Punctual Padé approximants as a regularization procedure for divergent and oscillatory partial wave expansions of the scattering amplitude[a)]

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Previous theorems on the convergence of the $[n,n+m]$ punctual Padé approximants to the scattering amplitude are extended. The new proofs include the cases of nonforward and backward scattering corresponding to potentials having $1/r$ and $1/r^2$ long-range behaviors, for which the partial wave expansions are divergent and oscillatory, respectively. In this way, the ability of the approximation scheme as a summation method is established for all of the long-range potentials of interest in potential scattering.

1. INTRODUCTION

In precedent papers[1,2] we have studied the evaluation of the scattering amplitude starting from its partial wave expansion

$$f(\theta)=\sum_{L=0}^{\infty} a_L P_L(\cos\theta), \tag{1.1}$$

where $a_L=(2L+1)[\exp(2i\delta_L)-1]/(2ik)$, k is the magnitude of the wave vector, i.e., $k=(2\mu E/\hbar^2)^{1/2}$, μ is the reduced mass of the system, the P_L are the Legendre polynomials, and the δ_L the phase shifts. We have considered interactions usual in atomic and molecular collision processes, which are characterized by long range potentials. This feature of the interactions determines, depending on μ and the energy E involved in the processes, a slow convergence of expansion (1.1). We dealt with potentials $V(r)$, which at great distances have the behavior

$$V(r) \underset{r\to\infty}{\sim} A/r^{\alpha+2}, \quad \alpha\geq 0 \tag{1.2}$$

where A is a constant and α an integer. For these cases, and when the series (1.1) is convergent, a large number of phase shifts is usually required to attain a reasonable accuracy when calculating differential cross-sections. To avoid this difficulty, its summation with the Punctual Padé Approximants (PPA) was proposed. A set of theorems were proven which showed that the rate of convergence of the PPA is higher, for any value of the scattering angle θ and of the coupling constant, than that of the partial wave sums of (1.1), when the latter are convergent.

From the mathematical point of view, we studied the convergence properties of the PPA when applied to sequences $\{S_m\}$, characterized by the asymptotic behavior

$$S_m \underset{m\to\infty}{\sim} f+A(m+a)^{-n-1/2}\sin(m\theta+b) \tag{1.3b}$$

and

$$S_m^{(\pm)} \underset{m\to\infty}{\sim} f+(\pm 1)^m A(m+a)^{-n}, \tag{1.3b}$$

where, following the nomenclature introduced by Shanks,[3] f is the base of the sequence, n is a positive integer, and A, a, b, and θ are parameters which define the convergent mathematical transients. The theorems proved in Ref. 1 for these cases represent a wide generalization of those by Wynn,[4] for monotonous and oscillating convergent Newton sequences, i.e., the sequences of Eq. (1.3b) with $n=1$.

In Ref. 2 we showed the numerical efficiency of the approach when calculating the differential cross section for e–He elastic scattering at intermediate energies and for the scattering by a Lennard–Jones potential. Furthermore, we also found fast numerical convergence in the cases of the scattering by Coulombian and repulsive inverse square potentials. In both cases, $f(\theta)$ is well defined for nonforward directions, although the partial wave expansion is divergent for any θ in the first, and oscillating for $\theta=\pi$ in the second. This suggested that the domain of convergence of the PPA is actually larger than that to which the theorems were restricted in Ref. 1.

In this paper we extend the convergence proofs for the PPA, to sequences $\{S_m\}$ with asymptotic behaviors of the type

$$\begin{aligned} &S_m \underset{m\to\infty}{\sim} f+A(m+a)^{\beta}\sin(m\theta+b), \\ &S_m \underset{m\to\infty}{\sim} f+(-1)^m[A+B(m+a)^{\beta}], \end{aligned} \tag{1.4}$$

with β a nonpositive integer complex number. They have the interesting property of being capable of having, depending on the values of the parameters, divergent or purely oscillating mathematical transients. In this way, we are able to include in our formalism, all of the long-range forces of interest in potential scattering covering all the cases for which $f(\theta)$ has finite meaningful values.

In Sec. 2 we introduce the PPA, and a set of lemmas are proven regarding their convergence when applied to sequences of the type satisfying Eqs. (1.4). By using these results in Sec. 3, we establish the convergence theorems for the PPA to the nonforward scattering amplitude, including the cases for which the partial wave expansions involved are divergent or oscillatory.

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2. PUNCTUAL PADÉ APPROXIMANTS

Given a formal power series

$$C(z)=\sum_{r=0}^{\infty} b_r z^r,$$

its $[N,M]_{C(z)}$ Padé approximant (PA) is defined[5] by

$$[N,M]_{C(z)}=R_M(z)/Q_N(z), \quad Q_N(0)=1,$$

where $R_M(z)$ and $Q_N(z)$ are polynomials in z of orders M and N, respectively, whose coefficients are uniquely determined by the requirements

$$C(z)\,Q_N(z)-R_M(z)=O[z^{M+N+1}].$$

The partial wave expansion (1.1) of $f(\theta)$ can be seen as a power series, by introducing a variable x and defining

$$C(x)=\sum_{L=0}^{\infty} a_L P_L(\cos\theta)\,x^L.$$

Then $f(\theta)=C(1)$ and we shall have an approximation for $f(\theta)$ by evaluating the PA to $C(x)$, calculated at $x=1$. The punctual Padé approximants (PPA) to the scattering amplitude,[1] so defined, determine a doubly infinite array of rational approximations. In this work, we shall restrict ourselves to consider the PPA $[n,n+m]_{f(\theta)}$, with $n, m \geq 0$.

Let us define the partial sums of expansion (1.1) by

$$S_m=\sum_{L=0}^{m} a_L P_L(\cos\theta).$$

Then, $[n,n+m]_{f(\theta)}$ can be expressed in the following way,[4]

$$[n,n+m]_{f(\theta)}=[n,n+m]_{\{S_r\}}=\frac{H_{n+1}^{(m)}\{S_r\}}{H_n^{(m)}\{\Delta^2 S_r\}}=\frac{H_{n+1}^{(0)}\{\Delta^r S_m\}}{H_n^{(2)}\{\Delta^r S_m\}}, \tag{2.1}$$

where, for $r\geq 1$, $\Delta^r S_m=\Delta^{r-1}S_{m+1}-\Delta^{r-1}S_m$, $\Delta^0 S_m=S_m$, and the Hankel determinants are defined for a given sequence $\{f_r\}$, by

$$H_k^{(m)}\{f_r\}=\begin{vmatrix} f_m & f_{m+1} & \cdots & f_{m+k-1} \\ f_{m+1} & f_{m+2} & \cdots & f_{m+k} \\ \vdots & \vdots & & \vdots \\ f_{m+k+1} & f_{m+k+2} & \cdots & f_{m+2k-2} \end{vmatrix}.$$

Furthermore, by using Eq. (2.1) it can be easily shown that if $S_r=A+BS'_r$, then

$$[n,n+m]_{\{S_r\}}=A+B[n,n+m]_{\{S'_r\}}. \tag{2.2}$$

Let us note that, for large n, the PPA are not readily computable with these determinantal quotients. Recurrent algorithms exist, however, which allow for an efficient calculation of the approximants.[2]

In what follows, we shall prove a set of lemmas which will be used in the next section, to derive our main proofs regarding the convergence of the $[n,n+m]_{f(\theta)}$.

Lemma 2.1: Given the sequence

$$g_m^{0,\beta}=(m+\tfrac{1}{2})^\beta \sin\Lambda_m, \tag{2.3}$$

where $\Lambda_m=(m+1)\,\theta-\pi/4$, $0<\theta<\pi$, and $\beta\neq 0,1,2,3,\cdots$, is a complex number, the sequences $\{g_m^{r,\beta}\}$ defined for fixed $r\geq 0$ by the recurrent relation

$$g_m^{r+1,\beta}=g_{m+1}^{r,\beta}+g_{m-1}^{r,\beta}-2\cos\theta\, g_m^{r,\beta}, \tag{2.4}$$

have, for large m, the following asymptotic behavior,

$$g_m^{r,\beta}\sim(-2\sin\theta)^r[\beta]_r(m+\tfrac{1}{2})^{\beta-r}\sin(\Lambda_m-r\pi/2)+O[m^{\beta-r-1}], \tag{2.5}$$

with $[\beta]_n=\beta(\beta-1)\cdots(\beta-n+1)$, for $n\geq 1$ and $[\beta]_0=1$.

Proof: Replacing (2.3) into (2.4) for $r=0$, it is easily seen that

$$g_m^{1,\beta}=-\sum_{k=1}^{\infty}\frac{[\beta]_k}{k!}[(-1)^k g_{m+1}^{0,\beta-k}+g_{m-1}^{0,\beta-k}]. \tag{2.6}$$

Assuming now that

$$g_m^{i,\beta}=-\sum_{k=1}^{\infty}\frac{[\beta]_k}{k!}[(-1)^k g_{m+1}^{i-1,\beta-k}+g_{m-1}^{i-1,\beta-k}], \tag{2.7}$$

it follows by using (2.4) that (2.7) holds also for i replaced by $i+1$, and then, by induction, that it is valid for all $i\geq 1$. The asymptotic equation (2.5) for $r=1$, can be readily obtained by replacing (2.3) into (2.6) and it is easily proven for $r>1$, again by induction, using Eq. (2.7).

Owing to the algebraic nature of the proof of Theorem 4.1 in Ref. 1, it is actually valid for any sequence to which a family of sequences may be associated by Eq. (2.4), and having the asymptotic behaviors given by Eq. (2.5) for all $r\geq 0$. This holds as long as β is restricted as in Lemma 2.1. Then, performing straightforward modifications in the statement of the theorem mentioned above, we can state the following:

Lemma 2.2: The PPA $[n,n+m]$ applied to the sequence $\{g_r^{0,\beta}\}$, defined in Lemma 2.1, have, for fixed n and large m, the following asymptotic behavior,

$$[n,n+m]_{\{g_r^{0,\beta}\}}\sim\frac{(\sin\theta)^{2(n-N)}[\beta]_N N!\,(\sin\Lambda_{m+n})^{2(2N-n)+1}(m+\frac{1}{2})^{\beta-2N}}{2^{2(n-N)}[\sin(\theta/2)]^{2n}}; \quad (\sin\Lambda_{m+n}\neq 0), \tag{2.8}$$

where $N=n/2$ for even n, and $N=(n-1)/2$ for odd n. As in Ref. 1, it should be noted that when $\sin\Lambda_{m+n}=0$ for a given θ, the asymptotic order of magnitude of the $[n,n+m]_{\{g_r^{0,\beta}\}}$ is somewhat smaller for even n, and somewhat larger for odd n, than that generally predicted by Eq. (2.8) without the oscillatory factor $\sin\Lambda_{m+n}$.

Lemma 2.3: The $[n,n+m]$ PPA to the sequence

$$G_r^\nu=(-1)^r[(r+\tfrac{1}{2})^\nu+E], \tag{2.9}$$

where E is a constant and ν a nonzero complex number have, for fixed $n>0$ and large m, the following asymptotic behavior,

$$[n,n+m]_{\{G_r^\nu\}}\sim(-1)^{m+n}2^{-2n}(m+\tfrac{1}{2})^{\nu-2n}\times\begin{cases}-(n-1)!\,[\nu]_{n+1}; & \mathrm{Re}\,\nu<0,\ E\neq 0, \quad (2.10a)\\ n!\,[\nu]_n; & \mathrm{Re}\,\nu>0, \text{ any } E, \\ \text{or } \mathrm{Re}\,\nu\leq 0, \ E=0. & \quad (2.10b)\end{cases}$$

Proof: We note that

$$\Delta^2 G_r^\nu = G_{r+2}^\nu + G_r^\nu - 2G_{r+1}^\nu \underset{r}{\sim}_\infty -4G_{r+1}^\nu + O[r^{\nu-2}],$$

and replace the first order asymptotic approximation for $\Delta^2 G_r^\nu$ thus obtained, in the expression (2.1) for the PPA $[n, n+m]_{\{G_r^\nu\}}$, to get

$$[n, n+m]_{\{G_r^\nu\}} = \frac{H_{n+1}^{(m)}\{G_r^\nu\}}{H_n^{(m)}\{\Delta^2 G_r^\nu\}} \underset{m}{\sim}_\infty \frac{(-1)^{m(m+1)} H_{n+1}^{(m)}\{(-1)^r G_r^\nu\}}{(-1)^{n(m+2)} 4^n H_n^{(m+1)}\{(-1)^r G_r^\nu\}}. \tag{2.11}$$

Let us first consider the case $\mathrm{Re}\nu < 0$, $E \neq 0$. Operating on the determinant $H_p^{(s)}\{(-1)^r G_r^\nu\}$ and using (2.9), we have

$$H_p^{(s)}\{(-1)^r G_r^\nu\} = H_p^{(0)}\{\Delta^r (-1)^s G_s^\nu\} = EH_{p-1}^{(2)}\{\Delta^r (s+\tfrac{1}{2})^\nu\} + H_p^{(0)}\{\Delta^r (s+\tfrac{1}{2})^\nu\}. \tag{2.12}$$

These Hankel determinants can be evaluated asymptotically by noting that

$$\Delta^r (s+\tfrac{1}{2})^\nu \sim [\nu]_r (s+\tfrac{1}{2})^{\nu-r}, \tag{2.13}$$

and the equality[6]

$$H_n^{(m)}\{[\nu]_r\} = \prod_{p=0}^{n-1} [\nu]_{m+p} (-1)^p p! \tag{2.14}$$

in order to obtain,

$$H_p^{(s)}\{(-1)^r G_r^\nu\} \underset{s}{\sim}_\infty (s+\tfrac{1}{2})^{(\nu-p)(p-1)} \left[\frac{E(-1)^{p-1}[\nu]_p}{\nu(p-1)!} + (s+\tfrac{1}{2})^\nu\right] \prod_{t=0}^{p-1} [\nu]_t (-1)^t t! \underset{s}{\sim}_\infty \frac{E(s+\tfrac{1}{2})^{(\nu-p)(p-1)}(-1)^{p-1}[\nu]_p \prod_{t=0}^{p-1}[\nu]_t (-1)^t t!}{\nu(p-1)!}. \tag{2.15}$$

In the other cases, i.e., $\mathrm{Re}\nu > 0$ and any E, or $\mathrm{Re}\nu \leq 0$ and $E = 0$, it is clear that

$$G_{r\ r}^\nu \sim_\infty (-1)^r (r+\tfrac{1}{2})^\nu,$$

and consequently,

$$H_p^{(s)}\{(-1)^r G_r^\nu\} \underset{s}{\sim}_\infty H_p^{(0)}\{\Delta^r (-1)^s (s+\tfrac{1}{2})^\nu\} = H_p^{(0)}\{\Delta^r (s+\tfrac{1}{2})^\nu\} \underset{s}{\sim}_\infty (s+\tfrac{1}{2})^{(\nu-p)(p-1)+\nu} \prod_{t=0}^{p-1} [\nu]_t (-1)^t t!, \tag{2.16}$$

where we have used Eqs. (2.13) and (2.14), as before

By using the asymptotic estimates given by Eqs. (2.15) and (2.16), in (2.11), Eqs. (2.10) follow.

3. THE NONFORWARD SCATTERING AMPLITUDE FOR LONG-RANGE POTENTIALS

Let us consider a central potential $V(r)$, which behaves at large distances as

$$V(r) \underset{r}{\sim}_\infty A/r^{\alpha+2}, \quad \alpha \geq -1, \tag{3.1}$$

where A is a constant and α an integer. We show in the Appendix that the corresponding partial wave amplitudes a_L in expansion (1.1), have, for large angular momentum L, the following asymptotic behavior,

$$a_{L\ L} \sim_\infty \sum_{i=1}^{J} B_i (L+\tfrac{1}{2})^{\beta_i} + O[L^{\beta_J + 1}], \tag{3.2}$$

where for $\alpha \geq 0$, $J = 2$,

$$B_1 = -Ak^{\alpha-1} I_\alpha, \quad B_2 = (i/2) A^2 k^{2\alpha-1} I_\alpha^2,$$

$$\beta_1 = -\alpha, \quad \beta_2 = -2\alpha - 1, \quad \beta_3 = -2\alpha - 2,$$

while for $\alpha = -1$, $J = 1$, and

$$B_1 = -i/k,$$

$$\beta_1 = 1 + i\chi, \quad \beta_2 = -1 + i\lambda,$$

I_α is a numeric factor dependent on α, and $\chi = A/k$. By noting the well-known properties of the Legendre polynomials

$$P_L(\cos\theta)\ {}_L\sim_\infty \left(\frac{2}{\pi \sin\theta}\right)^{1/2} \cos\Omega_L (L+\tfrac{1}{2})^{-1/2} + O[L^{-3/2}]$$

$$(0 < \theta < \pi, \ \Omega_L = (L+\tfrac{1}{2})\theta - \pi/4), \tag{3.3}$$

and

$$P_L(-1) = (-1)^L, \tag{3.4}$$

it follows that the sequence $\{S_m\}$ of partial sums of expansion (1.1),

$$S_m(\theta) = \sum_{L=0}^{m} a_L P_L(\cos\theta), \tag{3.5}$$

for the nonforward directions, is divergent for all θ when $\alpha = -1$, oscillatory for $\theta = \pi$ when $\alpha = 0$, and convergent otherwise. The scattering amplitude is well defined, for these anomalous cases. In what follows, we shall restrict ourselves to $\theta \neq 0$, and show the ability of the PPA to regularize the sequence (3.5) in those situations.

Let us introduce the regularizing factor[7] $(1 - \cos\theta)$ in (3.5), to obtain

$$(1-\cos\theta) S_m = \sum_{L=0}^{m} \bar{a}_L P_L + \frac{(m+1)}{2m+3} a_{m+1} P_m - \frac{(m+1)}{2m+1} a_m P_{m+1}, \tag{3.6}$$

where the coefficients

$$\bar{a}_L = a_L - \frac{L}{2L-1} a_{L-1} - \frac{L+1}{2L+3} a_{L+1}, \quad a_{-1} \equiv 0, \tag{3.7}$$

are those of the expansion

$$(1-\cos\theta) f(\theta) = \sum_{L=0}^{\infty} \bar{a}_L P_L(\cos\theta). \tag{3.8}$$

Taking account of the asymptotic behavior of the a_L as given by Eq. (3.2), it is easy to show that

$$\bar{a}_{L\ L} \sim_\infty -\tfrac{1}{2}(L+\tfrac{1}{2})^{-2} \sum_{i=1}^{J} B_i (\beta_i - 1)^2 (L+\tfrac{1}{2})^{\beta_i}, \tag{3.9}$$

and by using a procedure similar to that used to prove Lemma (3.1) of Ref. 1 we find for large m

$$\sum_{L=m+1}^{\infty} \bar{a}_L P_L(\cos\theta)\ {}_m\sim_\infty \begin{cases} O[a_m m^{-5/2}], & 0 < \theta < \pi, \quad (3.10a) \\ O[a_m m^{-2}], & \theta = \pi. \quad (3.10b) \end{cases}$$

This shows that expansion (3.8) will be convergent for the cases here considered, and we can then write,

$$S_m(\theta)=f(\theta)-(1-\cos\theta)^{-1}\left[\sum_{L=m+1}^{\infty}\bar{a}_L P_L - \frac{m+1}{2m+3}\,a_{m+1}P_m+\frac{m+1}{2m+1}\,a_m P_{m+1}\right], \tag{3.11}$$

and by using Eqs. (3.3), (3.4), and (3.10) we have for large m,

$$f_m(\theta)\underset{m}{\sim}\begin{cases} f(\theta)+D(\theta)\sin\Lambda_m B_1(m+\frac{1}{2})^{\beta_1-1/2}+O[a_m m^{-3/2}] \\ \qquad (0<\theta<\pi) \end{cases} \tag{3.12a}$$

$$\begin{cases} f(\pi)+\dfrac{(-1)^m}{2}\sum_{i=1}^{J} B_i(m+\frac{1}{2})^{\beta_i}+O[a_m m^{-1}] \end{cases} \tag{3.12b}$$

where $D(\theta)=-[2\pi\sin\theta\sin^2(\theta/2)]^{-1/2}$, $\Lambda_m=(m+1)\,\theta-\pi/4$, and J the $\{B_i\}$ and $\{\beta_i\}$, are defined as in Eq. (3.2).

By inspection of Eqs. (3.12) our previous assertions regarding the divergent and oscillatory nature of the sequence of partial wave sums can be clearly seen for the cases $\alpha=0$, -1, i.e., $\beta_1=0$, and $\beta_1=1+i\lambda$, which correspond to potentials having long-range behavior of the type $1/r^2$ and $1/r$, respectively. We can now state the following theorem:

Theorem 3.1: The PPA $[n,n+m]_{f(\theta)}$ to the scattering amplitude corresponding to a central potential having the long range tail

$$V(r)\underset{r}{\sim}A/r^{\alpha+2},\quad \alpha\geq -1,$$

where A is a constant and α an integer, has for fixed n and large m, the following asymptotic behavior:

$$[n,n+m]_{f(\theta)}\underset{m}{\sim} f(\theta)+\frac{D(\theta)\,B_1(\sin\theta)^{2(n-N)}[\beta_1]_N N!(\sin\Lambda_{m+n})^{2(2N-n)+1}}{2^{2(n-N)}(\sin\frac{1}{2}\theta)^{2n}(m+\frac{1}{2})^{2N-\beta_1+1/2}}, \tag{3.13a}$$

$$(0<\theta<\pi,\ \sin\Lambda_{m+n}\neq 0)$$

$$[n,n+m]_{f(\pi)}\underset{m}{\sim} f(\pi)+\begin{cases} B_1(-1)^{m+n}2^{-2n-1}(m+\frac{1}{2})^{\beta_1-2n}n![\beta_1]_n \\ \qquad (\alpha\neq 0) \end{cases} \tag{3.13b}$$

$$\begin{cases} B_1 2^{-1}(-1)^m\delta_{n0}+B_2(-1)^m 2^{-2n-1}(m+\frac{1}{2})^{-1-2n}\gamma_n(n+1)! \\ \qquad (\alpha=0), \end{cases} \tag{3.13c}$$

where the coefficients B_i and β_i are dependent on α and defined as in Eq. (3.2), $\gamma_n=(n-1)!$ for $n>0$, $\gamma_n=1$ for $n=0$, $D(\theta)$ and Λ_m are those of Eq. (3.12a), $N=n/2$ for even n, and $N=(n-1)/2$ for odd n.

Proof: We first note that according to Eqs. (3.12),

$$S_m(\theta)\underset{m}{\sim} f(\theta)+D(\theta)\,B_1 g_m^{0,\beta_1-1/2},\quad 0<\theta<\pi \tag{3.14}$$

$$S_m(\pi)\underset{m}{\sim} f(\pi)-E_1 G_m^{\nu}, \tag{3.15}$$

where $\{g^{0,\beta_1-1/2}\}$ is the sequence defined in Lemma 2.1, and $\{G_m^{\nu}\}$ is that of Lemma 2.3 with

$$\nu=-\alpha,\quad E_1=B_1/2,\quad E=0,\quad \text{for } \alpha>0,$$

$$\nu=-1,\quad E_1=B_2/2,\quad E=B_1/B_2,\quad \text{for } \alpha=0,$$

$$\nu=1+i\chi,\quad E_1=B_1/2,\quad E=0,\quad \text{for } \alpha=-1,$$

and by using Lemmas 2.2 and 2.3, and property (2.2) of the PPA, Eqs. (3.13) are readily obtained.

Theorem 3.1 generalizes Corollary 4.1 of Ref. 1.[8] It includes the latter for $0<\theta<\pi$ when $\alpha\geq 0$, and for $\theta=\pi$ when $\alpha>0$. Two new results are established: The convergence of the PPA $[n,n+m]$ to the nonforward scattering amplitude corresponding to a potential having a Coulombian long-range behavior, for $n\geq 2$ when $\theta\neq\pi$, and for $n\geq 1$ when $\theta=\pi$ [see Eqs. (3.13a)–(3.13b)] and to the backward scattering amplitude for the case in which the behavior included is of the $1/r^2$ type, for $n\geq 1$ [see Eq. (3.13c)]. This shows that the PPA are able to transform divergent or oscillatory sequences into others that converge to the right values, thus providing regularized sequences for the corresponding partial wave sums. Moreover the rate of convergence of the former is seen to increase rapidly with n.

The real physical interest in summing in a direct way the partial wave expansion when Coulomb forces are present, could be questioned. The usual method in this case, is to subtract in a closed form the Coulomb scattering amplitude, and to concentrate in the remaining convergent expansion.[9] However, the latter will be rapidly convergent only if the other forces of interest are short-range ones and the energy involved is relatively low. Otherwise, it will be poorly convergent and a summation method such as that of the PPA will be of value. This is the usual situation, for example, when studying ion–ion collisions, where long-range distorsion and polarization forces are present, apart from the Coulomb interaction. The PPA approach allows us to treat all of the long-range forces present in atomic and molecular collision processes, in a closed way, without further distinction.[10]

Finally, let us note that owing to the rational nature of the approximations, and their good behavior for physical values of $\cos\theta$, they can be expected to be a valuable means for the analytical continuation of the scattering amplitude in the complex $\cos\theta$ plane. This possibility deserves further study.

APPENDIX: ASYMPTOTIC BEHAVIOR OF THE PARTIAL WAVE AMPLITUDES FOR LONG-RANGE POTENTIALS

The partial wave amplitudes a_L are defined in terms of the phase shifts δ_L by

$$a_L=\begin{cases}\{\exp[2i\delta_L]-1\}(2L+1)/(2ik), & \alpha\geq 0,\\ \exp[2i\delta_L](2L+1)/(2ik), & \alpha=-1,\end{cases} \tag{A1}$$

where α characterizes the dominant long-range component of the potential [see Eq. (3.1)]. Moreover, it is well known that for these type of potentials the δ_L have the following asymptotic behavior, for $\alpha\geq 0$

$$\delta_L\underset{L}{\sim}-\frac{Ak^{\alpha}I_{\alpha}}{2(L+\frac{1}{2})^{\alpha+1}}+O[L^{-2\alpha-3}], \tag{A2a}$$

with[1]

$$I_\alpha = \begin{cases} \pi/2, & \alpha = 0, \\ \dfrac{(\alpha-1)!!}{\alpha!!}\,\dfrac{\pi}{2}, & \text{even } \alpha > 0, \\ \dfrac{(\alpha-1)!!}{\alpha!!}, & \text{odd } \alpha, \end{cases}$$

while for $\alpha = -1$, one has

$$\delta_L \underset{L\to\infty}{\sim} \frac{A}{2k}\log(L+\tfrac{1}{2}) + O[L^{-2}], \tag{A2b}$$

which can be obtained by considering the behavior of the Coulomb phase shifts,

$$\delta_L = \arg\Gamma[L+1+iA/(2k)],$$

for $L \gg 1$, $|A|/(2k)$.

For $\alpha \geq 0$ we expand $\exp[2i\delta_L]$ in powers of δ_L, in order to obtain, by using Eq. (A2a),

$$a_L = (L+\tfrac{1}{2})(2\delta_L + i2\delta_L^2 + \cdots)/k$$
$$\underset{L\to\infty}{\sim} \frac{-Ak^{\alpha-1}I_\alpha}{(L+\frac{1}{2})^\alpha} + \frac{iA^2k^{2\alpha-1}I_\alpha^2}{2(L+\frac{1}{2})^{2\alpha+1}} + O[L^{-2\alpha-2}], \tag{A3}$$

and using Eq. (A2b), we obtain, for $\alpha = -1$

$$a_L = -i(L+\tfrac{1}{2})\exp[2i\delta_L]/k$$
$$\underset{L\to\infty}{\sim} -i(L+\tfrac{1}{2})^{1+i\chi}/k + O[L^{-1+i\chi}], \tag{A4}$$

with $\chi = A/k$.

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[6] This equation can be obtained by using the same techniques applied in Appendix B 2 of Ref. 1.

[7] G.H. Hardy, *Divergent Series* (Oxford, London, 1949), p. 43; D.R. Yennie, D.G. Ravenhall, and R.N. Wilson, Phys. Rev. 95, 500 (1954).

[8] This theorem can also be seen as an extension of Theorem 11.4 of Ref. 5 on the convergence of PA to power series with "smooth" coefficients. We acknowledge the referee for pointing this out.

[9] L. Schiff, *Quantum Mechanics* (McGraw Hill, New York, 1968), p. 144.

[10] An alternative approach to the summation of partial wave expansions in potential scattering has been proposed recently, by using Legendre Padé approximants, by A.K. Common and T. Stacey (preprints UKC, England, April and July 1977). Other approaches, within the framework of Padé-type approximations, are referred to in Ref. 1.

Spectral and scattering inverse problems[a)]

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The reconstruction of a differential operator form discrete spectra is reduced to its reconstruction from an S-matrix. This method makes it possible to solve the singular Sturm–Liouville problems which determine certain modes of a sphere. The results pave the way for handling studies in which information on modes and scattering results would all be taken into account. They are applied to the earth inverse problem and partial answers are given to a well-known conjecture. Finally the relevance of the JWKB approximation in this kind of problem is briefly discussed.

1. INTRODUCTION

This paper is part of a study in which our purpose is to construct a method able to take into account altogether scattering *and* discrete spectra results in order to reconstruct the parameters of a differential system. Here we first show, in two general examples, how the problem of constructing the parameters of a second order differential equation on a finite domain from its "modes," the so-called "inverse Sturm Liouville problem," can be reduced to "inverse scattering problems." Such an approach, in some way, goes backwards in the sense of history. Inverse Sturm–Liouville problems were either studied for themselves,[1,2] or studied for their numerical analysis,[3] or studied for introducing and solving the fundamental analysis, or the numerical analysis, of inverse scattering problems.[4,5] But the various studies of collision theory have been so rich that it is now "*a priori*" justified to try this way of working. Besides, this is clearly a correct approach to the more general study quoted at the beginning. "*In fine,*" we feel justified by the results which have been obtained, both from the mathematical and from the physical point of view.

In Sec. 2, we consider a second-order linear differential problem on a finite interval of $\mathbb{R}$, in which the solution is imposed to vanish at the two end points. In a regular case, this is the usual inverse Sturm–Liouville problem. But thanks to the "scattering approach," nonintegrable singularities like R^{-2}, can be taken into account without additional difficulties, and the problem is completely solved.

In Sec. 3, again we consider a second order differential problem, on a finite interval of $\mathbb{R}$, but now the derivative of the solution should vanish at one or both end points. Again, the regular case reduces to the usual inverse Sturm–Liouville problem. Again, thanks to our approach, important singularities can be taken into account in a trivial way.

The physical justifications of our two general examples are clarified in Sec. 4. The first example is an acceptable scheme for the radial modes of a liquid ball. The second one is an acceptable scheme for the toroidal modes of a solid ball. The results are used to study a well-known conjecture concerning the earth inverse problem. In this problem, one tries to infer the density ρ and Lamé parameters λ, μ of the "spherical" earth, as functions of the radial variable R, from the information that is contained in the free oscillations. The central question is to determine what pieces of information are necessary and sufficient to determine the parameters. Backus and Gilbert[6] conjectured that the eigenvalues of three normal mode sequences are a sufficient amount of information. Our answer is more pessimistic. Let us state it as follows:

(1) Suppose that in a liquid ball, of radius R_∞, ρ and λ are finite positive and twice differentiable functions of R for any $0 < R \leq R_\infty$, with zero derivative at 0 and R_∞, and do not depend on θ or ϕ, and suppose the gravity can be neglected (this and the zero derivative assumptions are just for the sake of simplicity).

Suppose then we know:

(a) The sequences of radial mode eigenvalues $\{\omega_{l,n}\}$ for two values of the angular momentum l.

(b) The sequences of the corresponding values of either the derivative of the modes in the surface or the normalization factors. These sequences can be derived from the response to a fully analyzed known source.

Then we can reconstruct $\rho(R)$ and $\lambda(R)$ for any R.

(2) Suppose that in a solid ball, of radius R_∞, with a liquid core, of radius R_c, ρ and λ are finite, positive, twice differentiable functions of R for any $0 \leq R \leq R_\infty$, with zero derivative at 0 and R_∞, whereas μ is finite, positive, twice differentiable for any $R_c < R \leq R_\infty$, with zero derivative at R_∞, and is $(R - R_c)^\alpha$ times a twice differentiable function as R goes to R_c, with $0 \leq \alpha < 2$.

Suppose then we know the toroidal modes for two nontrivial values of l, again with both the eigenvalues and the normalization factors, or the amplitudes of the modes at R_∞. Then we can reconstruct $\rho(R)$ and $\mu(R)$ for $R > R_c$. The asymptotic behavior of the eigenvalues readily gives the value of α, which determines the method of reconstruction.

If μ was strictly positive for any $R \geq R_c$ (i.e., $\alpha = 0$), this toroidal modes problem would be an ordinary Sturm–Liouville problem and the result, henceforth, would be well known.[1] But for $\alpha \neq 0$ which is probably

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the physical case, the problem is singular, and, remarkably, it is simpler to treat it by the scattering approach than (with the same approach) in the regular case.

Suppose now that $1 < \alpha < 2$, and that we know in addition the $l=0$ radial modes, again in the sense of knowing both the eigenvalues and the normalization factors or the equivalent. Then, we can completely reconstruct $\lambda(R)$, $\rho(R)$, and $\mu(R)$ for any $R_c < R \leq R_\infty$.

Hence three spectra are sufficient to determine $\lambda(R)$, $\rho(R)$, and $\mu(R)$, but *only if we know altogether the eigenvalues and the normalization factors*, or equivalent information which follows from the response to a known source (e.g., toroidal mode amplitudes at R_∞, or derivative of the radial mode amplitudes at R_∞).

Let us emphasize at this point that we only pretend to give a reconstruction of *existing parameters*. Hence we do not try to clarify the necessary conditions (interlacing, asymptotic behaviors, etc.) that these spectra certainly must satisfy to correspond to a set of parameters. This question deserves a study by itself.

Of course, it would be interesting to study the information which is contained in several spheroidal modes, thus generalizing the "liquid" case to the "solid" one. Again, we know that it is possible to reduce the problem to a scattering problem, which is fully similar with one we have already studied.[7] Unfortunately, this is a *coupled channel problem*, and only partial solutions of the inverse problem are known in scattering theory. Again, this deserves a study by itself, and we shall not try to do it here.

Let us come back to the more general physical motivation of our study. Seismological problems often have two aspects, viz., a normal mode aspect, and a scattering aspect. Both have been taken in account in *local* (and oversimplified) studies, with respect to the *direct problem*. But, up to our knowledge, there never has been any *global* study, and taking into account altogether direct *and* inverse problems, altogether modes *and* scattering result. We tried to make a global study of the scattering results in previous papers,[7,10] but the finiteness of the earth was not taken into account. Only here do we really begin such a general study. At this point, a very natural question arises. What is the importance of our assumptions?.

First there are assumptions which are there only to simplify, or clarify, the results. The reader who is interested can drop them and follow our argument point for point, except for some complications or additional work. Such assumptions are of zero derivative of the parameters at end points and neglecting the gravity. A nonzero derivative at the origin can produce a R^{-1} singularity in the equivalent potential, and the remainders in inequalities get logarithmic terms. A nonzero derivative at R_∞ makes it necessary to investigate a little bit more carefully the asymptotic behavior of the eigenvalues. Taking into account the gravity in the $l=0$ radial mode is trivial.

It is likely that the assumption $1 < \alpha < 2$ in the earth problem can also easily be weakened up to $0 \leq \alpha < 2$.

Much more important is the differentiability condition. *It is not physical.* We should allow the parameters to be only piecewise continuous, with jumps. Unfortunately, these jumps produce δ' functions in the equivalent scattering problem, which is too singular to be treated in known generalizations of potential scattering theory.[6,8] Extending the scattering theory to these cases has been partially done, but many points deserve a study by themselves, and we shall not do it here.

The positivity condition is essential. It is connected with excluding the possibility of holes. A hole is a finite continuous domain in which ρ or at least two of the parameters are identically zero. When holes do not cut the domain in disconnected parts, they can be taken into account, and introduce important modifications in the theory (see for instance the problem of the "shape of a drum"[1,9]). In our radial case, a hole would introduce a cutoff between two parts of the ball, and hence a complete cutoff of the information. Thus it is not surprising that we cannot take it into account in our scattering approach.

In a short section (Sec. 5), we sketch the JWKB approximation of these problems. This just serves a pedagogical purpose, to understand certain points in the analysis of the eigenvalues, and to make a guess on the way to take into account various pieces of information. But when this method will be fully justified for piecewise continuous parameters, methods using its, as in the RKR method, can *certainly be of interest* in the earth inverse problem. It will be usefully combined with the ray theory, to which it is intimately connected.

To finish this Introduction, let us note that we do not pretend to give practical ways of reconstruction. We stop our study as soon as we get the scattering matrix, provided there exists a method like the Gel'fand—Levitan method, or Marchenko's method, or one of their generalizations, enabling us to obtain the functions we seek. In fact, we could have very easily used our results to describe *reconstruction methods for singular inverse Sturm—Liouville problems*, but this was not our purpose in the present paper, and we feel comfortable when a piece of information has been proved sufficient for deriving the parameters. The fact that such reconstruction methods are not deeply hidden in our results is very clear if one notices that the "external range" we have to introduce for $R > R_\infty$ is artificial, and the parameters are, to a large extent, arbitrary. Needless to say, when we shall try to analyze simultaneously modes and scattering results, the physical support will appear much more clearly.

Technical remarks: (1) It may be amusing to notice that the $l=0$ radial mode in Sec. 2 could have been studied by the method which is described in Sec. 4, provided the interest is focused on $\rho^{-1} d\Pi/dR$ instead of Π.

(2) With the differentiability assumptions, there are three formulations of the problem (space formulation, time formulation, Schrödinger formulation). We have thought it interesting to base the analysis of modes in certain cases on one formulation, for others on other formulations. The most physical one is the space formu-

lation, but in the present paper all the necessary analytic and asymptotic properties are derived in the Schrödinger formulation.

(3) Although they are very well known in scattering theory, techniques which are actually based on the use of R-matrix theory or of dispersion relations are given in such an elementary way that the paper is self contained even for a reader who is not acquainted with them. The properties of information which are behind these techniques (causality, etc.) are not recalled. We think it better to postpone remarks of this kind after a study of the problem for discontinuous media, where some of them may be modified.

2. DIFFERENTIAL PROBLEM OF THE FIRST KIND

We study the set of equations

$$\left(-\rho R^{-2}\frac{d}{dR}R^2\rho^{-1}\frac{d}{dR}+l(l+1)R^{-2}\right)$$

$$\times\Pi_l(\omega,R)=\omega^2\rho\lambda^{-1}\Pi_l(\omega,R) \tag{2.1}$$

in which l runs through the nonnegative integers, ρ and λ are nonnegative piecewise continuous functions, and ω is a real or complex continuous parameter. Equation (2.1) is completed by the following conditions:

$$R\to\Pi_l(\omega,R) \text{ should be absolutely continuous,} \tag{2.2a}$$

$$R\to\rho^{-1}\frac{d}{dR}\Pi_l(\omega,R) \text{ should be absolutely continuous,} \tag{2.2b}$$

$$[R\Pi_l(\omega,R)]_{R=0}=[\Pi_l(\omega,R)]_{R=R_\infty}=0. \tag{2.2c}$$

The condition (2.2) can be satisfied only for a certain set of values of ω, $\{\omega_{ln}\}$, which will be called the eigenvalues of the differential problem (2.1), (2.2), or its modes. The direct problem is that of deriving the sequences $\{\omega_{l,n}\}$ from ρ and λ. In the inverse problem we want to identify sets $\{\omega_{l,n}\}$ or related information which is sufficient to construct $\rho(R)$ and $\lambda(R)$. Because R is the variable in (2.1), we call this formulation of the problem its space formulation.

Time formulation: We introduce the physical assumption

$$\rho\lambda\neq 0 \quad \text{for any} \quad R. \tag{2.3}$$

This assumption enables us to introduce a new variable, called the time, which is *bijectively* related with R by

$$\tau(R)=\int_0^R[c(x)]^{-1}dx, \tag{2.4}$$

where the "local celerity" c is equal to

$$c=(\lambda/\rho)^{1/2}. \tag{2.5}$$

Thus we obtain the "time formulation" of (2.1),

$$\left(Z^2\frac{d}{d\tau}Z^{-2}\frac{d}{d\tau}+\omega^2-\frac{l(l+1)c^2}{R^2}\right)\Pi_l(\omega,R(\tau))=0, \tag{2.6}$$

where the "impedance" Z is

$$Z=R^{-1}(\rho c)^{1/2}, \tag{2.7}$$

and the conditions (2.2) are to be replaced by

$$\tau\to\Pi_l(\omega,R(\tau)) \text{ absolutely continuous,}$$

$$\tau\to Z^{-2}\frac{d\Pi_l}{d\tau} \text{ absolutely continuous,}$$

$$\tau[\Pi_l(\omega,R(\tau))]_{\tau=0}=[\Pi_l(\omega,R(\tau))]_{\tau=\tau_\infty}=0. \tag{2.8}$$

We use the index ∞ to denote the values at $R=R_\infty$ for $\tau=\tau_\infty$ and the notations $c(\tau)$, $Z(\tau)$, etc., for $c(R(\tau))$, $Z(R(\tau))$, etc., when there is no ambiguity.

"Schrödinger" formulation: We introduce the *strong mathematical assumption*: ρ and λ are twice differentiable functions of R, going to constants with zero derivative as $R\to 0$ or $R\to R_\infty$. It follows that Z is a twice differentiable function of τ. Setting

$$\varphi_l(\omega,\tau)=Z^{-1}\Pi_l(\omega,R(\tau)) \tag{2.9}$$

we obtain the "Schrödinger" formulation of (2.1),

$$\left(\frac{d^2}{d\tau^2}+\omega^2-W_l(\tau)-l(l+1)\tau^{-2}\right)\varphi_l(\omega,\tau)=0, \tag{2.10}$$

where

$$W_l(\tau)=V(\tau)-l(l+1)U(\tau),$$

$$V(\tau)=Z\frac{d^2}{d\tau^2}Z^{-1}, \quad U(\tau)=\tau^{-2}-R^{-2}c^2 \tag{2.11}$$

are continuous functions on $[0,\tau_\infty]$.

These formulations are completely similar to those of a scattering problem that we formerly studied and in which the inverse problem could be solved. The interest of the Schrödinger formulation, and of the strong mathematical assumption which enables it, is that many analytical properties are readily available. They are our main tool in the following. Since we use them in very precise forms, we have thought it convenient to sketch them and their proofs in Appendix A.

The scattering problem: We continue λ and ρ for $R>R_\infty$ by constant positive values λ' and ρ'. The equation (1.1) in this external range simply reads

$$\left(\frac{d^2}{dR^2}+\frac{\omega^2}{c'^2}-l(l+1)R^{-2}\right)R\Pi_l(\omega,R)=0, \tag{2.12}$$

where $c'^2=\lambda'/\rho'$. By this ansatz, Eqs. (2.6) and (2.10) are also continued for $\tau>\tau_\infty$. $V(\tau)$ is identically zero in this range. $U(\tau)$ is not, being exactly $\tau^{-2}-[\tau-\tau_\infty+R_\infty/c']^{-2}$. Thus $W(\tau)$ is twice differentiable for $0\leq\tau\leq\tau_\infty$ and for $\tau>\tau_\infty$, and is $O(\tau^{-3})$ as $\tau\to\infty$. Equation (1.10) can be considered as the partial wave equation for the scattering of a plane wave $\exp(i\omega\tau\cos\theta)$ whose propagation follows the Schrödinger equation with the l-dependent potential $W(\tau)$. The S-matrix s is diagonal and $s_l(\omega)$ is given by the ratio of the Jost functions $F_l(-\omega)/F_l(\omega)$, with

$$F_l(\omega)=(-\omega)^l[f_l(\omega,\tau)\varphi_l'(\omega,\tau)-f_l'(\omega,\tau)\varphi_l(\omega,\tau)], \tag{2.13}$$

where the prime indicates the derivative with respect to τ, $f_l(\omega,\tau)$ is the solution of (1.10) which asymptotically is $\exp[i(\omega\tau+l\pi/2)]$ as $\tau\to\infty$, and $\varphi_l(\omega,\tau)$ has been normalized to be $\tau^{l+1}/(2l+1)!!$ as $\tau\to 0$. We met the same problem (with $c'=c_\infty$) in our study of explosions in the earth[10] and a similar one later.[7] We know that, thanks to the positivity of Z, there cannot be[7,11] any bound state. Thus, if $s_l(\omega)$ is known for all real ω's, $W_l(\tau)$ can be reconstructed, for instance, by a generalization of Marchenko's method.[5,12] Knowing functions $s_l(\omega)$ for all real ω's and two values of l enables us to construct two functions $W_l(\tau)$, which readily yield $V(\tau)$ and $U(\tau)$. In turn, a knowledge of $V(\tau)$ and $U(\tau)$, together with R_∞, τ_∞, and Z_∞ (or equivalent information after c_∞ is known), enables us to reconstruct $\lambda(R)$ and $\rho(R)$. Let us again state this argument.

(a) $U(\tau)$ should satisfy two consistency conditions. First, for $\tau>\tau_\infty$, it must be equal to the exact function which was given above. Then for any τ, it must be not larger than τ^{-2}. In general, c' is not c_∞ so that $U(\tau)$ has a jump at $\tau=\tau_\infty$. We denote by the index ∞ the values which are in continuity with $\tau\leq\tau_\infty$.

(b) For $\tau\leq\tau_\infty$, $\alpha(\tau)=[\tau^{-2}-U(\tau)]^{-1/2}$, $R(\tau)$ and $c(\tau)$ are given by

$$R(\tau)=R_\infty\exp\int_{\tau_\infty}^{\tau}\alpha(x)dx,\quad c(\tau)=R(\tau)\alpha(\tau). \tag{2.14}$$

(c) For $\tau=\tau_\infty$, we know Z_∞ by assumption, and $Z^{-1}(d/d\tau)Z=\alpha(\tau_\infty)$. For $\tau\leq\tau_\infty$, Z^{-1} is the continuous solution of

$$\frac{d^2}{d\tau^2}Z^{-1}=V(\tau)Z^{-1}. \tag{2.15}$$

(d) From $Z(\tau)$, $c(\tau)$, $\tau(R)$, (2.7), and (2.5), we readily obtain $\lambda(R)$ and $\rho(R)$.

Thus, we are reduced to deriving $s_l(\omega)$ (real ω) from the free modes of (2.1).

Construction of $s_l(\omega)$: Since W is real, $f_l(\omega,\tau)$ has well-known symmetry properties, which can be combined with the parity of $\varphi_l(\omega,\tau)$ when $\omega\to-\omega$, to show that $[F_l(\omega)]^*=F_l(-\omega)$ for real ω. Thus we only need to construct $s_l(\omega)$ for positive ω. Now the equivalence of (2.6) and (2.10), together with (2.9) and (2.12), show that for $\tau\geq\tau_\infty$ (or $R\geq R_\infty$)

$$f_l(\omega,\tau)=\exp(-i\omega\tau')\mathcal{J}_l\left(\frac{\omega}{c'},\ R_\infty+c'(\tau-\tau_\infty)\right)\quad(\tau\geq\tau_\infty), \tag{2.16}$$

where

$$\mathcal{J}_l(k,R)=i\exp(il\pi)\left(\frac{\pi}{2}kR\right)^{1/2}H^{(1)}_{l+1/2}(kR), \tag{2.17a}$$

$$T'=R_\infty/c'-\tau_\infty=\Delta'-\tau_\infty. \tag{2.17b}$$

Hence $s_l(\omega)$ can be constructed from T' and the function

$$y_l(\omega)=[\varphi_l(\omega,\tau_\infty)]^{-1}\frac{\partial}{\partial\tau_\infty}\varphi_l(\omega,\tau_\infty) \tag{2.18}$$

which is real for real ω. Because of (2.2c), the poles of $y_l(\omega)$ are the modes of (2.1).

Properties of $\varphi_l(\omega,\tau_\infty)$: $\varphi_l(\omega,\tau_\infty)$ is an even function of ω. Its zeros are those of $\Pi_l(\omega,R_\infty)$. Besides,

(a) *All zeros are real and simple.*

Proof: Writing (2.1) for two different values of ω, ω and $\dot\omega$, we easily obtain

$$-R_\infty^2\left(\dot\Pi_l\rho^{-1}\frac{d}{dR}\Pi_l-\Pi_l\rho^{-1}\frac{d}{dR}\dot\Pi_l\right)_{R=R_\infty}$$
$$=(\dot\omega^2-\omega^2)\int_0^{R_\infty}\Pi_l\dot\Pi_l R^2\lambda^{-1}dR. \tag{2.19}$$

Setting $\dot\omega=\omega^*$, and noticing that the corresponding function $\dot\Pi_l$ is nothing but the conjugate Π_l^* of Π_l, we see that if ω is a zero of $\Pi_l(\omega,R_\infty)$, $\mathrm{Re}\,\omega\,\mathrm{Im}\,\omega=0$. On the other hand, it also follows from (2.1) that

$$\int_0^{R'}[\omega^2R^2\lambda^{-1}-l(l+1)\rho^{-1}]\Pi_l^2\,dR=\int_0^{R'}\rho^{-1}R^2\left(\frac{d}{dR}\Pi_l\right)^2dR$$
$$-\left(\Pi_lR^2\rho^{-1}\frac{d}{dR}\Pi_l\right)_0^{R'}. \tag{2.20}$$

For $R'=R_\infty$, the right-hand side reduces to the first term, which is positive, whereas the left-hand side is negative if $\mathrm{Re}\,\omega=0$. This completes the proof. In addition, we see that $\omega=0$ cannot be a mode and that, for $\omega=0$, neither Π_l nor its derivative vanish for any values of R (they both remain positive). Incidentally, making $R'=\infty$ in (2.20) enables one to prove that there cannot be any bound state. Incidentally also, one sees that different modes are orthogonal (weight R^2, λ^{-1}). It is well known that they form a complete sequence in $L_2(0,\tau_\infty)$.

(b) $\varphi_l(\omega,\tau_\infty)$ is an entire function of ω^2, of order $\frac{1}{2}$. The proof of this well-known result is recalled in Appendix A. Its very important consequence is that φ_l can be constructed from the sequence $\{\omega_{l,n}\}$ by Hadamard's product

$$\varphi_l(\omega,\tau_\infty)=\varphi_l(0,\tau_\infty)\prod_{n=1}^{\infty}(1-\omega^2/\omega_{l,n}^2). \tag{2.21}$$

$\varphi_l(0,\tau_\infty)$ and τ_∞ can be derived from the asymptotic behavior of φ_l for large $|\omega|$ in the upper half-plane, for instance, for $\mathrm{Re}\,\omega=0$,

$$2|\omega|^{l+1}\exp[-|\omega|\tau_\infty]\varphi_l(i|\omega|,\tau_\infty)=1+O(|\omega|^{-1}), \tag{2.22}$$

which follows from formula (A6), and is equivalent to the formula

$$\log[2\varphi_l(0,\tau_\infty)]+(l+1)\log|\omega|-|\omega|\tau_\infty+\sum_{n=1}^{\infty}\log\left(1+\frac{|\omega|^2}{\omega_{l,n}^2}\right)$$
$$=O(|\omega|^{-1}), \tag{2.23}$$

which gives the result. Hence the sequence $\{\omega_{l,n}\}$ completely determines the function $\varphi_l(\omega,\tau_\infty)$, but not $(\partial/\partial\tau_\infty)\varphi_l(\omega,\tau_\infty)$.

(c) That sequences $\{\omega_{l,n}\}$ do not determine $(\partial/\partial\tau_\infty)\times\varphi_l(\omega,\tau_\infty)$ most easily can be seen for $l=0$. If they did, then $s_0(\omega)$, and eventually $V(\tau)$, would be completely determined. However, it is clear in (2.6) that if we re-

place Z by its symmetric with respect to $\tau=\frac{1}{2}\tau_\infty$, or in (2.10) if we replace V by its symmetric with respect to $\tau=\frac{1}{2}\tau_\infty$, then symmetric solutions exist, and give the same sequences of modes $\{\omega_{0n}\}$. There are other transformations[13] of V keeping $\{\omega_{0n}\}$ (see below in Sec. 2). To prove that similar transformations exist also for other values of l, we first use Krein–Marchenko's transformations[5] to prove that there is a *regular* potential $\overline{W}_l(\tau)$, such that, if $\overline{W}_l$ is substituted for $[W_l - l(l+1)\tau^{-2}]$ in (2.10), the corresponding sequence of free oscillations still is $\{\omega_{l,n}\}$.

Proof: We know[5] that if φ is the regular solution of the equation

$$\varphi'' + (\omega^2 - U_l)\varphi = 0, \tag{2.24}$$

and if ψ_0 is *any* solution of the same equation for $\omega=\omega_0$, then the function

$$\varphi_1(\omega,\tau) = \frac{\varphi(\omega,\tau)\psi_0'(\omega_0,\tau) - \varphi'(\omega,\tau)\psi_0(\omega_0,\tau)}{(\omega^2-\omega_0^2)\psi_0(\omega_0,\tau)} \tag{2.25}$$

is the regular solution of

$$\varphi'' + \omega^2\varphi = (U_l + \Delta U_l)\varphi, \tag{2.26}$$

where

$$\Delta U_l = -2\frac{\partial}{\partial\tau}\frac{\psi'(\omega_0,\tau)}{\psi_0(\omega_0,\tau)} \tag{2.27}$$

In Appendix B, we prove that there exists a value of ω_0 and an irregular solution $\psi_0(\omega,\tau)$ which has its smallest zero at $\tau=\tau_\infty$. Let us use this function in (2.25). It is clear in (1.25) that $\varphi_1(\omega,\tau)$ has modes for all ω in $\{\omega_{ln}\}$. From (2.27) it follows[5] that the new potential $U_l+\Delta U_l$ has centrifugal barrier as $r\to 0$ corresponding to $(l-1)$ instead of l. To go back from $U_l+\Delta U_l$, it is possible to use the solution $\overline{\varphi}_1(\omega_0,\tau)=[\psi_0(\omega,\tau)]^{-1}$ in the formula

$$\varphi(\omega,\tau) = \frac{\varphi_1(\omega,\tau)\overline{\varphi}_1'(\omega_0,\tau) - \varphi_1'(\omega,\tau)\overline{\varphi}_1(\omega_0,\tau)}{\overline{\varphi}_1(\omega_0,\tau)}, \tag{2.28}$$

which has the meaning of an inverse of (2.25).

Thus the zeros φ_1 are also those of φ and both functions correspond to the same sequence $\{\omega_{ln}\}$. Using l times this method we are able to destroy the centrifugal singularity and construct $\overline{W}_l(\tau)$. Q.E.D. We can now construct potentials that are equivalent to $\overline{W}_l(\tau)$ like we did above, for instance its symmetric one. Going back l times, we are thus able to construct potentials which have in common with $W(\tau)$ the same sequence of modes. Thus giving the sequence $\{\omega_{ln}\}$ of normal modes is not sufficient to determine $W_l(\tau)$.

Now suppose that the response to a known source enables us to obtain the values of $(\partial/\partial\tau_\infty)\varphi(\omega_{l,n},\tau_\infty)$ for each mode in the l-sequence, up to a multiplicative constant. That such information can be obtained is easily seen with the following (slightly heuristic) argument. The Green's function (which is the response to a point explosion) can be expanded along with the normalized modes ($\overline{\Pi}$),

$$G(\mathbf{R}_0,\mathbf{R}_1) = \sum_{l,m,n} y_{l,m}(\theta_0,\phi_0,\theta_1,\phi_1)\frac{\overline{\Pi}_l(\omega_{l,n},R_0)\overline{\Pi}_l(\omega_{l,n},R_1)}{\omega_{ln}^2-\omega^2}, \tag{2.29}$$

where $\mathbf{R}$ stands for R,θ,ϕ, and y_{lm} stands for the product of spherical harmonics. The physical response is obtained by taking the Fourier transform (as a limit for $\mathrm{Im}\,\omega\to 0^+$) and convoluting with the source function. If one can fully analyze this response, one obtains $\overline{\Pi}_l(\omega_{l,n},R_0)\overline{\Pi}_l(\omega_{l,n},R_1)$. Now (this is the heuristic part), if R_0 and R_1 are very close to R_∞, this product is of the order of $(R_\infty-R_0)(R_\infty-R_1)[(\partial/\partial R_\infty)\overline{\Pi}_l(\omega_{l,n},R_\infty)]^2$. One can obtain this value rigorously if R_0 and R_1 are, together with R_∞, in a surface range where the parameters are constant. If not, the problem is more complicated but can also be disentangled. In all cases, one has to use as additional information the following formula, readily obtained from (2.19) by letting $\dot\omega$ go to $\omega_{l,n}$, $\omega=\omega_{ln}$,

$$\left(\frac{\partial\Pi_l(\omega,R_\infty)}{\partial\omega}\right)_{\omega=\omega_{l,n}}\left(\frac{\partial}{\partial R_\infty}\Pi_l(\omega_{l,n},R_\infty)\right)$$

$$= -\frac{2\rho_\infty\omega_{l,n}}{R_\infty^2}\int_0^\infty \Pi_l^2(\omega_{l,n},R)R^2\lambda^{-1}dR. \tag{2.30}$$

In the case quoted above, where we "know" $(\partial/\partial R_\infty)\overline{\Pi}$, and since we know [from (2.21) and (2.9)] $Z_\infty^{-1}(\partial/\partial\omega)\Pi$, we easily derive from (2.30) the value of $(\rho_\infty/c_\infty)\times(\partial/\partial\tau_\infty)\varphi(\omega,\tau_\infty)$ which is the desired result. Notice that it follows from (2.30), that the information $(1/\rho_\infty)\times(\partial/\partial R_\infty)\Pi_l(\omega_{ln},R_\infty)$ is equivalent to the information $\|\Pi_l(\omega_{l,n},R)\|$.

Thus we know the sequence $[y_l(\omega_{l,n})]$ equal to $(\rho_\infty/c_\infty)\times(y_l(\omega_{l,n}))$. From it, we can derive $y_l(\omega)$ for any ω.

Proof: Let us evaluate the integral of $z^{-2}(z-\omega)^{-1}y(z)$ on an infinite circle in the z plane. Because of the asymptotic behavior of $y(z)$ [see (A12)], this integral is equal to zero. The residue theorem yields

$$y_l(\omega) = y_l(0) - 2\sum_{n=1}^{\infty}\omega^2[\omega_{l,n}\mathcal{R}'(\omega_{l,n})(\omega_{l,n}^2-\omega^2)]^{-1}, \tag{2.31}$$

where

$$\mathcal{R}'(\omega_{l,n}) = \left(\frac{\partial}{\partial\tau_\infty}\varphi(\omega_{l,n},\tau_\infty)\right)^{-1}\frac{\partial}{\partial\omega_{l,n}}\varphi(\omega_{l,n},\tau_\infty) \tag{2.32}$$

is known up to the multiplicative constant c_∞/ρ_∞, but it follows from (A12) that the leading asymptotic behavior of $y_l(\omega)$ as $|\omega|\to\infty$ must be $\omega\cot(\omega\tau - l\pi/2)$. Hence the constant can be determined. If $[\mathcal{R}']=\mathcal{R}'c_\infty/\rho_\infty$, we can write,

$$\rho_\infty/c_\infty = 2\lim_{|\omega|\to\infty}\sum_{n=1}^{\infty}|\omega|[\omega_{l,n}[\mathcal{R}'(\omega_{l,n})](\omega_{l,n}^2+|\omega|^2)]^{-1}. \tag{2.33}$$

Hence, we obtain $\mathcal{R}'(\omega_{l,n})$ from $[\mathcal{R}'(\omega_{l,n})]$ and we can insert the result into (2.31). It remains to determine $y_l(0)$. This is done by writing (2.31) for $W_l=0$, obtaining $y_l^0(\omega)$, which is perfectly well known, and subtracting from (2.31), then taking the limit when $\mathrm{Im}\,\omega\to\infty$, $\mathrm{Re}\,\omega=0$, using (A12). This yields the formula

$$y_l(0)-y_l^{(0)}(0)=2\lim_{|\omega|\to\infty}\sum_{n=1}^{\infty}|\omega|^2\{[\omega_{l,n}^{(0)}R'^{(0)}(\omega_{l,n}^{(0)})$$

$$\times(\omega_{l,n}^0)^2+|\omega|^2)]^{-1}-[\omega_{l,n}R'(\omega_{l,n})(\omega_{ln}^2+|\omega|^2)]^{-1}\}. \tag{2.34}$$

Hence $y_l(\omega)$ is completely determined by (2.31) Q.E.D.

We also know τ_∞ by (2.23), and therefore $f_l(\omega,\tau_\infty)$ and $(\partial/\partial\tau_\infty)f_l(\omega,\tau_\infty)$ by (2.16). From y_l, f_l, and $(\partial/\partial\tau_\infty)f_l$, we readily obtain $s_l(\omega)$ and thus we can construct W_l. From two values of W_l, we first obtain c_∞, which is easily combined with ρ_∞/c_∞ to give Z_∞, λ_∞, ρ_∞, and we easily achieve the whole determination of λ and ρ.

Remark: The assumption that $\lambda(R)$ and $\rho(R)$ have zero derivative for $R\to R_\infty^0$ is a simplifying assumption. It is not essential, but we shall leave to the reader the tedious complications which come in when it is suppressed.

3. DIFFERENTIAL PROBLEM OF THE SECOND KIND

We study the set of equations

$$-\frac{d}{dR}\left(\mu R\frac{d}{dR}R^{-1}T_l\right)-3\mu\frac{d}{dR}(R^{-1}T_l)$$

$$+[(l+2)(l-1)\mu R^{-2}-\rho\omega^2]T_l=0 \tag{3.1}$$

in which l runs through the positive integers, ρ and μ are nonnegative piecewise continuous functions, and ω is a real or complex continuous parameter. Equation (3.1) is completed by the following conditions, in which R_c is a positive number:

$$R\to T_l(\omega,R) \text{ should be absolutely continuous,} \tag{3.2a}$$

$$R\to T_l'=\mu\frac{d}{dR}[R^{-1}T_l(\omega,R)] \text{ should be absolutely continuous,} \tag{3.2b}$$

$$T_l'(\omega,R_c)=T_l'(\omega,R_\infty)=0. \tag{3.2c}$$

Again the conditions (3.2) can be satisfied only for a certain set of values of ω, $\{\omega_{l,n}\}$, which will be called the modes. Again, the inverse problem is to determine information on the modes which is bijectively related to μ, ρ.

Time formulation: We introduce the physical assumption

$$\rho\mu\neq 0 \text{ for any } R\geq R_c, \tag{3.3}$$

and the new variables

$$c(R)=(\mu/\rho)^{1/2},\quad \tau(R)=\int_{R_c}^{R}[c(x)]^{-1}dx,\quad A=(\rho c)^{1/2}R^2. \tag{3.4}$$

Thus we obtain the "time formulation" of (3.1),

$$\left(A^{-2}\frac{d}{d\tau}A^2\frac{d}{d\tau}+\omega^2-\frac{(l-1)(l+2)}{R^2}c^2\right)t_l(\tau)=0, \tag{3.5}$$

where $t_l(\tau)=R^{-1}T_l$, and the conditions (3.2) are to be replaced by

$\tau\to 1$, and $\tau\to A^2\frac{dt_l}{d\tau}$ absolutely continuous,

$$\frac{d}{d\tau}t_l=0 \text{ for } \tau=0 \text{ and } \tau=\tau_\infty. \tag{3.6}$$

Schrödinger formulation: Again we introduce the *strong mathematical assumption*: ρ and μ are twice differentiable functions, going to constants with zero derivative as $R\to R_\infty$. It follows that A is a twice differentiable function of τ. Setting

$$\chi_l(\omega,\tau)=A(\tau)t_l(\omega,\tau), \tag{3.7}$$

we obtain the "Schrodinger formulation" of (3.1),

$$\left(\frac{d^2}{d\tau^2}+\omega^2-V(\tau)-(l+2)(l-1)c^2R^{-2}\right)\chi_l(\omega,\tau)=0, \tag{3.8}$$

where

$$V(\tau)=A^{-1}\frac{d^2}{d\tau^2}A. \tag{3.9}$$

With the assumptions, V is a regular potential for any $0\leq\tau\leq\tau_\infty$ as well as c^2R^{-2}, and χ_l is the continuously differentiable solution of (3.8) which satisfies the boundary conditions

$$\frac{d}{d\tau}[A^{-1}\chi_l(\omega,\tau)]=0 \text{ for } \tau=\tau_\infty. \tag{3.10}$$

Let us now introduce the auxiliary scattering problem. For $R>R_\infty$, we continue μ and ρ by the positive numbers μ' and ρ' which can be equal, or not, to μ_∞ and ρ_∞. For each value of l, we consider the scattering *of an S-wave by the potential*

$$W(l,t)=V(\tau)+(l+2)(l-1)c^2R^{-2}. \tag{3.11}$$

For each potential $W(l,\tau)$, we can define the (S-wave) functions φ_0, f_0, F_0, $s_0(\omega)$, exactly as in Sec. 1. In the following, in all functions we drop the index 0 referring to the absence of centrifugal singularity, and use l as an additional variable only when we want to refer to a particular $W(l,\tau)$ or emphasize the dependence on l. Thus the regular solution of (3.8), which vanishes at $\tau=0$, will be denoted by $\varphi(\omega,\tau)$, or $\varphi(l,\omega,\tau)$ when it is necessary. The scattering "matrix" will be denoted by $s(\omega)$ or $s(l,\omega)$ instead of $s_0(l,\omega)$, which could have been used more correctly. Now, thanks to the positivity of μ and ρ for any $R>R_c$, no bound state can correspond to a potential $W(l,\tau)$. Indeed, for such a potential, it is well known that ω^2 necessarily would be negative, and the regular solution [$\varphi(l,\omega,\tau)$, or its product by $[A(\tau)]^{-1}$, say, $r(l,\omega,\tau)$], would decrease exponentially as $\tau\to\infty$. But $r(\omega,\tau)$ would be a solution of (3.5) so that, multiplying both sides by r and integrating by parts, we would get

$$0=-\int_0^\infty A^2(\tau)\left(\frac{d}{d\tau}r(\omega,\tau)\right)^2d\tau+\int_0^\infty\left(\omega^2-\frac{(l-1)(l+2)c^2}{R^2}\right)$$

$$\times A^2(\tau)r^2(\omega,\tau)d\tau, \tag{3.12}$$

which is contradictory for negative ω^2.

Hence $s(l,\omega)$ is bijectively related to $W(l,\tau)$. On the other hand, it is easy to derive μ and ρ from the values of $W(l,\tau)$ for two values of l since they give $V(\tau)$ and c^2R^{-2} from which μ and ρ can be derived, exactly like we did for λ and ρ in Sec. 1, and provided τ_∞ and Z_∞ (or equivalent information once c_∞ is known) are given. Hence we are led to construct $s(l,\omega)$ from the modes. This will be done in three steps. First we study the analytic properties of the function $\chi(\omega,\tau)$ in the ω plane, and those of its Wronskian with $f(\omega,\tau)$, which is in some sense the "Jost function" of this particular solution of the Schrödinger equation. Then we show how the modes can give this "Jost function." It remains to show how one can get the true Jost function and the S-matrix from it.

Analytic properties of $\chi(\omega,\tau)$: Let us recall that $\varphi(\omega,\tau)$ is the solution of (3.8) which goes to zero, with derivative equal to one, as τ goes to zero. We define the solution $\psi(\omega,\tau)$ as the solution of (3.8) which goes to one, with zero derivative, as $\tau\to 0$. From (3.7), and if we normalize $\chi(\omega,\tau)$ by imposing the value 1 at $\tau=0$, we obtain

$$\chi(\omega,\tau)=\frac{A'(0)}{A(0)}\varphi(\omega,\tau)+\psi(\omega,\tau). \tag{3.13}$$

$\psi(\omega,\tau)$ is a solution of Volterra's integral equation

$$\psi(\omega,\tau)=\cos\omega\tau+\int_0^\tau \frac{\sin[\omega(\tau-\tau')]}{\omega}W(\tau')\psi(\omega,\tau')d\tau'. \tag{3.14}$$

The Green's function which appears in (3.14) can be bounded by means the formula (A5) (used for $l=0$), and $|\cos\omega\tau|$ can be bounded by $C\exp[\tau|\mathrm{Im}\,\omega|]$. Using these bounds, we easily prove that $\psi(\omega,\tau)$ is an even entire function of ω, and satisfies the inequalities[14]

$$|\psi(\omega,\tau)-\cos\omega\tau|<C\int_0^\tau |W(\tau')|d\tau'\,\frac{\tau}{1+|\omega|\tau}\times\exp|\mathrm{Im}\omega|\tau, \tag{3.15}$$

$$\left|\psi(\omega,\tau)-\cos\omega\tau-\int_0^\tau\frac{\sin\omega(\tau-\tau')}{\omega}W(\tau')\cos\omega\tau'd\tau'\right| < C\int_0^\tau|W(\tau')|d\tau'\,\frac{\tau}{1+|\omega|\tau}\exp|\mathrm{Im}\omega|\tau \times\int_0^\tau\frac{\tau'|W(\tau')|d\tau'}{1+|\omega|\tau'}. \tag{3.16}$$

The derivative of ψ with respect to τ is given by

$$\psi'(\omega,\tau)=-\omega\sin\omega\tau+\int_0^\tau\cos[\omega(\tau-\tau')]W(\tau')\psi(\omega,\tau')d\tau'. \tag{3.17}$$

and satisfies the inequality

$$\left|\psi'(\omega,\tau)-\left[-\omega\sin\omega\tau+\int_0^\tau\cos\omega(\tau-\tau')W(\tau')\cos\omega\tau'\,d\tau'\right]\right| < C\int_0^\tau|W(\tau')|d\tau'\exp(|\mathrm{Im}\omega|\tau)\int_0^\tau\frac{\tau'|W(\tau')|d\tau'}{1+|\omega|\tau'}. \tag{3.18}$$

Collecting these properties and those of $\varphi(\omega,\tau)$, which are given in Appendix A, and using (3.13) and (3.7), we are able to prove that

(1) $\chi(\omega,\tau)$ and $t(\omega,\tau)$ are entire functions of ω^2, of order $\frac{1}{2}$.

(2) $\chi'(\omega,\tau)$ and $t'(\omega,\tau)$ are entire functions of ω^2, of order $\frac{1}{2}$.

(3) For large $|\omega|$, and taking into account the differentiability of W in (3.13) and (3.18) to integrate by parts and evaluate the integral on the left-hand side, we obtain for t and t' the asymptotic behavior ($\tau\leq\tau_\infty$)

$$t(\omega,\tau)=\frac{\cos\omega\tau}{A(\tau)}+\frac{\sin\omega\tau}{\omega A(\tau)}\left(\frac{A'(0)}{A(0)}+\frac{1}{2}\int_0^\tau W(\tau')d\tau'\right)+O(|\omega|^{-2}\exp|\mathrm{Im}\omega|\tau), \tag{3.19}$$

$$t'(\omega,\tau)=-\frac{\omega\sin\omega\tau}{A(\tau)}+\frac{\cos\omega\tau}{A(\tau)}\left(\frac{A'(0)}{A(0)}-\frac{A'(\tau)}{A(\tau)}+\tfrac{1}{2}\int_0^\tau W(\tau')d\tau'\right)+O(|\omega|^{-1}\exp|\mathrm{Im}\omega|\tau). \tag{3.20}$$

Construction of $t'(\omega,\tau)$: The modes are the zeros of $t'(\omega,\tau_\infty)$. They have the following properties:

(a) All zeros are real and simple: From (2.5) we obtain the equation

$$\left[A^2\left(\dot t\frac{d}{d\tau}t-t\frac{d}{d\tau}\dot t\right)\right]_{\tau=\tau_\infty}=(\dot\omega^2-\omega^2)\int_0^{\tau_\infty}t\dot t A^2\,d\tau, \tag{3.21}$$

where ω and $\dot\omega$ are two different values of ω, and t and $\dot t$ are the corresponding functions $t(\omega,\tau)$. Setting $\dot\omega=\omega^*$, and noticing that the corresponding function $\dot t$ is nothing but the conjugate t^* of t, we see that if ω is a zero of $t(\omega,\tau_\infty)$, $\mathrm{Re}\,\omega\,\mathrm{Im}\omega=0$. On the other hand, it also follows from (3.5) that

$$-\int_0^{\tau_\infty}A^2\left(\frac{d}{d\tau}t_l\right)^2d\tau=\int_0^{\tau_\infty}\left((l+2)(l-1)\frac{c^2}{R^2}A^2-\omega^2A^2\right)t_l^2(\tau)\,d\tau, \tag{3.22}$$

which yields a contradiction if ω^2 is negative. Q.E.D.

In addition, we see that $\omega=0$ cannot be a mode, and that, for $\omega=0$, neither t_l nor its derivative vanish for any value of R. They both remain positive. It also follows from (3.21) that the functions t of two different modes are orthogonal on $[0,\tau_\infty]$ weight $A^2(\tau)$. On the other hand, one knows that they form a complete set.

(b) Since $t_l'(\omega,\tau_\infty)$ is entire, of order $\frac{1}{2}$, and not zero for $\omega=0$, it can be constructed from the sequence $\{\omega_{l,n}\}$ by Hadamard's product

$$t'(\omega,\tau_\infty)=\prod_{n=1}^{\infty}(1-\omega^2/\omega_n^2)\,t'(0,\tau_\infty). \tag{3.23}$$

It follows from (3.20) that

$$-\frac{A(\tau_\infty)t'(\omega,\tau_\infty)}{\omega\sin(\omega\tau_\infty)}=1+O(|\omega|^{-1})\quad(|\omega|\to\infty). \tag{3.24}$$

Hence, for large imaginary ω ($\omega=i|\omega|$), we obtain τ_∞ by the formula

$$\sum_{n=1}^{\infty} \log \frac{\omega_n^2+4|\omega|^2}{\omega_n^2+|\omega|^2} = |\omega|\tau_\infty + \log 2 + O(|\omega|^{-1}). \quad (3.25)$$

On the other hand, using Hadamard's product for $x^{-1}\sin x$, we easily derive from (3.23) and (3.24) the formula

$$\sum_{n=1}^{\infty} \log \frac{1+|\omega|^2/\omega_n^2}{1+|\omega^2|\tau_\infty^2/n^2\pi^2} - 2\log(|\omega|\tau_\infty) + \log[\tau_\infty A(\tau_\infty) t'(0,\tau_\infty)] = O(|\omega|^{-1}), \quad (3.26)$$

which yields $A(\tau_\infty)t'(0,\tau_\infty)$, achieving the determination of $t'(\omega,\tau_\infty)$ up to the constant A_∞.

(c) That the sequences $\{\omega_{l,n}\}$ do not determine ρ and μ has been shown by Gerver and Kazhdan.[13] The most simple example of nonuniqueness is obtained by replacing $A(\tau)$ and $c(\tau)/R(\tau)$ in (3.5) by $A(\tau-\tau_\infty)$ and $c(\tau-\tau_\infty)/R(\tau-\tau_\infty)$. Obviously $t(\tau-\tau_\infty)$ is a mode of (3.5) with the new parameters if $t(\tau)$ is a mode with the former ones. But clearly also, unless $t(\tau)$ happens to have the same value at 0 and τ_∞, the normalization factor $\int_0^{t_\infty} t^2(\tau)A^2(\tau)\,d\tau$ [with $t(\tau)$ uniformly standardized at $\tau=0$, e.g., by $t(0)=1$] is not conserved in this symmetry. Other examples have been given[13] when $A(\tau)$ and $c(\tau)/R(\tau)$ are periodic functions, with its period equal to $\tau_\infty N^{-1}$ (N is a positive integer). Then a symmetry (as given above) inside a period is possible and transforms a mode into a mode. The new solution of (3.5) is easily obtained by the same transformations, taking care of the continuity of $t(\tau)$ (since the derivative itself is trivially continuous, being zero at both ends of any period).

(d) Suppose now we know in addition either the values $\bar{t}(\omega_n,\tau_\infty)$ (the bar means a normalized function), or the normalization factors $[\int_0^{\tau_\infty} t^2(\omega_n,\tau)A^2(\tau)\,d\tau]^{1/2}$. They are related with each other by the formula

$$-A_\infty t(\omega_n,\tau_\infty)\left(A_\infty \frac{\partial^2}{\partial\tau_\infty\,\partial\omega}\, t(\omega,\tau_\infty)\right)_{\omega=\omega_n} = 2\omega_n \int_0^{\tau_\infty} t^2(\omega_n,\tau)A^2(\tau)\,d\tau, \quad (3.27)$$

which is obtained from (3.21) by setting $\omega=\omega_n$ and letting $\dot{\omega}$ go to ω_n. Using it, we easily see that if we know $\bar{t}(\omega_n,\tau_\infty)$ (which is obtained from the Green's function more easily than in Sec. 1), and since we know $A_\infty(\partial^2/\partial\tau_\infty\partial\omega_n)t(\omega_n,\tau_\infty)$, we know $A_\infty^{-1}t(\omega_n,\tau_\infty)$. Calculating on an infinite circle of the z plane the integral $\int_C[(z-\omega)t'(z,\tau_\infty)]^{-1}t(z,\tau_\infty)\,dz$, and using the asymptotic behavior (3.19)–(3.20), we obtain zero. Thus the residue theorem yields

$$\frac{t(\omega,\tau_\infty)}{t'(\omega,\tau_\infty)} = 2\sum_{n=1}^{\infty} \omega_n t(\omega_n,\tau_\infty)/(\omega_n^2-\omega^2)\left(\frac{\partial}{\partial\omega_n}\, t'(\omega_n,\tau_\infty)\right). \quad (3.28)$$

Comparing the asymptotic behavior of both sides we obtain the value of A_∞^2,

$$A_\infty^{-2} = 2\lim_{|\omega|\to\infty} \sum_{1}^{\infty} \omega_n|\omega|[A_\infty^{-1}t(\omega_n\tau_\infty)] \times\left\{(\omega_n^2+|\omega|^2)\frac{\partial}{\partial\omega_n}[A_\infty t'(\omega_n,\tau_\infty)]\right\}^{-1}, \quad (3.29)$$

and reinserting it in (2.27), we obtain

$$\frac{t(\omega,\tau_\infty)}{t'(\omega,\tau_\infty)} = 2A_\infty^2 \sum_{n=1}^{\infty} \omega_n[A_\infty^{-1}t(\omega_n,\tau_\infty)] \times\left\{(\omega_n^2-\omega^2)\frac{\partial}{\partial\omega_n}[A_\infty t'(\omega_n,\tau_\infty)]\right\}^{-1}. \quad (3.30)$$

Hence, at this point of our study, we know τ_∞, A_∞, and $t(\omega,\tau_\infty)/t'(\omega,\tau_\infty)$. We are now in a position to calculate the S matrix.

(e) For $R\geq R_\infty$, Eq. (2.1) reduces to

$$\frac{d^2\xi_l}{dR^2} + \left(\frac{\omega^2}{c'^2} - \frac{l(l+1)}{R^2}\right)\xi_l = 0, \quad (3.31)$$

where $\xi_l(\omega,R)=\chi_l(\omega,\tau)$. Hence the Jost solution $f(l,\omega,\tau)$ [for $f_0(l,\omega,\tau)$] of (2.8) can be derived for $\tau\geq\tau_\infty$. This Jost function goes to $\exp[i\omega\tau]$ as $\tau\to\infty$, and thus differs from (3.17) by the additional factor $\exp(-il\pi/2)$. The Wronskian $H(\omega)$ of $\chi(\omega,\tau)$ with $f(\omega,\tau)$ is constant. It is readily calculated at $\tau=\tau_\infty$ by using (3.7), $t(\omega,\tau_\infty)$, and $t'(\omega,\tau_\infty)$ [of course, for the S-matrix, which is the ratio $f(-\omega,\tau)/f(\omega,\tau)$, t/t' is sufficient]. Since W is real, $f(-\omega,\tau)$ is the conjugate of $f(\omega,\tau)$, and since $\chi(\omega,\tau)$ is an even function, $H(-\omega)$ is the conjugate of $H(\omega)$. For $t=0$, one readily obtains

$$H(\omega) = f(\omega,0)A'(0)/A(0) - f'(\omega,0) \quad (3.32)$$

and

$$\mathrm{Im}\frac{f(\omega,0)}{H(\omega)} = \frac{\omega}{|H(\omega)|^2} = \mathrm{Im}\frac{F(\omega)}{H(\omega)}, \quad (3.33)$$

where $F(\omega)$ is the Jost function. This result of course suggests that we calculate F from H by a dispersion relation. We need some analytic and asymptotic properties of F and H.

(1) It is well known [and it readily follows from (A13)] that $F(\omega)$ is holomorphic for $\mathrm{Re}\,\omega\geq 0$ and behaves for $|\omega|\to\infty$, $\mathrm{Re}\,\omega\geq 0$, like $1+O(|\omega|^{-1})$. Let $G(\omega)$ be the Wronskian of $f(\omega,\tau)$ with $\psi(\omega,\tau)$. From (3.14), letting $\tau\to\infty$, and using the asymptotic behavior of $f(\omega,\tau)$, we obtain the formula

$$G(\omega) = -i\omega + \int_0^{\infty} \exp(i\omega\tau')W(\tau')\psi(\omega,\tau')\,d\tau' \quad (3.34)$$

and inserting in (3.33) the asymptotic behavior appearing in (3.15) and (3.18), we obtain that for $\mathrm{Re}\,\omega\geq 0$, and $|\omega|\to\infty$,

$$G(\omega) = -i\omega + \int_0^{\infty} \exp(i\omega\tau')W(\tau')\cos(\omega\tau')\,d\tau' + O(|\omega|^{-1}). \quad (3.35)$$

From the definition of $H(\omega)$ and (3.13), we finally obtain the asymptotic behavior of $H(\omega)$ in the upper half-plane,

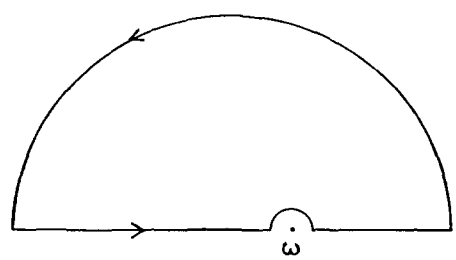

FIG. 1.

$$H(\omega)=-i\omega+\left(\frac{A'(0)}{A(0)}+\int_0^\infty \exp(i\omega\tau')W(\tau')\cos\omega\tau'\,d\tau'\right)$$
$$+O(|\omega|^{-1}). \qquad (3.36)$$

(2) That $H(\omega)$ has no zero in the upper half-plane can be seen as one does for $F(\omega)$ in ordinary potential scattering. If $H(\omega)$ had a zero, then for this value $\chi(\omega,\tau)$ would be proportional to $f(\omega,\tau)$ and hence would decrease exponentially as $\tau\to\infty$. This is also so for $t(\omega,\tau)$. Then writing (3.21) for $\tau=\infty$, instead of $\tau=\tau_\infty$, we again prove that $\mathrm{Re}\omega=0$. Then writing (3.12) for $t(\omega,\tau)$ we obtain a contradiction.

(3) Now, let us calculate the integral, for real ω.

$$\int_C \frac{F(\omega')/H(\omega')}{\omega-\omega'}\,d\omega',$$

where C is given in Fig. 1 and the radius of the half-circle increases to ∞. Since $F(\omega)/H(\omega)$ is $O(|\omega|^{-1})$ on this circle, the corresponding part of the integral vanishes, and since $H(\omega)$ has no zero in the upper half-plane, we obtain after separating the real and imaginary part,

$$\mathrm{Re}\left(\frac{F(\omega)}{H(\omega)}\right)=\frac{1}{\pi}V_p\int_{-\infty}^{+\infty}\frac{\mathrm{Im}[F(\omega')/H(\omega')]}{\omega'-\omega}d\omega'$$
$$=\frac{1}{\pi}V_p\int_{-\infty}^{+\infty}\frac{\omega'}{\omega'-\omega}\,\frac{d\omega'}{|H(\omega')|^2}. \qquad (3.37)$$

So $F(\omega)$ can be calculated from $H(\omega)$.

And $S(\omega)$ is determined from $F(\omega)$, and $W(r')$ can be determined from $F(\omega)$. This closes this part of our study.

Case $\mu\to 0$ as $R\to R_c$: Since $\mu=0$ for $R\le R_c$, it seems necessary to study this case, which makes the Sturm–Liouville problem singular. If $\mu\to 0$ like $(R-R_c)^\alpha$ ($\alpha>0$), whereas ρ remains positive, c goes to zero like $(R-R_c)^{\alpha/2}$. For $\alpha\ge 2$, formula (3.4) cannot define $\tau(R)$ since it does not converge. This case is related both to a "physical singularity" (uncontrolled travel time), and to a very strong mathematical singularity. This case will be discarded in the following.

For $\alpha<2$, $\tau(R)$ goes to zero like $(R-R_c)^{1-\alpha/2}$, and therefore $(R-R_c)$ is $O(\tau^{2/2-\alpha})$. A is $O(R-R_c)^{\alpha/2}$ or $O(\tau^{(\alpha/2)/(2-\alpha)})$. Hence, for $\tau\to 0$,

$$V(\tau)=A^{-1}\frac{d^2}{d\tau^2}A=s(s+1)\tau^{-2}+O(\tau^{-1}), \qquad (3.38)$$

where

$$s=\tfrac{1}{2}(3\alpha-4)/(2-\alpha). \qquad (3.39)$$

The conditions (3.3c) or (3.10) imply that $\chi(\omega,\tau)$ is the solution—say, $\varphi_s(\omega,\tau)$, of (3.8), which is $O(\tau^{1+s})$ as $\tau\to 0$, viz. the "regular solution" of (3.8). The modes are the zeros of $t'(\omega,\tau_\infty)$. Now it follows from (3.7) and the results of Appendix A on the functions φ_s and φ_s' that $t'(\omega,\tau_\infty)$ is an entire function of ω^2 of order $\frac{1}{2}$. It can be constructed from the sequence $\{\omega_n\}$ of its zeros. Again the formulas (3.21) and (3.22) show that all the zeros are real, simple, and $\omega=0$ is not one. From (A9), (A11), and (A16), it is easy to see that for any $s>-1$, there exists a positive number ϵ such that

$$\frac{A(\tau_\infty)t'(\omega,\tau_\infty)}{\omega^{-s}\cos(\omega\tau_\infty-\frac{1}{2}\pi s)}=1+O(|\omega|^{-\epsilon}). \qquad (3.40)$$

Hence, for large imaginary ω ($\omega=i|\omega|$), *we get s and τ_∞* by the formula

$$\sum_{n=1}^{\infty}\log\frac{\omega_n^2+4|\omega|^2}{\omega_n^2+|\omega|^2}=|\omega|\tau_\infty-s\log 2+O(|\omega|^{-\epsilon}). \qquad (3.41)$$

It is important to notice that (3.41) is a straightforward generalization of (3.25), which would correspond to $s=-1$. Thus, investigating the asymptotic behavior of $\{\omega_n\}$ is a way to see that μ goes to zero as R goes to R_c. Now there are two cases, which correspond to different cases in the factorization of $\cos(\omega\tau_\infty-\frac{1}{2}\pi s)$.

(a) If s is an odd integer, $s=(2k+1)$, factorizing $\cos(\omega\tau_\infty-\frac{1}{2}\pi s)$ and using (3.40) yields for large $|\omega|$, and $\omega=i|\omega|$,

$$\sum_{n=1}^{\infty}\log\frac{1+|\omega|^2/\omega_n^2}{1+|\omega|^2\tau_\infty^2/n^2\pi^2}$$
$$+2k\log|\omega\tau_\infty|+\log[\tau_\infty^{-s}t'(0,\tau_\infty)A(\tau_\infty)]=O(|\omega|^{-\epsilon}), \qquad (3.42)$$

which reduces to (3.26) for $s=k-1$.

(b) For other values of $s>-1$, we obtain

$$\sum_{n=1}^{\infty}\log\left\{\left(1+\frac{|\omega|^2}{\omega_n^2}\right)\Big/\left[1+\left(\frac{|\omega|\tau_\infty+\frac{1}{2}is\pi}{(n-\frac{1}{2})\pi}\right)^2\right]+s\log|\omega\tau_\infty|\right|$$
$$-is\tfrac{1}{2}\pi+\log[\tau_\infty^{-s}t'(0,\tau_\infty)A(\tau_\infty)]=O(|\omega|^{-\epsilon}). \qquad (3.43)$$

Thus we are able to determine $t'(0,\tau_\infty)A(\tau_\infty)$, and hence $t'(\omega,\tau_\infty)A(\tau_\infty)$. Again, the response to a known source may give, directly or not, the values $t(\omega_n,\tau_\infty)$, with an additional and uniform factor which involves μ_∞ and ρ_∞. From (A15), (A16) (if $-1<s<0$), (A6), and (A9) (for $s\ge 0$), it follows that there exists ϵ positive and such that, as $|\omega|$ and $\mathrm{Im}\omega\to\infty$,

$$\frac{t(\omega,\tau_\infty)}{t'(\omega,\tau_\infty)}\,\frac{\omega u_s'(\omega\tau_\infty)}{u_s(\omega\tau_\infty)}=1+O(|\omega|^{-\epsilon}). \qquad (3.44)$$

Hence formulas similar to (3.28)–(3.30) can be obtained and yield $t(\omega,\tau_\infty)/t'(\omega,\tau_\infty)$ and $\chi(\omega,\tau_\infty)/\chi'(\omega,\tau_\infty)$.

From this point, this "singular case" is no longer a straightforward generalization of the regular one, because it is simpler! Indeed, since $\chi(\omega,\tau)$ is now the "regular solution, the S-matrix is simply obtained by matching χ and the Jost solution at τ_∞. Of course, to be consistent with the singularity $\tau^{-2}s(s+1)$, we have to define the Jost solution $f_s(\omega,\tau)$ as the solution of (3.8) which behaves asymptotically like $i^l\exp(i\omega\tau)$. The Jost function is the Wronskian of $\chi(\omega,\tau)$ with this Jost solution, and the S-matrix is given, for real ω, by

$$S_s(\omega,\tau_\infty)=\frac{f_s'(-\omega,\tau_\infty)\chi_s(\omega,\tau_\infty)/\chi_s'(\omega,\tau_\infty)-f_s(-\omega,\tau_\infty)}{f_s'(\omega,\tau_\infty)\chi_s(\omega,\tau_\infty)/\chi_s'(\omega,\tau_\infty)-f_s(\omega,\tau_\infty)}. \qquad (3.45)$$

From this S-matrix, using the generalized Marchenko's method,[12] we construct the effective potential, viz., the difference between $U_l(\tau)$ and $s(s+1)\tau^{-2}$ for two values of l. Hence we can achieve the determination of parameters as in the regular case.

4. THE EARTH INVERSE PROBLEM

In the "liquid" approximation $\mu = 0$, where the only modes are radial modes, this problem has been fully treated in Sec. 1. In the general case, we shall only study the information that is contained in the $l = 0$ radial modes and in the toroidal modes. For the sake of simplicity, we shall assume that λ and ρ are positive and twice differentiable functions of R, with zero derivative as $R \to R_\infty$, and that μ is identically zero for $R < R_c$, is $O(R - R_c)^\alpha$, with $1 < \alpha < 2$, for $R \to R_c^+$, and strictly positive and twice diffrentiable for $R > R_c$, with zero derivative as $R \to R_\infty$.

With these assumptions, the toroidal modes problem clearly is the one which has been studied in Sec. 2, in the solvable "singular" range. Hence, a knowledge of two sequences of normal modes, with both eigenvalues and surface derivatives or normalization factors, yields the functions $\rho(R)$ and $\mu(R)$ for $R_c \leq R \leq R_\infty$. Let us now study the radial ($l = 0$) modes. They are given by the equations[14]

$$\frac{d}{dR}\mathcal{R}^* + 4\mu \frac{d}{dR}(R^{-1}\mathcal{R}) = -\rho\omega^2 R, \tag{4.1}$$

$$\mathcal{R}^* = \lambda R^{-2} \frac{d}{dR}(R^2\mathcal{R}) + 2\mu \frac{d\mathcal{R}}{dR}, \tag{4.2}$$

$$\mathcal{R}(\omega, 0) = \mathcal{R}^*(\omega, R_\infty) = 0, \tag{4.3}$$

where $\mathcal{R}$ and $\mathcal{R}^*$ must be continuous functions of R. Actually, it follows from our assumptions that $\mathcal{R}$ and $d\mathcal{R}/dR$ must be continuous. The condition (4.3) can be satisfied only for the spectral values of ω, say, ω_n. The Eqs. (4.1)—(4.3) are the space formulation of the problem. Setting

$$c = (\lambda + 2\mu)^{1/2}\rho^{-1/2}, \tag{4.4}$$

$$\tau = \int_0^R [c(x)]^{-1}\, dx, \tag{4.5}$$

$$Z = R^{-1}(\rho c)^{1/2}, \tag{4.6}$$

and taking into account the differentiability assumptions, we obtain the "Schrödinger" formulation of the problem

$$\frac{d^2 v}{d\tau^2} + [\omega^2 - W(\tau) - V(\tau)]v = 0, \tag{4.7}$$

where

$$v(\omega, \tau) = ZR^2\mathcal{R}(\omega, R(\tau)), \tag{4.8}$$

$$W(\tau) = 4Z^{-2}R^{-3}\frac{d\mu}{d\tau}, \tag{4.9}$$

$$V(\tau) = Z^{-1}\frac{d^2}{d\tau^2}Z. \tag{4.10}$$

In this section, as in previous ones, we use $c(\tau)$, etc., for $c(R(\tau))$, etc., when this is not confusing. Now it follows from (4.4)—(4.6) and the differentiability assumptions that $V(\tau)$ is $2\tau^{-2}[1 + O(\tau^2)]$ as $\tau \to 0$, while $W(\tau)$ is identically zero for any τ smaller than $\tau(R_c) = \tau_c$. Taking into account (4.3), we see that $v(\omega, \tau)$ is the regular solution of the P-wave equation (4.7), and should satisfy in addition (for $\omega = \omega_n$), the second condition (4.3). The potentials $V(\tau)$ and $W(\tau)$ are twice differentiable for any $\tau > 0$, except τ_c, where $V(\tau)$ is $O(\tau - \tau_c)^{\alpha-2}$ when $\tau \to \tau_c^+$, and remains finite when $\tau \to \tau_c^-$, and the derivative of $W(\tau)$ is singular like $V(\tau)$ whereas $W(\tau)$ itself is continuous.

The modes are the zeros of $\mathcal{R}^*(\omega, R_\infty)$. Their properties can be derived with the help of two equations which are easily derived from (4.1), (4.2), and (4.3), by using Wronskian properties as in Secs. 2 and 3. For any $R_0 > 0$, and ω and $\mathring{\omega}$, we can write for regular solutions $\mathcal{R}(\omega, R)$ and $\mathring{\mathcal{R}}(\mathring{\omega}, R)$,

$$-\int_0^{R_0} \rho\omega^2 R^2\, dR = [R^2\mathcal{R}\mathcal{R}^*]_{R=R_0} - \int_0^{R_0} \lambda R^{-2}\left(\frac{d}{dR}(R^2\mathcal{R})\right)^2 dR - 4\int_0^{R_0} \mu\mathcal{R}^2\, dR \tag{4.11}$$

and

$$R_0^2[\mathring{\mathcal{R}}\mathcal{R}^* - \mathcal{R}\mathring{\mathcal{R}}^*]_{R=R_0} = (\mathring{\omega}^2 - \omega^2)\int_0^{R_0} \rho\mathcal{R}\mathring{\mathcal{R}}\, R^2\, dR. \tag{4.12}$$

If $\omega = \omega_n$, and $\mathring{\omega} = \omega^*$ is the conjugate value, $\mathring{\mathcal{R}} = \mathcal{R}^*$, the left-hand side in (4.12) vanishes, the integral in the right-hand side is positive, and hence $\mathrm{Re}\omega_n$ or $\mathrm{Im}\omega_n$ is zero. But if $\mathrm{Re}\omega_n$ was zero, then (4.11), in which the first term of the right-hand side vanishes for $\omega = \omega_n$, would be contradictory. Hence all modes are real. They are simple because there is only one regular solution. It is also easy to prove from (4.11) and (4.12) that there is no bound state (same argument with $R_0 = \infty$) and from (4.11) that $\omega = 0$ is not a mode, and both $\mathcal{R}$ and $\mathcal{R}^*$ (as well as $d\mathcal{R}/dR$) cannot vanish for $R > 0$ if $\omega = 0$.

Again, we continue the parameter for $R > R_\infty$ by constant values (not necessarily those for $R = R_\infty$), so that (4.1) and (4.2) become there

$$\left(\frac{d^2}{dR^2} + \frac{\omega^2}{c'^2} - \frac{2}{R^2}\right) R\mathcal{R} = 0. \tag{4.13}$$

Replacing R by $R_\infty + c'(\tau - \tau_\infty)$ and $R\mathcal{R}$ by v gives the corresponding equation in the Schrödinger time formulation. As in previous problems, we are led to construct the logarithmic derivative of $v(\omega, \tau)$ at $\tau = \tau_\infty$. We shall construct it from $\mathcal{R}(\omega, R_\infty)$ and $\mathcal{R}^*(\omega, R_\infty)$.

The analytic and asymptotic properties of $\mathcal{R}(\omega, R_\infty)$ and $\mathcal{R}^*(\omega, R_\infty)$ can be derived from those of the P wave, $v(\omega, R_\infty)$, and its derivative, which are given in Appendix A, and the formula

$$\mathcal{R}^*(\omega, R_\infty) = Z_\infty\left(\frac{dv(\omega, \tau)}{d\tau}\right)_{\tau=\tau_\infty} + \frac{\lambda_\infty - 2\mu_\infty}{Z_\infty R_\infty^3} v(\omega, \tau_\infty), \tag{4.14}$$

which is derived from (4.2) and (4.8). Since the potential is integrable, $(1 + |\omega|\tau)^{-1}\tau$ can be replaced by $|\omega|^{-1}$ in the remainders.

Thus $\mathcal{R}^*(\omega, R_\infty)$ is an entire function of ω^2, of order $\frac{1}{2}$, which does not vanish for $\omega = 0$, and can be reconstructed as Hadamard's product of its zeros ω_n^2,

$$\mathcal{R}^*(\omega, R_\infty) = \mathcal{R}^*(0, R_\infty)\prod_{n=1}^{\infty}(1 - \omega^2/\omega_n^2). \tag{4.15}$$

From (A9), we obtain the asymptotic behavior of $\mathcal{R}^*(\omega, R_\infty)$,

$$\mathcal{R}^*(\omega, R_\infty) = Z_\infty\omega^{-1}\sin[\omega\tau_\infty] + O(|\omega|^{-2}\exp[|\mathrm{Im}\omega|\tau_\infty]). \tag{4.16}$$

Hence, we derive τ_∞, and $Z_\infty^{-1}\mathcal{R}^*(0,R_\infty)$ by the formulas

$$\sum_{n=1}^{\infty}\log\frac{1+4|\omega|^2/\omega_n^2}{1+|\omega|^2/\omega_n^2}=|\omega|\tau_\infty-\log 2+O(|\omega|^{-1}), \quad (4.17)$$

$$\sum_{n=1}^{\infty}\log\frac{1+|\omega|/\omega_n^2}{1+|\omega|^2\tau_\infty^2/n^2\pi^2}+\log\frac{\mathcal{R}^*(\omega,R_\infty)}{Z_\infty\tau_\infty}=O(|\omega|^{-1}). \quad (4.18)$$

Hence we know $Z_\infty^{-1}\mathcal{R}^*(\omega,R_\infty)$. However, this is not sufficient to determine V and W (one can construct counterexamples as in previous sections), but let us assume in addition that the response to a known source has given the normalized values $\bar{\mathcal{R}}(\omega_n,R_\infty)$. This is tantamount to saying that we know $\mathcal{R}(\omega_n,R_\infty)$ up to a constant factor, since it follows from (4.12) that

$$-R_\infty^2\mathcal{R}(\omega_n,R_\infty)\frac{\partial}{\partial\omega_n}\mathcal{R}^*(\omega_n,R_\infty)=2\omega n\,\|\mathcal{R}(\omega_n,\cdot)\|^2. \quad (4.19)$$

Indeed, $Z_\infty^{-1}\mathcal{R}^*(\omega,R_\infty)$ gives $Z_\infty^{-1}(\partial/\partial\omega_n)\mathcal{R}^*(\omega_n,R_\infty)$, which can be combined with $\bar{\mathcal{R}}(\omega_n,R_\infty)$ to give $Z_\infty^{-1}\mathcal{R}(\omega_n,R_\infty)$. Thus we know $[(\partial/\partial\omega_n)\mathcal{R}^*(\omega_n,R_\infty)]^{-1}\mathcal{R}(\omega_n,R_\infty)$. The integral of $[(z-\omega)\mathcal{R}^*(z,R_\infty)]^{-1}\mathcal{R}(z,R_\infty)$ on an infinite circle in the z plane is zero, thanks to (4.16) and to the corresponding formula for $\mathcal{R}(\omega,R_\infty)$,

$$\mathcal{R}(\omega,R_\infty)=-\omega^{-2}(\rho_\infty c_\infty)^{-1/2}R_\infty^{-1}\cos(\omega\tau_\infty)+O(\omega^{-2}\exp(|\mathrm{Im}\,\omega|\tau). \quad (4.20)$$

The residue theorem yields

$$\frac{\mathcal{R}(\omega,R_\infty)}{\mathcal{R}^*(\omega,R_\infty)}=-2\sum_1^\infty\frac{\omega_n\mathcal{R}(\omega_n,R_\infty)}{(\partial/\partial\omega_n)\mathcal{R}^*(\omega_n,R_\infty)(\omega_n^2-\omega^2)}. \quad (4.21)$$

Comparing the asymptotic behavior of both sides, we obtain

$$R_\infty^{-2}Z_\infty^2=\lim_{|\omega|\to\infty}\left(-2\sum_1^\infty\omega_n|\omega|\mathcal{R}(\omega_n,R_\infty)\times\left[(\omega_n^2+|\omega|^2)\frac{\partial}{\partial\omega_n}\mathcal{R}^*(\omega_n,R_\infty)\right]^{-1}\right). \quad (4.22)$$

Hence we can construct $\mathcal{R}(\omega,R_\infty)$ from (4.21), (4.22), and $Z_\infty^{-1}\mathcal{R}^*(\omega,R_\infty)$, which we already know. From Z_∞, and since the toroidal modes gave μ_∞ and ρ_∞, we can derive λ_∞. Using (4.8) and (4.14), we construct $v(\omega,\tau_\infty)$ and $[dv(\omega,\tau)/d\tau]_{\tau=\tau_\infty}$. The Jost function in the external range $\tau\geq\tau_\infty$ is readily obtained from (4.13), and is equal to the function given in (2.16) for $l=1$. Hence $s_1(\omega)$ can be constructed and since there is no bound state, one can derive from it $\bar{W}(\tau)=W(\tau)+V(\tau)$. We have now to derive $\lambda(R)$ from this function and a knowledge of $\rho(R)$, $\mu(R)$, $\lambda(R_\infty)$, and $\lambda'(R_\infty)=0$. From (4.9) and (4.10), and replacing $d\mu/d\tau$ by $\mu'(R)\,c(\tau)$, and then using (4.6), we obtain for $R(\tau)$ and $Z(\tau)$ the system of equations

$$\frac{d^2Z}{d\tau^2}+\frac{4\mu'(R(\tau))}{R(\tau)\rho(R(\tau))}Z(\tau)=\bar{W}(\tau)Z(\tau), \quad (4.23)$$

$$Z^2(\tau)=\rho(R(\tau))[R(\tau)]^{-2}\frac{dR}{d\tau}. \quad (4.24)$$

So as to reduce this system, we notice that (4.24) is equivalent to

$$\int_{\tau_\infty}^{\tau}Z^2(x)\,dx=\int_{R_\infty}^{R(\tau)}R^{-2}\rho(R)\,dR. \quad (4.25)$$

The function $R\to B=\int_{R_\infty}^{R}t^{-2}\rho(t)\,dt$ is monotone, and continuous. Let D be the inverse function $R=D(B)$. Instead of (4.25), we can write down

$$R(\tau)=D\left(\int_{\tau_\infty}^{\tau}Z^2(x)\,dx\right). \quad (4.26)$$

Then inserting (4.26) in (4.23) yields the unique equation

$$\frac{d^2Z}{d\tau^2}+\left[F\left(\int_{\tau_\infty}^{\tau}Z^2(x)\,dx\right)-\bar{W}(\tau)\right]Z(\tau)=0, \quad (4.27)$$

where

$$F(u)=\frac{4\mu'(D(u))}{\rho(D(u))\,D(u)} \quad (4.28)$$

and Z is the unknown function. Once Z is known, R can be derived by (4.26), then c by (4.6), and, from c and μ, λ is derived by (4.4).

For $\tau<\tau_c$, Eq. (4.27) reduces to an ordinary linear differential equation, which can be solved if we know R_c, ρ_c, λ_c, and their derivatives with respect to τ, all these being continuous at τ_c. Thus we obtain $Z(\tau)$ for $0\leq\tau<T_c$, but we cannot derive λ from Z since we do not know $\rho(R)$ for $R<R_c$.

Usually $W(\tau)$, which involves $d^2Z/d\tau^2$, has a singularity like $(\tau-\tau_c)^{\alpha-2}$ for $\tau\to\tau_c^+$, while V is continuous. Thus $\bar{W}(\tau)$ has the same singularity and, in that case, τ_c is known offhand. If not, τ_c is known as the value of τ for which $R(\tau)=R_c$ which is known from the function $\mu(R)$. Hence it is sufficient to study Eq. (4.27) for $\tau>\tau_c$. We study it for $\tau\in[\tau_c+\epsilon,\tau_\infty]$, where ϵ can be arbitrarily small, but must be positive. On this interval, it is a matter of elementary transformations of (4.27), taking care of Z and its derivative at τ_∞, to obtain the integral equation

$$Z=Z_0(\tau)+\int_{\tau_\infty}^{\tau}(t-\tau)\left\{F\left(\int_{\tau_0}^{t}Z^2(x)\,dx\right)-W(t)\right\}Z(t)\,dt, \quad (4.29)$$

where

$$Z_0(\tau)=Z_\infty-\rho_\infty^{-1}Z_\infty^2(\tau-\tau_\infty). \quad (4.30)$$

It is proved in Appendix C that (4.29) has a unique solution, which can be obtained by a constructive method. From $Z(\tau)$, $R(\tau)$ is derived by (4.25), c by (4.6), λ by (4.4), λ therefore is obtained for any $R\geq R_c$.

Remarks: (1) It is of interest to notice that the method we use to study (4.29) in Appendix C can probably be generalized to take into account more general behavior of $\mu(R)$ as $R\to R_c$. But since there are many other simplifying assumptions in this paper, we do not think it is useful to study generalizations.

(2) Core oscillations and their coupling with mantle oscillations can be studied in the same way, provided their coupling can be described in the elastic theory. Such a study would make it possible to get λ, μ, ρ, from $R=0$ to $R=R_\infty$.

(3) In the regular case, c/R may be a monotone function of τ. Let us take it as a new variable and make a Liouville transform of (3.8). For large l, the transformed equation is the Hankel equation plus a comparatively small perturbation. For $l\to\infty$, it is possible to show in this case that two sequences $\{\omega_{ln}\}$ determine the parameters. Compare this with the JWKB result at the end of Sec. 5 (for a differentiable potential, the

JWKB approximation asymptotically gives the correct result).

5. JWKB INFORMATION

The Schrödinger equations we obtained can be studied by approximate methods. The JWKB method is justified for large values of ω_n, when the differentiability assumptions hold. It can be used to understand the nature of information which is given by the asymptotic behavior of the modes. Take the example of toroidal modes, with Eq. (3.8), first in the regular case. Then $\chi(\omega,\tau)$ is approximately

$$\chi(\omega,\tau)\sim[\omega^2-W(\tau)]^{-1/4}\cos\left(\int_0^\tau[\omega^2-W(t)]^{1/2}\,dt\right) \quad (5.1)$$

and the modes are given by the condition

$$\int_0^{\tau_\infty}[\omega_n^2-W(\tau)]^{1/2}\,dt=(n-\tfrac{1}{2})\pi, \quad (5.2)$$

where $W(\tau)$ is given by (3.11). This asymptotically yields

$$\omega_n=(n-\tfrac{1}{2})\pi+O(n^{-1}). \quad (5.3)$$

Inserting (5.3) and transforming the sum into an integral, enables one to check, for instance, the leading terms in (3.25).

In the singular case, the argument of the periodic function in the approximate value of χ is an integral whose lower bound is the turning point instead of 0. For large ω, this turning point is completely determined by the centrifugal singularity (3.38). Thus the asymptotic behavior of ω_n should give information on s—and this is readily checked in (3.40).

Similar remarks can be made for all sequences of modes. Apart from these pedagogical remarks, is it possible to use this approximation as a practical inversion method?

One certainly thinks of the Rydberg–Klein–Rees method of analyzing data on atom–atom interactions.[5] This method works beautifully in chemical physics when many (vibration-rotation) modes are available. In the earth problem, there are also many available modes, but the smooth differentiable functions which usually justify this approximation are lacking in the crust. Nevertheless, let us look at what it would be for the example of toroidal modes (the others would be similar).

At least for the first modes, which are the best known, turning points appear. The simplest case is the one in which $W(\tau)$ is monotone decreasing, and there is only one turning point. Hardly more complicated is the case in which $W(\tau)$ has a minimum, with two monotone branches. In both cases, the condition (5.2) becomes

$$\int_{TP_1}^{TP_2}[\omega_n^2-W(\tau)]^{1/2}\,dt=(n-\epsilon_n)\,\pi, \quad (5.4)$$

where TP_1 is the first turning point (always present in the singular case) and TP_2 is either the second turning point [if $W(\tau)$ has a minimum, and $\omega_n^2<W(\tau_\infty)$], or τ_∞. ϵ_n is equal to $\frac{1}{2}$ if there is zero or two turning points, $\frac{3}{4}$ if there is one only. n is the ordinal number of the mode (numbered in our paper from 1). A very important additional assumption of the method is that ω_n is so smooth that it justifies interpolation towards $n=\epsilon_n$, which yields the minimum of $W(\tau)$ [or $W(\tau_\infty)$ in the monotone decreasing case]. It is equivalent to say that we can fit the curve $n(\omega)$ from $n=\epsilon_n$.

Apply now to both sides of (5.4) the semi-integration operator between $W_{\min}$ and ω^2, $D^{-1/2}$, defined by

$$[D^{-1/2}f]_{\omega^2}=\pi^{-1/2}\int_{W_{\min}}^{\omega_2}(\omega^2-\omega'^2)^{-1/2}f(\omega'^2)\,d(\omega'^2). \quad (5.5)$$

We obtain

$$I(\omega^2)=\int_{TP_1(\omega^2)}^{TP_2(\omega^2)}[\omega^2-W(\tau)]\,dt=2\pi^{-1/2}D^{-1/2}([n(\omega^2)-\epsilon_n]\pi), \quad (5.6)$$

where $TP_1(\omega^2)$ stands either for the first turning point when it is positive or for 0, $TP_2(\omega^2)$ stands either for the second turning point when it is smaller than τ_∞, or for τ_∞ when it is not. From (5.6), one readily gets the difference $\chi=[TP_2(\omega^2)-TP_1(\omega^2)]$

$$\chi(\omega^2)=\frac{\partial}{\partial\omega^2}\{2\pi^{-1/2}D^{-1/2}([n(\omega^2)-\tfrac{1}{2}]\pi)\}. \quad (5.7)$$

Hence we see again in this approximate model that the modes do not determine $W(\tau)$ but rather the separation between its two branches (in this relatively simple case). It is only when $W(\tau)$ is monotone that it is completely determined, since TP_2 is τ_∞ (another well-posed case would occur if the two branches were symmetric). It is also interesting to notice that when ω^2 is larger than than any $W(\tau)$ (in the regular case), the left-hand side of formula (5.6) should simply reduce to $[\omega^2\tau^2-\int_0^{\tau_\infty}W(\tau)\,dt]$. This yields a simple way to check the relevancy of the JWKB method in the range of values of n which are accessible. But a negative result does not prove anything since one then cannot know whether these large values of ω have been reached or not.

Information contained in the amplitudes at τ_∞: This information can be analyzed in the JWKB approximation. From well-known connection formulas,[15] it is not difficult to see that the amplitude at τ_∞, of modes which are standardized at $\tau=0$, yields the ratio

$$(-1)^n\,|u(0)/u(\tau_\infty)|^{1/2}\exp\left[\int_0^{TP_1}u\,dt-\int_{TP_2}^{\tau_\infty}u\,dt\right], \quad (5.8)$$

where

$$u(\tau)=[W(\tau)-\omega^2]^{1/2}, \quad (5.9)$$

and we assumed that there are two turning points for $\omega=\omega_n$. We saw above that the parts of $W(\tau)$ where there is only one turning point are determined by (5.7). Thus, if we are, for instance, in the case of Fig. 2, $W(\tau)$ is known from $\tau=0$ to $\tau_0=TP_1(W(\tau_\infty))$, $W(\tau_\infty)$ is known, and so are $u(0)$ and $u(\tau_\infty)$. Thus, from (5.8), we know by interpolation between the modes [since we know $\omega(n)$], the value of

$$\Delta(\omega^2)=\int_{\tau_0}^{TP_1}[W(\tau)-\omega^2]^{1/2}dt-\int_{TP_2}^{\tau_\infty}[W(\tau))-\omega^2]^{1/2}dt. \quad (5.10)$$

In other cases, we know $W(\tau)$ near $W(\tau_\infty)$ and replace τ_∞ by another point τ_1. In the singular case, $u(0)$ is infinite and (5.8) has to be modified to take into account a convenient standardization at $\tau=0$, but again we obtain (5.10). Now let us apply to both sides of (5.10) the

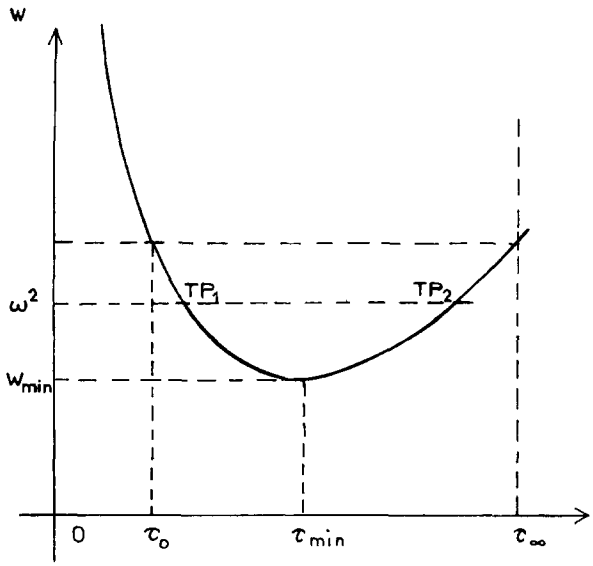

FIG. 2.

semi-integration operator between ω^2 and (in the case of Fig. 2) $W(\tau_\infty)$, in any case, the value of ω^2 which corresponds to the new end points. We obtain

$$Y = 2\pi^{-1/2} D^{-1/2}[\Delta(\omega^2)]$$
$$= \int_{\tau_0}^{TP_1(\omega^2)} [W(\tau) - \omega^2] \int_{TP_2(\omega^2)}^{\tau_\infty} [W(\tau) - \omega^2]\, d\tau \qquad (5.11)$$

and obviously

$$\frac{\partial Y}{\partial \omega^2} = \tau_0 + \tau_\infty - TP_1(\omega^2) - TP_2(\omega^2). \qquad (5.12)$$

Hence, these amplitudes (which are equivalent to the normalization factors, etc., see previous sections) give information that are complementary of those given by $\{\omega_n\}$. Comparing (5.12) and (5.7) readily yields TP_1 and TP_2, and hence $W(\tau)$. Again the result suggested by this approximation method confirms the one obtained in Sec. IV.

Information contained in different values of l: The function $I(\omega^2)$ which is obtained in (5.6) actually depends on l since W is a function of l and τ [see (3.11)]. If we know two sequences with the sequences of amplitudes, this can of course be used as in the exact solution of Sec. 4. But in the RKR method, one can derive TP_1 and TP_2 from (5.6) if one knows its value for different values of l. This is easy to understand: The potential $W(l,\tau)$ which appears in chemical physics contains l in one term, which is exactly known, and which is $(l+\frac{1}{2})^2/\tau^2$ (with the present notation). Hence

$$\frac{\partial(I, (l+\frac{1}{2})^2)}{\partial(l+\frac{1}{2})^2} = -\int_{TP_1(\omega^2)}^{TP_2(\omega^2)} \tau^{-2} dt \qquad (5.13)$$

and this result obviously can be combined with (5.6) to give TP_1 and TP_2. But if we come back to our method, the corresponding ansatz will give

$$T(\omega^2) = \int_{TP(\omega^2)}^{TP_2(\omega^2)} c^2(\tau) R^{-2}(\tau) d\tau, \qquad (5.14)$$

which gives $c(t)R^{-1}(\tau)$ if we know both TP_1 and TP_2, but not if we know their difference.

It is interesting to notice that when l vary, the various values of $X(\omega^2)$ and $T(\omega^2)$ which are obtained depend on l only through the turning points, which should be zero for $\omega^2 - W(l,\tau)$, but not formally. This, however, does not mean that all l values give the same information. Actually, for large l, the term containing l becomes so large that $W(l,\tau)$ is dominated by this term. If it is monotone, between 0 and τ_∞, then everything can be determined, even if, for small l, $V(\tau)$ introduces turning points.

Similar results hold for other mode problems.

Combined information: Suppose we have information which comes altogether from scattered waves[10] (seismic waves in the earth problem) and by modes. The most commonly available modes are the lower ones, whereas the scattering involve much larger values of ω. The JWKB phase shifts involve essentially the same function, $[\omega^2 - W(\tau)]^{1/2}$, and its integral, which appear in the JWKB analysis of modes. Hence it is very easy to combine information on the modes and on scattering data in this approximation. This is not so obvious in the exact case, in which determining a function from its first zeros and its asymptotic behavior is not so easy (nevertheless it can be done, e.g., by using continued fractions or Padé analysis). Here we shall not go deeper in this problem.

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APPENDIX A: REGULAR SOLUTION OF (1.10)

$\varphi_l(\omega,\tau)$, which is normalized as in (1.12), is given by Volterra's integral equation,

$$\varphi_l(\omega,\tau) = \omega^{-l-1} u_l(\omega\tau)$$
$$+ \int_0^\tau G_l(\omega,\tau,\tau') W_l(\tau') \varphi_l(\omega,\tau') d\tau', \qquad (A1)$$

where u_l is the free wavefunction $(\frac{1}{2}\pi\omega\tau)^{1/2} J_{l+1/2}(\omega\tau)$ and G_l is the Green's function, which can be written in terms of the free Jost functions or wavefunctions

$$G_l = \frac{i}{2\omega}(-1)^l [f_l^0(\omega,\tau') f_l^0(-\omega,\tau)$$
$$- f_l^0(\omega,\tau) f_l^0(-\omega,\tau')] \qquad (A2a)$$
$$= (-1)^l \omega^{-1} [u_l(\omega\tau) f_l^0(\omega,\tau')$$
$$- u_l(\omega\tau') f_l^0(\omega,\tau)] \qquad (A2b)$$
$$= (\omega \sin\pi\lambda)^{-1} [\bar{u}_\lambda(\omega\tau)\bar{u}_{-\lambda}(\omega\tau') - \bar{u}_\lambda(\omega\tau')\bar{u}_{-\lambda}(\omega\tau)], \qquad (A3)$$

where $\lambda = l + \frac{1}{2}$, $\bar{u}_{l+1/2} = u_l$. Using the bounds[16] (valid for any Z, any ω, τ, τ' real, and $\tau \geq \tau' \geq 0$):

$$|u_l(Z)| < C|Z|^{-l-1}(1 + |Z|^{-l-1}\exp(|\mathrm{Im}Z|), \tag{A4}$$

$$|G_l(\omega,\tau,\tau')|^{-1}\left(\frac{|\omega|\tau}{1+|\omega|\tau}\right)^{l+1}\left(\frac{|\omega|\tau'}{1+|\omega|\tau'}\right)^{-l}$$

$$\times\exp[|\mathrm{Im}\,\omega|(\tau-\tau')], \tag{A5}$$

we easily show that the series of successive approximations which solves (A1) is absolutely and uniformly convergent. Hence (since G_l and $\omega^{-l-1}u_l$ are entire functions), $\varphi_l(\omega,\tau)$ is an entire function of ω.

Besides

$$|\varphi_l(\omega,\tau) - \omega^{-l-1}u_l(\omega\tau)| \leq C\left(\frac{\tau}{1+|\omega|\tau}\right)^{l+1}\exp(|\mathrm{Im}\,\omega|\tau)$$

$$\times\int_0^\tau \frac{\tau'}{1+|\omega|\tau'}|W_l(\tau')|d\tau'. \tag{A6}$$

From (A1), we obtain a formula for the derivative of φ_l,

$$\frac{\partial}{\partial\tau}\varphi_l(\omega,\tau) = \omega^{-1}u_l'(\omega\tau) + \int_0^\tau\left(\frac{\partial}{\partial\tau}G_l(\omega,\tau,\tau')\right)W_l(\tau')$$

$$\times\varphi_l(\omega,\tau')d\tau'. \tag{A7}$$

Using the recurrence formula for Bessel functions, formula (A4), and the symmetry of the Green's function, we obtain for $\tau \geq \tau' \geq 0$ the bound

$$\left|\frac{\partial}{\partial\tau}G_l(\omega,\tau,\tau')\right|$$

$$< C\left(\frac{|\omega|\tau}{1+|\omega|\tau}\right)^{l}\left(\frac{|\omega|\tau'}{1+|\omega|\tau'}\right)^{-l}\exp[|\mathrm{Im}\omega|(\tau-\tau')]. \tag{A8}$$

Inserting it in (A7), we get

$$\left|\frac{\partial}{\partial\tau}\varphi_l(\omega,\tau) - \frac{\partial}{\partial\tau}\omega^{-l-1}u_l(\omega\tau)\right|$$

$$< C(\tau^{-1}+|\omega|)\left(\frac{\tau}{1+|\omega|\tau}\right)^{l+1}\exp(|\mathrm{Im}\omega|\tau)$$

$$\times\int_0^\tau \frac{\tau'}{1+|\omega|\tau'}|W_l(\tau')|d\tau'. \tag{A9}$$

For large $|\omega|$, in nonreal directions, $|u_l(\omega\tau)|$ is asymptotic to $|\sin(\omega\tau - l\pi/2)|$, and $|u_l'(\omega\tau)|$ to $|\cos(\omega\tau - l\pi/2)|$. Iterating Eq. (A1) once, and using (A6) and (A9), we easily prove that for large $|\omega|$, in nonreal directions, we can write for a regular potential $W_l(\tau)$:

$$\omega^{l+1}\varphi_l(\omega,\tau) = u_l(\omega\tau) + \int_0^\tau G_l(\omega,\tau,\tau')W_l(\tau')u_l(\omega\tau')d\tau'$$

$$+ O(|\omega|^{-2}\exp(|\mathrm{Im}\omega|\tau)), \tag{A10}$$

$$\omega^l\frac{\partial}{\partial\tau}\varphi_l(\omega,\tau) = u_l'(\omega\tau) + \omega^{-1}\int_0^\tau \frac{\partial}{\partial\tau}G_l(\omega,\tau,\tau')$$

$$\times W_l(\tau')u_l(\omega\tau')d\tau' + O(|\omega|^{-2}\exp(|\mathrm{Im}\omega|)), \tag{A11}$$

$$\omega^{-1}\frac{\partial}{\partial\tau}\varphi_l(\omega,\tau)\,/\,\varphi_l(\omega,\tau) - \frac{u_l'(\omega\tau)}{u_l(\omega\tau)}$$

$$= O(|\omega|^{-1}|\mathrm{Im}\omega|^{-1}) + O(|\omega|^{-2}). \tag{A12}$$

Jost function: $F(\omega)$ (for $l=0$), is given by the formula

$$F(\omega) = 1 + \int_0^\infty \exp(i\omega\tau')W(\tau')\varphi(\omega,\tau')d\tau', \tag{A13}$$

which is easily obtained from (A1) (for $l=0$), the definition of $F(\omega)$, and by letting $\tau\to\infty$. Inserting (A6) and (A9) into (A13), we obtain the asymptotic behavior of $F(\omega)$,

$$F(\omega) = 1 + \omega^{-1}\int_0^\infty \exp(i\omega\tau')W(\tau')\sin(\omega\tau')d\tau' + O(|\omega|^{-2}), \tag{A14}$$

where we used the integrability of W on $\mathbf{R}$.

Generation: Let us introduce the continuous variable $\lambda = l + \frac{1}{2}$, and $\mu = \mathrm{Re}\lambda$. For noninteger λ and $\mu \geq 0$, the bounds (A4) and (A5) are readily extended provided $(l+1)$ is replaced by $\mu + \frac{1}{2}$, $-l$ by $-\mu + \frac{1}{2}$. The bounds (A6)—(A14) are thus readily extended with obvious modifications. For integer $\lambda \geq 0$, our method does not apply. From (A3), one can obtain a limit form for G_λ, in which $\log\omega$ appears. It is nevertheless possible to prove that $\varphi_l(\omega,\tau)$ is entire and that the bounds we obtained can be generalized with some modifications in the remainders, but we shall not do it. For $\mathrm{Re}\lambda < 0$, the parity of G_λ enables one to get bounds. In particular, if $-\frac{1}{2} < \mathrm{Re}\lambda < \frac{1}{2}$, with $\lambda \neq 0$, it is easy to see that $|G_\lambda|$ is smaller than $C|\omega|^{-1}\exp[|\mathrm{Im}\omega|(\tau-\tau')|$, whereas $|u_\lambda(z)|$ is smaller than $C\exp[|\mathrm{Im}z|]$. Inserting these bounds, we easily prove from (A1) that $\varphi_l(\omega,\tau)$ is an entire function of ω and $(-1 < l < 0,\ l \neq -\frac{1}{2})$

$$|\varphi_l(\omega,\tau) - \omega^{-l-1}u_l(\omega\tau)|$$

$$< C|\omega|^{-1}\exp(|\mathrm{Im}\omega|\tau)\int_0^\tau |W_l(\tau')|d\tau'. \tag{A15}$$

Bounds for $(\partial/\partial\tau)G_l$ can be obtained from (A8) by noticing the parity of G_l as a function of λ. Inserting them in (A7), we obtain for $-1 < l < 0$, $l \neq -\frac{1}{2}$,

$$\left|\frac{\partial}{\partial\tau}\varphi_l(\omega,\tau) - \omega^{-l}u_l'(\omega\tau)\right|$$

$$< C\left(\frac{|\omega|\tau}{1+|\omega|\tau}\right)^{|l|}\exp(|\mathrm{Im}\omega|\tau)\int_0^\tau |W_l(\tau')|d\tau'. \tag{A16}$$

APPENDIX B

We give some properties of the zeros of the solutions of (2.1), or (2.10), for $l \neq 0$. The regular solution φ is normalized as in (2.13), and we also consider an "irregular solution" ψ such that

$$\psi\varphi' - \psi'\varphi = 1. \tag{B1}$$

(1) $\Pi_l(\omega_{l0}, R)$ has no zero for $R \in]0, R_\infty[$.

Proof: Π_l is the function for which the minimum of the functional $F(\Pi)$ on $\tilde{C}_1(0,R_\infty)$ is achieved, where

$$F(\Pi) = \int_0^{R_\infty}[R^2\rho^{-1}\Pi'^2 - l(l+1)\rho^{-1}\Pi^2 - \omega^2R^2\lambda^{-1}\Pi^2]dR \tag{B2}$$

and

$$\tilde{C}_1(0,R_\infty)=\{y\,|\,y\in C_1(0,R_\infty)\,;\,y(0)=y(R_\infty)=0\}. \tag{B3}$$

In fact, ω_{l0} is fixed by this condition[17] and the additional constraint $\int_0^{R_\infty} R^2\lambda^{-1}\Pi^2\,dR=1$. If there was a zero R_0 in $]0,R_\infty[$, we could replace Π' by 0 in a small interval, of width Δ, containing R_0, in such a way that Π remains continuous. Now $\mathrm{Inf}\,|\Pi'|$ in this interval is not zero (remember that Π and Π' cannot vanish simultaneously) and $\sup|\Pi'|$ is not infinite. It is easy to see that the first term in the right-hand side of (B2) is reduced by a term which is at least $O(\Delta\,\mathrm{Inf}\,|\Pi'|)$, whereas the other ones are reduced by a term which is at most $O(\Delta^3\mathrm{Inf}\,|\Pi'|)$. Thus for the new function Π, $F(\Pi)$ is smaller, which contradicts the fact that is should be minimum Q.E.D.

(2) For $\omega\leq\omega_{l0}$, each zero has a continuous trajectory.

Proof: The zeros are solutions of

$$\Pi(\omega,R(\omega))=0. \tag{B4}$$

Because the differential equation (21) is a linear second order equation, Π and $(\partial/\partial R)\Pi$ cannot simultaneously vanish. Hence the implicit function theorem says that for a couple ω_0, R_0, and an open neighborhood of ω_0, U_0, there exists for all connected open neighborhoods U of ω_0 contained in U_0, a unique continuous mapping $R(\omega)$ such that $R(\omega_0)=R_0$ and (B3) holds. This can be continued in the domain in which we work. Q.E.D.

(3) For ω small enough, there cannot be any zero between 0 and R_∞.

Proof: For any ω such that

$$\omega^2R_\infty^2\lambda^{-1}-l(l+1)\rho^{-1}<0, \tag{B5}$$

such a zero R', when inserted in (2.20), would yield a contradiction.

(4) For $\omega<\omega_{l0}$, there is no zero between 0 and R_∞.

Proof: One can prove very simply that there is a ball free of zeros around $R=0$ (proof left to the reader). Now suppose that there is a zero for $\omega<\omega_{l0}$, and let us make ω decrease. The zero can only go beyond R_∞ since there is no zero for ω small enough. Thus it should reach the value R_∞ for a certain ω smaller than ω_{l0}, which is a contradiction.

(5) All these properties are readily extended to $\varphi_l(\omega,\tau)$ by using the definition of φ_l from Π_l and that of τ from R.

(6) Consider now an irregular solution of (1.10), say $\psi_l(\tau)$. Giving the Wronskian of ψ with φ, as in (B1), is not sufficient to define ψ, since one can add to ψ the product of φ by an arbitrary constant λ (we use in the following the notation ψ_λ). From the analysis given above, we know that the regular solution for $\omega=\omega_{l0}$ is positive for $\tau<\tau_\infty$ and zero at $\tau=\tau_\infty$, and for $\omega=\omega_0\in\,]0,\omega_{l0}[$, is positive for $\tau<\tau_0$, zero at $\tau=\tau_0$, for a certain value τ_0 larger than τ_∞. On the other hand, any solution ψ_λ satisfying (B1) is asymptotic to $\tau^{-l}/(2l-1)!!$ as $\tau\to0$, and is therefore positive. From (B1), it is readily seen that any solution $\psi_\lambda(\omega_0,\tau)$ is negative at $\tau=\tau_0$, and any solution $\psi_\lambda(\omega_{l0},\tau)$ is negative at $\tau=\tau_\infty$.

Now, since φ is positive between 0 and τ_∞, there is a value of λ above which $\psi_\lambda(\omega_0,\tau)$ is positive for $0\leq\tau\leq\tau_\infty$. Fix this value of λ and consider $\psi_\lambda(\omega,\tau)$ for $\omega_0\leq\omega\leq\omega_{l0}$. This function of ω has its first zero in τ smaller than τ_∞ for $\omega=\omega_{l0}$, and larger than τ_∞ for $\omega=\omega_0$. Thanks to the continuity of the zero, there is a value of ω for which $\psi_\lambda(\omega,\tau)$ is positive for $\tau<\tau_\infty$, and zero for $\tau=\tau_\infty$. This result is used in (2.28).

APPENDIX C

Let τ_0 be a number in $[\tau_c,\tau_\infty]$. Let $\mathcal{T}$ be the operator which maps any real function $Z(\tau)$, defined in $[\tau_0,\tau_\infty]$, into a function $\mathcal{T}(Z)$, whose value at τ is

$$[\mathcal{T}(Z)]_\tau=Z_0(\tau)+\int_{\tau_\infty}^{\tau}(t-\tau)[F(\int_{\tau_\infty}^{t}Z^2(x)\,dx-W(t)]Z(t)\,dt. \tag{C1}$$

Any solution of (4.29) is a fixed point of $\mathcal{T}(Z)$ in a conveniently chosen set. Now, in addition to the function $D(B)$ which is defined in (4.26), let us define, for any number $0\leq\epsilon\leq R_\infty-R_c$, the function D_ϵ,

$$D_\epsilon(B)=\begin{cases}D(B) & \text{for } B(R_c+\epsilon)\leq B\leq B(R_\infty)=0,\\ R_c+\epsilon & \text{for } B\leq B(R_c+\epsilon).\end{cases} \tag{C2}$$

In particular, using $D_0(B)$ in (4.28) instead of $D(B)$ enables us to continue F for any real negative argument. F is thus a continuous function, which is equal to zero for $\int_{\tau_\infty}^{\tau}Z^2(x)\,dx<B(R_c)$. In the following, we use this definition of F in (C1). Since $W(t)$ is integrable, and Z_0 is continuous, it follows that $\mathcal{T}$ is a mapping of $C(\tau_0,\tau_\infty)$ into $C(\tau_0,\tau_\infty)$. In the following, we look for the solution of (C1) as a fixed point of $\mathcal{T}$ in $C(\tau_0,\tau_\infty)$, where τ_0 can be any number in $[\tau_c,\tau_\infty]$.

With our definition, F is uniformly bounded for any Z. Let $\bar{F}$ be an upper bound for $|(t-\tau)F|$, $\bar{W}$ be an upper bound for $|(t-\tau)W|$, C_0 their sum, and, for any other function, e.g., Z, let us define the number $\bar{Z}$,

$$\bar{Z}=\sup_{\tau_0\leq\tau\leq\tau_\infty}\left|\exp(-p(\tau_\infty-\tau))\,Z(\tau)\right|, \tag{C3}$$

where p is a positive parameter. One readily shows the inequality

$$\mathcal{T}(\bar{Z})<\bar{Z}_0+p^{-1}C_0\bar{Z}. \tag{C4}$$

Hence, if we choose p larger than C_0, $\mathcal{T}$ maps the set $\beta=\{f\,|\,\bar{f}<\bar{Z}_0(1-p^{-1}C_0)^{-1}\}$ into itself. It follows that any continuous solution Z of (C1) must satisfy the inequality

$$|Z(\tau)|<p(p-C_0)^{-1}\exp(p(\tau_\infty-\tau))\,|Z_0(\tau)| \tag{C5}$$

for any p larger than C_0. We shall set in the following $p=(C_0+1)$. Let us now introduce the function $F_\epsilon(B)$ by substituting D_ϵ for D in (4.28), and the operator $\mathcal{T}_\epsilon$ by substituting F_ϵ in (C1). All the results which have been obtained above remain valid.

Now, consider the algorithm

$$Z_{n+1}(\tau)=Z_0(\tau)+\int_{\tau_\infty}^{\tau}(t-\tau)[F_\epsilon(\int_{\tau_\infty}^{t}Z_n^2(x)dx)-W(t)]Z_n(t)\,dt \tag{C6}$$

which begins at $Z_0(\tau)$. Since Z_0 belongs to β, so does each Z_i, and they satisfy inequality (C5). Let us introduce in $C(\tau_0,\tau_\infty)$ the norm

$$\|Z\| = \sup_{0 \le \tau \le \infty} \{\exp(-q(\tau_\infty - \tau))|Z(\tau)|\}, \quad \text{(C7)}$$

where q is a positive number. $C(\tau_0, \tau_\infty)$ is complete for this norm. From (4.28), (4.25), (4.26) and (C2), it follows that there exists a constant f such that

$$|F_\epsilon(\int_{\tau_\infty}^{t} Z_i^2(x)dx) - F_\epsilon(\int_{\tau_\infty}^{t} Z_j^2(x)dx)| \le f\epsilon^{\alpha-2}\int_t^{\tau_\infty} |Z_i^2(x) - Z_j^2(x)|\,dx. \quad \text{(C8)}$$

From (C6), (C7), and (C8), we obtain

$$\|Z_{n+1} - Z_n\| \le L\|Z_n - Z_{n-1}\|, \quad \text{(C9)}$$

where

$$L \le \frac{2p^2 f(\tau_\infty - \tau_0)}{(2p+q)(p+q)} \exp(2p(\tau_\infty - \tau_0)) + \frac{\bar{F} + \bar{W}}{q}. \quad \text{(C10)}$$

It is always possible to define q so large that $L < 1$, and the algorithm converges for the corresponding norms. Its limit is a continuous function $Z_\epsilon(\tau)$. Since the mapping $\mathcal{T}_\epsilon$ is contracting in $C(\tau_0, \tau_\infty)$ for the norm (C7), $Z_\epsilon(\tau)$ is the unique fixed point of $\mathcal{T}_\epsilon$. Now, two functions F_{ϵ_1} and F_{ϵ_2} are obviously identical for any Z such that

$$D[\int_{\tau_\infty}^{t} Z^2(x)\,dx] > R_c + \sup(\epsilon_1, \epsilon_2) \quad \text{(C11)}$$

and hence $Z_{\epsilon_1}(\tau)$ and $Z_{\epsilon_2}(\tau)$ are identical in this range. It follows that $Z_\epsilon(\tau)$ converges in β. Its limit is continuous for any $\tau > \tau_c$, bounded for $\tau = \tau_c$, and since (4.29) maps bounded functions into continuous functions, it is continuous for any $\tau \ge \tau_c$. That $R(\tau_c)$ must be equal to R_c is a consistency condition, since R_c is known from the toroidal modes, whereas τ_c appears as a singularity of $W(\tau)$.

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Renormalized plane wave-projected and Coulomb-projected T-matrices

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The plane wave-projected formulation of the half-shell T-matrix for ionization and the Coulomb-projected formulation of the half-shell T-matrices for excitation and ionization are shown to converge to zero in the energy-shell limit. "Renormalized" plane wave-projected and Coulomb-projected half-shell T-matrices are defined and are shown to have physical energy-shell limits.

I. INTRODUCTION

The plane-wave-projected (PP) and Coulomb-projected (CP) formulations of the scattering amplitude have been used as a basis for the computation of the excitation and ionization cross sections.[1] In particular the PP formulation of the scattering amplitude has been used to justify the Born approximation for ionization and the CP formulation of the scattering amplitudes leads to the Coulomb-projected Born approximation for excitation and ionization.[1]

In Sec. III of this paper we define PP and CP half-shell T matrices which formally reduce to the integral expressions for the PP and CP excitation and ionization scattering amplitudes on the energy shell. The time-dependent theory of Coulomb scattering is used to show that the PP half-shell T matrix for ionization and the CP half-shell T matrices for excitation and ionization converge to zero in the energy-shell limit.

In Sec. IV of this paper we apply the techniques developed in Ref. 2 to define "renormalized" plane-wave-projected (RPP) and Coulomb-projected (RCP) half-shell T matrices. The convergence of the RPP and RCP half-shell T matrices for ionization and the RCP half-shell T matrix for excitation to the corresponding physical S matrices for ionization and excitation is shown.

A short discussion of the Born approximation and the Coulomb-projected Born approximation is given in Sec. V.

II. PRELIMINARIES

In this paper we consider three spinless particles, assumed to be distinguishable, with a Hamiltonian H given by

$$H = H_0 + V_1(\mathbf{x}_1) + V_2(\mathbf{x}_2) + V_{12}(\mathbf{x}_1 - \mathbf{x}_2),$$

$$H_0 = -\frac{1}{2m_1}\nabla_1^2 - \frac{1}{2m_2}\nabla_2^2,$$

$$V_{12}(\mathbf{x}_1 - \mathbf{x}_2) = \frac{e_1 e_2}{|\mathbf{x}_1 - \mathbf{x}_2|}, \quad V_i(\mathbf{x}_i) = \frac{e_i e_N}{|\mathbf{x}_i|}, \quad i = 1, 2,$$

where m_i, e_i, and $\mathbf{x}_i$, $i = 1, 2$, represent respectively the mass, charge, and position coordinate of particle i and e_N denotes the charge of the "nucleus" which is assumed to be infinitely heavy.

We assume that the initial channel α is made up of an uncharged fragment, consisting of particle 2 bound to the nucleus ($e_N + e_2 = 0$) and a particle 1 which is free. The bound state wavefunction of the particle two-nucleus system is denoted by $\phi_\alpha(\mathbf{x}_2)$ and satisfies

$$H_2\phi_\alpha(\mathbf{x}_2) = E_\alpha\phi_\alpha(\mathbf{x}_2),$$

where

$$H_i = -\frac{1}{2m_i}\nabla_i^2 + V_i(\mathbf{x}_i), \quad i = 1, 2.$$

In the case of excitation the bound state wavefunction $\phi_\beta(\mathbf{x}_2)$ corresponding to the final channel β satisfies

$$H_2\phi_\beta(\mathbf{x}_2) = E_\beta\phi_\beta(\mathbf{x}_2),$$

where $E_\beta \neq E_\alpha$. For ionization the final channel corresponds to the free channel, $\beta = 0$, which is made up of three free particles.

Since there is only one charged fragment in the initial channel α the usual wave operators exist and are given by[3]

$$W_\pm^{(\alpha)} = \text{s-}\lim_{t\to\pm\infty} \exp(iHt)\exp(-iH_\alpha t)P^{(\alpha)}$$

where $H_\alpha = H_0 + V_2$ and $P^{(\alpha)}$ is the projector onto the α-channel subspace $\mathcal{H}^{(\alpha)}$. The "modified" or "renormalized" wave operators which are required in this paper are defined as follows[3]

$$\Omega_\pm^{(0)} = \text{s-}\lim_{t\to\pm\infty} \exp(iHt)\exp[-iH_0 - iG^{(0)}(t)],$$

$$\Omega_\pm^{(j)} = \text{s-}\lim_{t\to\pm\infty} \exp(iH_j t)\exp\left[-i\left(-\frac{1}{2m_j}\nabla_j^2\right)t - iG^{(j)}(t)\right],$$

$$j = 1, 2,$$

where

$$G^{(0)}(t) = G^{(1)}(t) + G^{(2)}(t) + \epsilon(t)\frac{m_1 m_2 e_1 e_2}{|m_2\mathbf{p}_1 - m_1\mathbf{p}_2|}\log\left[\frac{2|t||m_2\mathbf{p}_1 - m_1\mathbf{p}_2|^2}{m_1 m_2(m_1 + m_2)}\right],$$

$$G^{(i)}(t) = \epsilon(t)\frac{m_i e_i e_N}{|\mathbf{p}_i|}\log\left[\frac{2|t||\mathbf{p}_i|^2}{m_i}\right],$$

$$i = 1, 2, \epsilon(t) = \begin{cases} 1, & t > 0, \\ -1, & t < 0, \end{cases}$$

with $\mathbf{p}_i$ the momentum coordinates of particle, i, $i = 1, 2$.

We will asume the usual relation between the wave operator $W_-^{(\alpha)}$ and the three-particle Coulomb wave-

 0022-2488/78/1912-2426$1.00

function $\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1)$, that is,

$$(W_-^{(\alpha)}\phi)(\mathbf{x}_1,\mathbf{x}_2)=\text{l.i.m.}\int d\mathbf{p}_1\,\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1)\hat{\phi}(\mathbf{p}_1), \quad (2.1)$$

where $\phi(\mathbf{x}_1,\mathbf{x}_2)=\psi(\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2)$, $\psi\in L^2(R^3)$ and $\hat{\psi}$ denotes the Fourier transform of ψ. Furthermore, we will require that there exists a constant C for each $\hat{\phi}\in C_0^\infty(R^3\backslash\{0\})$ such that

$$\int d\mathbf{p}_1\,|\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1)\hat{\phi}(\mathbf{p}_1)|<C \quad (2.2)$$

for almost all $\mathbf{x}_1,\mathbf{x}_2\in R^3$. The asumptions (2.1) and (2.2) are sufficient to derive the relationship between the various Riemann—Stieltjes integral expressions of Sec. III and IV and the corresponding half-shell T matrices.

The renormalized wave operators $\Omega_\pm^{(i)}$ can be expanded in terms of the two-particle Coulomb wavefunctions $\psi_\mp(\mathbf{x}_i,\mathbf{p}_i)$, $i=1,2$ as follows[3]:

$$(\Omega_\pm^{(i)}\phi)(\mathbf{x}_i)=\text{l.i.m.}\int d\mathbf{p}_i\;\psi_\mp(\mathbf{x}_i,\mathbf{p}_i)\hat{\phi}(\mathbf{p}_i), \quad i=1,2 \quad (2.3)$$

for each $\phi\in L^2(R^3)$. Using the explicit form of the two-particle wavefunction, one can show that there exists a constant C for each $\phi\in C_0^\infty(R^3\backslash\{0\})$ such that

$$\int d\mathbf{p}_i\,|\psi_\mp(\mathbf{x}_i,\mathbf{p}_i)\hat{\phi}(\mathbf{p}_i)|<C \quad (2.4)$$

for all $\mathbf{x}_i\in R^3$, $i=1,2$.

III. THE PLANE WAVE AND COULOMB-PROJECTED T MATRICES

In this section we define PP and CP forms of the half-shell T matrix and apply the time-dependent theory of Coulomb scattering to examine their behavior near the energy shell. The PP formulation of the half-shell T matrix for ionization and the CP formulation of the half-shell T matrices for excitation and ionization are shown to converge to zero [in the sense of distributions, see Eqs. (3.4), (3.5), and (3.6)] in the energy-shell limit. We conclude from this result that the PP and CP half-shell T matrices are not continuous on the energy shell. Thus the usual integral expressions[1] for the PP scattering amplitude for ionization and the CP scattering amplitudes for excitation and ionization are not mathematically well defined.

The plane wave-projected half-shell T matrix for ionization $\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{pp}}^i|\mathbf{p}_1'\rangle$ and the Coulomb-projected half-shell T matrices for excitation and ionization, denoted respectively by $\langle\mathbf{p}_1|T_{\text{CP}}^e|\mathbf{p}_1'\rangle$ and $\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{CP}}^i|\mathbf{p}_1'\rangle$, are defined as follows:

$$\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{PP}}^i|\mathbf{p}_1'\rangle=\lim_{R\to\infty}\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{PP}}^i(R)|\mathbf{p}_1'\rangle,$$

$$\begin{aligned}\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{PP}}^i(R)|\mathbf{p}_1'\rangle&=\int d\mathbf{x}_1d\mathbf{x}_2\,(2\pi)^{-3/2}\exp(-i\mathbf{p}_1\mathbf{x}_1)\overline{\psi_-(\mathbf{x}_2,\mathbf{p}_2)}\\&\times\exp[-(1/R)(|\mathbf{x}_1|+|\mathbf{x}_2|)][V_1(\mathbf{x}_1)+V_{12}(\mathbf{x}_1-\mathbf{x}_2)]\\&\times\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1'),\end{aligned} \quad (3.1)$$

$$=\lim_{R\to\infty}\langle\mathbf{p}_1,|T_{\text{CP}}^e(R)|\mathbf{p}_1'\rangle,$$

$$\begin{aligned}\langle\mathbf{p}_1|T_{\text{CP}}^e(R)|\mathbf{p}_1'\rangle&=\int d\mathbf{x}_1d\mathbf{x}_2\,\overline{\psi_-(\mathbf{x}_1,\mathbf{p}_1)}\overline{\phi_\beta(\mathbf{x}_2)}\\&\times\exp[-(1/R)|\mathbf{x}_1|]V_{12}(\mathbf{x}_1-\mathbf{x}_2)\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1'),\end{aligned} \quad (3.2)$$

and

$$\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{CP}}^i|\mathbf{p}_1'\rangle=\lim_{R\to\infty}\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{CP}}^i(R)|\mathbf{p}_1'\rangle,$$

$$\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{CP}}^i(R)|\mathbf{p}_1'\rangle=\int d\mathbf{x}_1\,d\mathbf{x}_2\,\overline{\psi_-(\mathbf{x}_1,\mathbf{p}_1)}\,\overline{\psi_-(\mathbf{x}_2,\mathbf{p}_2)} \quad (3.3)$$

$$\times\exp[-(1/R)(|\mathbf{x}_1|+|\mathbf{x}_2|)]V_{12}(\mathbf{x}_1-\mathbf{x}_2)\,\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1'),$$

where the limit $R\to\infty$ is to be taken in the sense of distributions. If we formally set the initial energy equal to the final energy in (3.1), (3.2), and (3.3), we obtain the PP and CP formulations of the scattering amplitudes.[1]

In the following we show that the PP and CP formulations of the half-shell T matrices given by (3.1), (3.2), and (3.3) converge to zero in the energy-shell limit, that is,

$$\lim_{\epsilon\to+0}\lim_{R\to\infty}\int d\mathbf{p}_1d\mathbf{p}_2d\mathbf{p}_1'\,\overline{\hat{f}(\mathbf{p}_1,\mathbf{p}_2)}\hat{g}(\mathbf{p}_1')$$

$$\times\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{PP}}^i(R)|\mathbf{p}_1'\rangle\,\frac{\epsilon}{(E^0-E^\alpha)^2+\epsilon^2}=0, \quad (3.4)$$

$$\lim_{\epsilon\to+0}\lim_{R\to\infty}\int d\mathbf{p}_1d\mathbf{p}_1'\,\overline{\hat{h}(\mathbf{p}_1)}\hat{g}(\mathbf{p}_1')$$

$$\times\langle\mathbf{p}_1|T_{\text{CP}}^e(R)|\mathbf{p}_1'\rangle\,\frac{\epsilon}{(E^\beta-E^\alpha)^2+\epsilon^2}=0, \quad (3.5)$$

and

$$\lim_{\epsilon\to+0}\lim_{R\to\infty}\int d\mathbf{p}_1d\mathbf{p}_2d\mathbf{p}_1'\,\overline{\hat{f}(\mathbf{p}_1,\mathbf{p}_2)}\hat{g}(\mathbf{p}_1')$$

$$\times\langle\mathbf{p}_1,\mathbf{p}_2|T_{\text{CP}}^i(R)|\mathbf{p}_1'\rangle\,\frac{\epsilon}{(E^0-E^\alpha)^2+\epsilon^2}=0 \quad (3.6)$$

for each $\hat{f}\in C_0^\infty(R^6)$, $\hat{f}(\mathbf{p}_1,\mathbf{p}_2)=0$ in a neighborhood of $\mathbf{p}_i=0$ for each i, $i=1,2$, $\hat{g}$, $\hat{h}\in C_0^\infty(R^3\backslash\{0\})$ with $E^\alpha=|\mathbf{p}_1'|^2/2m_1+E_\alpha$, $E^\beta=|\mathbf{p}_1|^2/2m_1+E_\beta$, and $E^0=|\mathbf{p}_1|^2/2m_1+|\mathbf{p}_2|^2/2m_2$.

By a lengthy but straightforward argument (see the proof of Theorem 7.2, Ref. 2) one can show, using (2.1), (2.2), (2.3), and (2.4), that (3.4), (3.5), and (3.6) are consequences of the following respective results:

$$\text{w-}\lim_{\epsilon\to+0}\int_{-\infty}^{+\infty}d_\lambda E_\lambda^{H_0}\Omega_+^{(2)*}[V_1+V_{12}]W_-^{(\alpha)}\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}=0, \quad (3.7)$$

$$\text{w-}\lim_{\epsilon\to+0}\int_{-\infty}^{+\infty}d_\lambda E_\lambda^{H_\beta}P^{(\beta)}\Omega_+^{(1)*}V_{12}W_-^{(\alpha)}\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}=0, \quad (3.8)$$

and

$$\text{w-}\lim_{\epsilon\to+0}\int_{-\infty}^{+\infty}d_\lambda E_\lambda^{H_0}\,(\Omega_+^{(1)}\Omega_+^{(2)})^*V_{12}W_-^{(\alpha)}\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}=0, \quad (3.9)$$

where $E_\lambda^{H_0}$ and $E_\lambda^{H_\beta}$ denote the spectral functions corresponding to H_0 and H_β respectively.[4,5] Thus, in order to show the convergence of the PP and CP formulations of the half-shell T matrices to zero, we must verify (3.7), (3.8) and (3.9). Only the proof of (3.9) is given in the following since (3.7) and (3.8) can be verified in a similar fashion.

The intertwining properties[4] together with the following equalities[5]:

$$\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_1+H_2}(H-\lambda)\frac{1}{H-\lambda\pm i\epsilon} = \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_1+H_2}\ V_{12}\frac{1}{H-\lambda\pm i\epsilon}$$

and

$$\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_1+H_2}\frac{\pm i\epsilon}{H-\lambda\pm i\epsilon} = (\mp)\int_0^{\mp\infty} dt \exp\left[\pm t + \frac{i(H_1+H_2)t}{\epsilon}\right]\exp\left(-\frac{iHt}{\epsilon}\right)$$

yield

$$\begin{aligned}
&\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_0}(\Omega_+^{(1)}\Omega_+^{(2)})^* V_{12} W_-^{(\alpha)} \frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2} \\
&= (2i)^{-1}(\Omega_+^{(1)}\Omega_+^{(2)})^* \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_1+H_2} \\
&\quad\times V_{12}\left(\frac{1}{H-\lambda-i\epsilon}-\frac{1}{H-\lambda+i\epsilon}\right) W_-^{(\alpha)} \\
&= (2i)^{-1}(\Omega_+^{(1)}\Omega_+^{(2)})^* \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_1+H_2} \\
&\quad\times\left(\frac{i\epsilon}{H-\lambda+i\epsilon}+\frac{i\epsilon}{H-\lambda-i\epsilon}\right) W_-^{(\alpha)} \\
&= I_1(\epsilon)+I_2(\epsilon), \qquad (3.10)
\end{aligned}$$

where

$$I_1(\epsilon) = (-2i)^{-1}(\Omega_+^{(1)}\Omega_+^{(2)})^* \int_0^{-\infty} dt \times\exp[t+i(H_1+H_2)t/\epsilon]\exp(-iHt/\epsilon)W_-^{(\alpha)}$$

and

$$I_2(\epsilon) = (-2i)^{-1}(\Omega_+^{(1)}\Omega_+^{(2)})^* \int_0^{+\infty} dt \times\exp[-t+i(H_1+H_2)t/\epsilon]\exp(-iHt/\epsilon)W_-^{(\alpha)}.$$

$I_1(\epsilon)$ converges strongly to zero since

$$\text{s-}\lim_{\epsilon\to+0}\left\{\exp\left[\frac{i(H_1+H_2)t}{\epsilon}\right]\exp\left(\frac{-iHt}{\epsilon}\right)W_-^{(\alpha)} - \exp\left(\frac{iH_1t}{\epsilon}\right)\exp\left[i\left(\frac{1}{2m_1}\nabla_1^2\right)\frac{t}{\epsilon}\right]P^{(\alpha)}\right\}=0$$

for $t<0$ and $\Omega_+^{(2)*}P^{(\alpha)}=0$.

The following result for $t>0$,

$$\text{s-}\lim_{\epsilon\to+0}\{\exp(iHt/\epsilon)\exp[-i(H_1+H_2)t/\epsilon]\Omega_+^{(1)}\Omega_+^{(2)} - \exp(iHt/\epsilon)\exp[-iH_0t/\epsilon - iG^{(1)}(t/\epsilon) - iG^{(2)}(t/\epsilon)]\}=0,$$

together with Corollary A.2 yields

$$\text{w-}\lim_{\epsilon\to+0}(\Omega_+^{(1)}\Omega_+^{(2)})^*\exp[i(H_1+H_2)t/\epsilon]\exp(-iHt/\epsilon)=0$$

for $t>0$. Thus $I_2(\epsilon)$ converges weakly to zero, which verifies (3.9).

IV. RENORMALIZED PLANE WAVE AND COULOMB-PROJECTED T MATRICES

An inadequate formulation of the asymptotic condition for Coulomb scattering is responsible for the breakdown of the PP and CP forms of the half-shell T matrix in the energy-shell limit. In this section we define "renormalized" versions of the PP and CP half-shell T matrices which correctly take into account the asymptotic condition for Coulomb scattering.

The "renormalized" plane wave-projected (RPP) half-shell T matrix for ionization and the "renormalized" Coulomb-projected (RCP) half-shell T matrices for excitation and ionization are defined respectively as follows:

$$\langle \mathbf{p}_1,\mathbf{p}_2|T^i_{\mathrm{RPP}}|\mathbf{p}_1'\rangle = \lim_{R\to\infty}\Lambda_{\mathrm{PP}}(\epsilon)\langle \mathbf{p}_1,\mathbf{p}_2|T^i_{\mathrm{PP}}(R)|\mathbf{p}_1'\rangle, \quad (4.1)$$

$$\langle \mathbf{p}_1|T^e_{\mathrm{RCP}}|\mathbf{p}_1'\rangle = \lim_{R\to\infty}\Lambda^e_{\mathrm{CP}}(\epsilon)\langle \mathbf{p}_1|T^e_{\mathrm{CP}}(R)|\mathbf{p}_1'\rangle, \quad (4.2)$$

$$\langle \mathbf{p}_1,\mathbf{p}_2|T^i_{\mathrm{RCP}}|\mathbf{p}_1'\rangle = \lim_{R\to\infty}\Lambda^i_{\mathrm{CP}}(\epsilon)\langle \mathbf{p}_1,\mathbf{p}_2|T^i_{\mathrm{CP}}(R)|\mathbf{p}_1'\rangle, \quad (4.3)$$

where the limit $R\to\infty$ is to be taken in the sense of distributions and

$$\Lambda_{\mathrm{PP}}(\epsilon) = \Gamma\left(1-i\left(\frac{m_1m_2e_1e_2}{|m_2\mathbf{p}_1-m_1\mathbf{p}_2|}+\frac{m_1e_1e_N}{|\mathbf{p}_1|}\right)\right)^{-1} \times\exp\left\{-i\frac{m_1m_2e_1e_2}{|m_2\mathbf{p}_1-m_1\mathbf{p}_2|}\log\left[\frac{\epsilon m_1m_2(m_1+m_2)}{2|m_2\mathbf{p}_1-m_1\mathbf{p}_2|^2}\right] - i\frac{m_1e_1e_N}{|\mathbf{p}_1|}\log\left(\frac{\epsilon m_1}{2|\mathbf{p}_1|^2}\right)\right\}, \quad (4.4)$$

$$\Lambda^e_{\mathrm{CP}}(\epsilon) = \Gamma\left(1+\frac{im_1e_1e_N}{|\mathbf{p}_1|}\right)^{-1}\exp\left[i\frac{m_1e_1e_N}{|\mathbf{p}_1|}\log\left(\frac{\epsilon m_1}{2|\mathbf{p}_1|^2}\right)\right], \quad (4.5)$$

$$\Lambda^i_{\mathrm{CP}}(\epsilon) = \Gamma\left(1-\frac{im_1m_2e_1e_2}{|m_2\mathbf{p}_1-m_1\mathbf{p}_2|}\right)^{-1} \times\exp\left\{-i\frac{m_1m_2e_1e_2}{|m_2\mathbf{p}_1-m_1\mathbf{p}_2|}\log\left[\frac{\epsilon m_1m_2(m_1+m_2)}{2|m_2\mathbf{p}_1-m_1\mathbf{p}_2|^2}\right]\right\}. \quad (4.6)$$

In the following we show the convergence of the renormalized half-shell T matrices (4.1), (4.2), and (4.3) to the corresponding physical S matrices for excitation and ionization.

The S operators for excitation and ionization are defined respectively by $S_{\alpha\beta}=-(1/2\pi i)W_+^{(\beta)*}W_-^{(\alpha)}$ and $S_{\alpha 0}=-(1/2\pi i)\Omega_+^{(0)*}W_-^{(\alpha)}$. The physical S matrices for excitation and ionization, denoted respectively by $\langle \mathbf{p}_1|S^e|\mathbf{p}_1'\rangle_{E^\beta=E^\alpha}$ and $\langle \mathbf{p}_1,\mathbf{p}_2|S^i|\mathbf{p}_1'\rangle_{E^0=E^\alpha}$, exist as distributions[6] and satisfy

$$\langle h_1|S_{\alpha\beta}g_1\rangle = \int_{E^\beta=E^\alpha} d\mathbf{p}_1d\mathbf{p}_1'\,\overline{\hat h(\mathbf{p}_1)}\,\hat g(\mathbf{p}_1')\langle \mathbf{p}_1|S^e|\mathbf{p}_1'\rangle_{E^\beta=E^\alpha} \quad (4.7)$$

and

$$\langle f|S_{\alpha 0}g_1\rangle = \int_{E^0=E^\alpha} d\mathbf{p}_1d\mathbf{p}_2d\mathbf{p}_1'\,\overline{\hat f(\mathbf{p}_1,\mathbf{p}_2)}\,\hat g(\mathbf{p}_1')\langle \mathbf{p}_1,\mathbf{p}_2|S^i|\mathbf{p}_1'\rangle_{E^0=E^\alpha} \quad (4.8)$$

for each $f\in S(R^6)$ and $h_1=h\phi_\beta$, $g_1=g\phi_\alpha$, $h,g\in S(R^3)$. Let $\chi_\delta(\mathbf{y})$ be a C^∞ function which satisfies

$$|\chi_\delta(|\mathbf{y}|)|\le 1,\quad \chi_\delta(|\mathbf{y}|)=\begin{cases}1 & \text{if } |\mathbf{y}|\ge\delta,\\ 0 & \text{if } |\mathbf{y}|\le\delta/2.\end{cases}$$

Let

$$\mathcal{D} = \{\phi(\mathbf{x}_1,\mathbf{x}_2)\,|\,\hat\phi(\mathbf{p}_1,\mathbf{p}_2) = \chi_\delta(|\mathbf{p}_1|)\chi_\delta(|\mathbf{p}_2|)\chi_\delta(|m_2\mathbf{p}_1-m_1\mathbf{p}_2|)\hat\psi(\mathbf{p}_1,\mathbf{p}_2)$$

for some $\delta>0$ where $\hat\psi\in C_0^\infty(R^6)\}$. $\mathcal{D}$ is dense in $L^2(R^6)$.

The renormalized half-shell T matrices and physical S-matrices are related as follows:

$$\int_{E^0=E^\alpha} d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_1' \overline{\hat{f}(\mathbf{p}_1,\mathbf{p}_2)}\,\hat{g}(\mathbf{p}_1')\langle \mathbf{p}_1,\mathbf{p}_2|S^i|\mathbf{p}_1'\rangle_{E^0=E^\alpha}$$
$$= \lim_{\epsilon\to+0}\lim_{R\to\infty}\int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_1' \overline{\hat{f}(\mathbf{p}_1,\mathbf{p}_2)}\,\hat{g}(\mathbf{p}_1')$$
$$\times\Lambda_{PP}(\epsilon)\langle \mathbf{p}_1,\mathbf{p}_2|T^i_{PP}(R)|\mathbf{p}_1'\rangle \frac{\epsilon}{(E^0-E^\alpha)^2+\epsilon^2}$$
$$= \lim_{\epsilon\to+0}\lim_{R\to\infty}\int d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_1' \overline{\hat{f}(\mathbf{p}_1,\mathbf{p}_2)}\, g(\mathbf{p}_1')$$
$$\times\Lambda^i_{CP}(\epsilon)\langle \mathbf{p}_1,\mathbf{p}_2|T^i_{CP}(R)|\mathbf{p}_1'\rangle \frac{\epsilon}{(E^0-E^\alpha)^2+\epsilon^2} \tag{4.9}$$

and

$$\int_{E^\beta=E^\alpha} d\mathbf{p}_1 d\mathbf{p}_1' \overline{\hat{h}(\mathbf{p}_1)}\,\hat{g}(\mathbf{p}_1')\langle \mathbf{p}_1|S^e|\mathbf{p}_1'\rangle_{E^\beta=E^\alpha}$$
$$= \lim_{\epsilon\to+0}\lim_{R\to\infty}\int d\mathbf{p}_1 d\mathbf{p}_2 \overline{\hat{h}(\mathbf{p}_1)}\,\hat{g}(\mathbf{p}_1')$$
$$\times\Lambda^e_{CP}(\epsilon)\langle \mathbf{p}_1|T^e_{CP}(R)|\mathbf{p}_1'\rangle \frac{\epsilon}{(E^\beta-E^\alpha)^2+\epsilon^2}, \tag{4.10}$$

where $f\in\mathcal{D}$ and $\hat{g}$, $\hat{h}\in C_0^\infty(R^3\backslash\{0\})$.

Using (2.1)–(2.4) together with (4.7) and (4.8), one can show that (4.9) and (4.10) are consequences of the following Riemann–Stieltjes integral representations of the S operators:

$$\langle f_1|S_{\alpha 0}g_1\rangle = \lim_{\epsilon\to+0}\left\langle (\Lambda_{PP}(\epsilon))^* f_1 \left| (\pi^{-1})\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_0}\,\Omega_+^{(2)*}\right.\right.$$
$$\left.\left.\times[V_1+V_{12}]W_-^{(\alpha)}\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}g_1\right\rangle\right., \tag{4.11}$$

$$\langle f_2|S_{\alpha 0}g_1\rangle = \lim_{\epsilon\to+0}\left\langle (\Lambda^i_{CP}(\epsilon))^* f_2 \left| (\pi^{-1})\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_0}\,(\Omega_+^{(1)}\Omega_+^{(2)})^*\right.\right.$$
$$\left.\left.\times V_{12}W_-^{(\alpha)}\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}g_1\right\rangle\right., \tag{4.12}$$

and

$$\langle h_1|S_{\alpha\beta}g_1\rangle = \lim_{\epsilon\to+0}\left\langle (\Lambda^e_{CP}(\epsilon))^* h_1 \left| (\pi^{-1})\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta}\,\Omega_+^{(1)*}\right.\right.$$
$$\left.\left.\times V_{12}W_-^{(\alpha)}\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}g_1\right\rangle\right., \tag{4.13}$$

where $g_1\in\mathcal{H}^{(\alpha)}$ and $f_1\in\mathcal{H}$, $f_2\in\mathcal{H}$, $h_1\in\mathcal{H}^{(\beta)}$ are such that $(\Lambda_{PP}(\epsilon))^* f_1\in\mathcal{H}$, $(\Lambda^i_{CP}(\epsilon))^* f_2\in\mathcal{H}$ and $(\Lambda^e_{CP}(\epsilon))^* h_1\in\mathcal{H}^{(\beta)}$ for each $\epsilon>0$. Only the proof of (4.12) is given in the following since (4.11) and (4.13) are verified by an analogous argument.

Using (3.10) yields

$$\left\langle (\Lambda^i_{CP}(\epsilon))^* f_2 \left| (\pi^{-1})\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_0}\,(\Omega_+^{(1)}\Omega_+^{(2)})^* V_{12}W_-^{(\alpha)}\right.\right.$$
$$\left.\left.\times\frac{\epsilon}{(\lambda-H_\alpha)^2+\epsilon^2}g_1\right\rangle\right. \tag{4.14}$$
$$= \pi^{-1}\langle(\Lambda^i_{CP}(\epsilon))^* f_2|I_1(\epsilon)g_1\rangle + \pi^{-1}\langle(\Lambda^i_{CP}(\epsilon))^* f_2|I_2(\epsilon)g_1\rangle$$

for $g_1\in\mathcal{H}^{(\alpha)}$ and $f_2\in\mathcal{H}$ such that $(\Lambda^i_{CP}(\epsilon))^* f_2\in\mathcal{H}$, $\epsilon>0$.

The term involving $I_1(\epsilon)$ in (4.14) converges to zero as $\epsilon\to+0$ since $I_1(\epsilon)$ converges strongly to zero. The term involving $I_2(\epsilon)$ can be written as follows

$$\pi^{-1}\langle(\Lambda^i_{CP}(\epsilon))^* f_2|I_2(\epsilon)g_1\rangle = (-2\pi i)^{-1}\int_0^{+\infty} dt\exp(-t)$$
$$\times\langle\exp(iHt/\epsilon)\exp[-i(H_1+H_2)t/\epsilon]$$
$$\times\Omega_+^{(1)}\Omega_+^{(2)}(\Lambda^i_{CP}(\epsilon))^* f_2|W_-^{(\alpha)}g_1\rangle. \tag{4.15}$$

In order to complete the proof of (4.12), we must show that (4.15) converges to $\langle f_2|S_{\alpha 0}g_1\rangle$.

By a similar argument as used to verify Theorem A.1 we have

$$\text{s-}\lim_{\epsilon\to+0}\{\exp(iHt/\epsilon)\exp[-i(H_1+H_2)t/\epsilon]\Omega_+^{(1)}\Omega_+^{(2)}$$
$$\times\exp[-iG^{12}(t/\epsilon)]-\Omega_+^{(0)}\}=0$$

for each $t>0$. Thus for each fixed $t>0$

$$\text{s-}\lim_{\epsilon\to+0}\exp(iHt/\epsilon)\exp[-i(H_1+H_2)t/\epsilon]\Omega_+^{(1)}\Omega_+^{(2)}(\Lambda^i_{CP}(\epsilon))^* f_2$$
$$= \text{s-}\lim_{\epsilon\to+0}\exp(iHt/\epsilon)\exp[-i(H_1+H_2)t/\epsilon]\Omega_+^{(1)}\Omega_+^{(2)}$$
$$\times\exp[-iG^{12}(t/\epsilon)]\exp[iG^{12}(t)](\tilde{\Lambda}^i_{CP})^* f_2$$
$$= \Omega_+^{(0)}\exp[iG^{12}(t)](\tilde{\Lambda}^i_{CP})^* f_2, \tag{4.16}$$

where $(\Lambda^i_{CP}(\epsilon))^* f_2\in\mathcal{H}$ and

$$(\Lambda^i_{CP}(\epsilon))^* = \exp\left(\frac{im_1m_2e_1e_2}{|m_2\mathbf{p}_1-m_1\mathbf{p}_2|}\log\epsilon\right)(\tilde{\Lambda}^i_{CP})^*.$$

From (4.16) it follows that (4.15) converges to $\langle f_2|S_{\alpha 0}g_1\rangle$, which verifies (4.12).

V. CONCLUDING REMARKS

The usual Born approximation for ionization and the Coulomb-projected Born approximations for excitation and ionization have been derived from the PP and CP formulations of the scattering amplitudes by replacing the three-particle wavefunction $\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1')$, appearing in these expressions, by $(2\pi)^{-3/2}\exp(i\mathbf{p}_1'\cdot\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2)$.[1] This derivation is not adequate since the PP and CP formulations of the scattering amplitudes are not defined.

Presumably these approximations can be justified by defining formal "renormalized" series expansions for the RPP and RCP half-shell T matrices in analogy with the two-particle case.[7] For example, a renormalized series expansion for the RCP half-shell T matrix for ionization can be defined by expanding (4.3) via the Lippmann–Schwinger equations for $\psi^{(\alpha)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}_1)$, multiplying the result by the series expansion of $\Lambda^i_{CP}(\epsilon)$ and collecting all terms which are multiplied by the same powers of the expansion parameters e_1e_2 and e_1e_N. The term multiplied by e_1e_2 is given by

$$\lim_{R\to+\infty} e_1e_2\int d\mathbf{x}_1 d\mathbf{x}_2\,\overline{\psi_-(\mathbf{x}_1,\mathbf{p}_1)}\,\overline{\psi_-(\mathbf{x}_2,\mathbf{p}_2)}\exp[-(1/R)(|\mathbf{x}_1|+|\mathbf{x}_2|)]$$
$$\times|\mathbf{x}_1-\mathbf{x}_2|^{-1}(2\pi)^{-3/2}\exp(i\mathbf{p}_1'\cdot\mathbf{x}_1)\phi_\alpha(\mathbf{x}_2). \tag{5.1}$$

Using the techniques of this paper one can show that (5.1) has a well-defined energy shell limit which is given by the usual Coulomb-projected Born approximation for ionization.[1] The terms from the expansion of $\Lambda^i_{CP}(\epsilon)$ which are divergent in the limit $\epsilon\to+0$ appear in the renormalized series expansion for (4.3) in the coefficients of $(e_1e_2)^l$, $l>1$, and thus do not effect the validity of the Coulomb-projected Born approximation. Thus if one is willing to accept the validity of a renormalized series expansion for (4.3) then the Coulomb-projected

Born approximation can be justified via the RCP expressions for the half-shell T matrix.

The approach adopted in this paper is also applicable to the problem of multiple ionization. One can define RPP and RCP half-shell T matrices for multiple ionization and show the convergence of these expressions to the physical S matrix.

APPENDIX

We assume that $H = H_0 + V$, where H_0 is the usual N-particle kinetic energy operator and V consists of a sum of two-body Coulomb-like potentials, i.e., $V = \sum_{i<j} V_{ij}$, $V_{ij} = V_{ij}^c + V_{ij}^s$, $V_{ij}^s = V_{ij}^1 + V_{ij}^2$, $V_{ij}^1 \in L^2(R^3)$, $V_{ij}^2 \in L^p(R^3)$, $2 < p < 3$. The results of this appendix are also valid for the scattering situation considered in this paper where one particle is assumed to be infinitely heavy.

The renormalized wave operators $\Omega_{\pm}^{(\beta)}$ for N-particle Coulomb scattering are defined by

$$\Omega_{\pm}^{(\beta)} = \text{s-}\lim_{t \to \pm\infty} \exp(iHt) \exp[-iH_\beta t - iG_2^{(\beta)}(t)] P^{(\beta)}, \tag{A1}$$

where $G^{(\beta)}(t)$ consists of a sum of terms connecting the various charged fragments making up the channel β.[3] Let $G_1^{(\beta)}(t)$ consist of a fixed number of these terms and set $G_2^{(\beta)}(t) = G^{(\beta)}(t) - G_1^{(\beta)}(t)$. Let the bound state wavefunction corresponding to the lth fragment, $1 \leq l \leq n_\beta$, where n_β is the number of complex fragments making up the channel β, be denoted by $n_l(x_l)$ where x_l denotes collectively the internal coordinates associated with the lth fragment.

We have the following technical result (see Ref. 8 for the case of two-particle scattering involving a general class of long-range potentials):

Theorem A.1: Assume that for $l = 1, \ldots, n_\beta$ –

$$\int d\mathbf{x}_l \, |n_l(x_l)|^2 |\mathbf{x}_l|^\beta < \infty$$

for some $\beta > 0$ and each $\mathbf{x}_l$ making up x_l; then

$$\text{s-}\lim_{t \to \pm\infty} \{\exp(iHt) \exp[-iH_\beta t - iG_2^{(\beta)}(t)] P^{(\beta)} - \Omega_{\pm}^{(\beta)} \exp[iG_1^{(\beta)}(t)]\} = 0. \tag{A2}$$

Outline of proof: We have for a dense set of $\psi \in \mathcal{H}^{(\beta)}$ $(t > 0)$

$$\|\{\exp(iHt) \exp[-iH_\beta t - iG_2^{(\beta)}(t)] P^{(\beta)} - \Omega_{+}^{(\beta)} \exp[iG_1^{(\beta)}(t)]\}\psi\| \leq \int_t^{+\infty} du \left\| \left(V^{(\beta)} - \frac{dG^{(\beta)}(u)}{du} \right) \exp[-iH_\beta u - iG^{(\beta)}(u) + iG_1^{(\beta)}(t)]\psi \right\|,$$

where $V^{(\beta)} = H - H_\beta$. It is straightforward to generalize Dollard's estimates[3] to show that the above integral converges to zero as $t \to +\infty$.

The following result is an immediate consequence of Theorem A1.

Corollary A.2: Suppose the hypothesis of Theorem A.1 is satisfied and assume that

$$\text{w-}\lim_{t \to \pm\infty} \exp[iG_1^{(\beta)}(t)] = 0; \tag{A3}$$

then

$$\text{w-}\lim_{t \to \pm\infty} \exp(iHt) \exp[-iH_\beta t - iG_2^{(\beta)}(t)] P^{(\beta)} = 0. \tag{A4}$$

In Ref. 2 the convergence of the N-particle off-shell wavefunctions for Coulomb scattering to zero in the limit to physical energies was shown to be a consequence of the following result:

$$\text{w-}\lim_{\epsilon \to +0} W_{\pm\epsilon}^{(\beta)} = 0,$$

$$W_{\pm\epsilon}^{(\beta)} = (\pm) \int_0^{\pm\infty} dt \exp(\mp t + iHt/\epsilon) \exp(-iH_\beta t/\epsilon) P^{(\beta)}. \tag{A5}$$

The proof of (A5) given in Ref. 2 required the asymptotic completeness of H. Corollary A.2 allows us to drop the asymptotic completeness of H assumption. Setting $G_1^{(\beta)}(t) = G^{(\beta)}(t)$ in Corollary A.2 yields

$$\text{w-}\lim_{t \to \pm\infty} \exp(iHt) \exp(-iH_\beta t) P^{(\beta)} = 0.$$

Thus (A5) is valid under the hypothesis of Corollary A.2 together with the assumptions stated in the first paragraph concerning H.

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An illustration of the Lie group framework for soliton equations: Generalizations of the Lund–Regge model

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The Lie group framework for soliton equations is illustrated. It is shown that the original Lund–Regge model is one of an infinite family of similar relativistically invariant models that possess associated eigenvalue problems and isospectral flows. The models are explicitly found and their associated structures displayed. The group theoretic significance of the soliton equations and associated structures are given in accordance with the general theory.

1. INTRODUCTION

In this paper it is shown that a relativistically invariant set of field equations studied by Lund and Regge[1] and Lund[2] and shown by them to possess an associated eigenvalue problem and isospectral flow is one example of an infinite family of similar models. This family of models is defined and the associated eigenvalue problem and isospectral flows are explicitly computed. The calculations in this paper are all carried out from the point of view of a recently developed Lie group framework of soliton equations[3,4] and are illustrations both of the logic of this approach to soliton equations and the computational procedure that yields soliton equations in the Form (2.2) below with $C^l_{np} \neq 0$.

Equation (2.2) is the necessary and sufficient condition for the local existence of parameters (coordinates) that themselves depend, for a Lie group G (specified by the structure constants C^k_{np}), on two space–time points. It was pointed out in Refs 3 and 4 that (2.2) is formally equivalent to defining a Yang–Mills field with zero field strength. Thus soliton equations can be thought of as defining vector potentials, denoted below by f^k_λ, that describe part of the Yang–Mills vacuum. A particular soliton equation does not describe the entire vacuum of the gauge field associated with G since for a particular soliton equation the f^k_λ are of particular form. In a loose sense the soliton equation fixes the gauge. It is not clear whether this last statement can be made precise.

The interpretation of (2.2) as defining a Yang–Mills field with zero field strength is slightly labored since when the Yang–Mills field vanishes the field equations vanish without a trace, so to speak, since they reduce to $0=0$ and leave no artifact in the formalism. However the identification has a certain heuristic value and is quite natural from the point of view of Yang's integral formulation of gauge fields.[14]

Once the bilocal parameters of G are defined, group actions are considered. In accordance with the general theory[4] the linear group action is the eigenvalue problem and isospectral flow associated with the soliton equation. Some nonlinear group actions are also considered.

The Lie group framework for soliton equations offers a clear and unambiguous Lie group theoretic interpretation of the inverse scattering equations and has a unique generalization when the number of space–time dimesions is greater than two. If the framework is accepted in two dimensions as an appropriate description of soliton equations and associated structures, then it follows that in more than two dimensions it should be possible to write soliton equations in the form (2.2)[3,4] and that the higher dimensional generalization of the inverse scattering equations continue to be the linear group action, i.e., of the form (4.3) below.

The Lie group framework provides a group theoretic interpretation of "pseudopotentials" that is incompatible with the understanding of these objects as defining generalizations of conservation laws. It will be recalled that "pseudopotentials" were introduced in Ref. 5 as generalizations of the potentials of classical conservation laws, hence the name. The most recent exposition of this point of view can be found in the papers by Estabrook, Hermann, and Wahlquist in Ref. 6 and Hermann in Ref. 7. As a generalization of conservation laws, when three dimensions are present the "prolongation structure" should be defined by 2-forms, in four dimensions by 3-forms and so on. The reason for this is that the vanishing of an exterior derivative of an $(N-1)$-form in n-dimensional space–time is, in coordinates, a vanishing of the N-divergence of an n-vector, i.e., a conservation law. Indeed Morris[8] adapted, with some success, the differential-form prolongation ideas to nonlinear wave equations in more variables by doing precisely this (see Hermann's introduction to Ref. 7). The present author also investigated "pseudopotentials" from this point of view.[9,10]

In the Lie group approach the "pseudopotentials" in $N=2$ are elements of a representation space on which G acts. They retain this interpretation in all dimensions. In essence the difference in how these objects are understood comes down to the observation that it is possible in two dimensions to interpret the exterior derivative of a 1-form as whether the specialization of the exterior derivative of an $(N-1)$-form in N-dimensional space–time *or* as the specialization of the exterior derivative of a 1-form in N-dimensional space–time. The Wahlquist–Estabrook approach takes the first interpretation. If soliton equations and the associated inverse scattering equations are to be given a Lie group theoretic interpretation the second interpretation is the only possible choice.

The above remarks were included in the spirit of "truth in advertising," that is, the reader should be clearly aware of the forseeable implications of adopt-

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ing one or another approach. Precisely because on one hand the characteristics of solitons in higher dimensions are obscure and on the other two dimensions has so many special characterisitics, it is extremely important to draw careful distinctions between interpretations of two-dimensional soliton equations and associated structures, if the eventual object of the investigation is to produce a fomulation that generalizes in a useful way, with respect to solitons, to higher dimensions. There is, of course, no question of the logical consistency, in two dimensions, of the Wahlquist–Estabrook approach, the Lie group approach, or most of the other two-dimensional interpretations given in the literature, some of which are mentioned in the concluding section of this paper.

2. FIELD EQUATIONS AS INTEGRABILITY CONDITIONS

Attention will be focused on pairs of real field equations of the form

$$\Theta_{\alpha\beta} - g(\Theta) + h(\Theta)\lambda_\alpha\lambda_\beta = 0, \tag{2.1a}$$

$$\lambda_{\alpha\beta} = p(\Theta)(\lambda_\alpha\Theta_\beta + \lambda_\beta\Theta_\alpha). \tag{2.1b}$$

Subscripts denote differentiation with respect to the indicated variable and $g(\Theta)$, $h(\Theta)$, and $p(\Theta)$ are, for the moment, arbitrary functions of Θ. Clearly with appropriate choices of $g(\Theta)$, $h(\Theta)$, and $p(\Theta)$, (2.1) become the systems discussed in Refs. 1 and 2. It will be shown that these are but two of an infinite number of equations of the form (2.1) that have soliton properties.

When can the system (2.1) be written as the integrability conditions for a bilocal Lie group?[4] That is, for which g, h, and p is this possible? More exactly, when can (2.1) be written in the form

$$\frac{\partial f^l_\mu}{\partial x^\lambda} - \frac{\partial f^l_\lambda}{\partial x^\mu} = C^l_{np} f^n_\lambda f^p_\mu, \tag{2.2}$$

where l, n, $p = 1, \cdots, f$, C^l_{np} are the structure constants for an f-papameter Lie group G, $\lambda = 0, 1, \cdots, N-1$, and N = dimension of the underlying space–time.

In this work attention will be restricted to the above question with the stipulation that $f = 3$ so that $l, n, p = 1, 2, 3$, and $C^l_{np} = \epsilon_{lnp}$, where ϵ_{lnp} is the completely antisymmetric tensor with $\epsilon_{123} = 1$. Further $N = 2$ and the space–time coordinates (which should be thought of as light-cone coordinates) are denoted by α and β.

It is convenient to note the components of f^l_μ, $\mu = \alpha, \beta$ by

$$f^l_\alpha \equiv -A^l, \quad f^l_\beta \equiv -B^l, \tag{2.3}$$

and to introduce the vectors

$$\mathbf{A} = (A^1, A^2, A^3), \quad \mathbf{B} = (B^1, B^2, B^3). \tag{2.4}$$

With this notation (2.2) becomes

$$\mathbf{A}_\beta - \mathbf{B}_\alpha = \mathbf{A}\times\mathbf{B}. \tag{2.5}$$

It is now required that (2.5) becomes a re-expression of (2.1) with a suitable identification of **A** and **B** as functions of the field variables and their independent derivatives, these being Θ, Θ_α, Θ_β, λ_α, and λ_β. It will become clear in this example, and it is true in general, that the identification of the f^l_μ so that the original field equations are expressed in the form (2.2) is a computational problem with a well-defined line of attack. This point was not stressed in Ref. 4; see, however, Refs. 9–12.

It is thus required that

$$\mathbf{A} = \mathbf{A}(\Theta, \Theta_\alpha, \lambda_\alpha), \tag{2.6a}$$

$$\mathbf{B} = \mathbf{B}(\Theta, \Theta_\beta, \lambda_\beta), \tag{2.6b}$$

where no Θ_β or λ_β dependence is assumed in **A** since this can quickly be seen to be impossible by arguments similar to those used below, likewise with Θ_α and λ_α in **B**.

Using (2.6), (2.5) becomes

$$\mathbf{A}_\Theta\Theta_\beta + \mathbf{A}_{\Theta_\alpha}\Theta_{\alpha\beta} + \mathbf{A}_{\lambda_\alpha}\lambda_{\alpha\beta} - \mathbf{B}_\Theta\Theta_\alpha - \mathbf{B}_{\Theta_\beta}\Theta_{\alpha\beta} - \mathbf{B}_{\lambda_\beta}\lambda_{\alpha\beta} = \mathbf{A}\times\mathbf{B}. \tag{2.7}$$

Using (2.1) this becomes

$$\mathbf{A}_\Theta\Theta_\beta - \mathbf{B}_\Theta\Theta_\alpha + [g(\Theta) - h(\Theta)\lambda_\alpha\lambda_\beta](\mathbf{A}_{\Theta_\alpha} - \mathbf{B}_{\Theta_\beta}) + p(\Theta)(\lambda_\alpha\Theta_\beta + \lambda_\beta\Theta_\alpha)(\mathbf{A}_{\lambda_\alpha} - \mathbf{B}_{\lambda_\alpha}) = \mathbf{A}\times\mathbf{B}. \tag{2.8}$$

Following the computation method discussed in detail in Refs. 9 and 11, it can be shown that **A** and **B** must be of the form

$$\mathbf{A} = \Theta_\alpha\mathbf{C}^1 + \lambda_\alpha\mathbf{A}^2(\Theta) + \mathbf{F}(\Theta), \tag{2.9a}$$

$$\mathbf{B} = \Theta_\beta\mathbf{C}^2 + \lambda_\beta\mathbf{B}^2(\Theta) + \mathbf{G}(\Theta), \tag{2.9b}$$

where $\mathbf{C}^1$ and $\mathbf{C}^2$ are constant vectors. When this result is used in (2.8) and the independence of Θ_α, Θ_β, λ_α, and λ_β is used to balance the coefficients of monomials in these quantities it follows that

$$\mathbf{C}^1\times\mathbf{C}^2 = 0, \tag{2.10a}$$

$$\mathbf{G}_\theta = \mathbf{G}\times\mathbf{C}^1 \tag{2.10b}$$

$$\mathbf{F}_\Theta = \mathbf{F}\times\mathbf{C}^2, \tag{2.10c}$$

$$\mathbf{F}\times\mathbf{G} = g(\Theta)(\mathbf{C}^1 - \mathbf{C}^2), \tag{2.10d}$$

$$\mathbf{A}^2\times\mathbf{G} = 0, \tag{2.11a}$$

$$\mathbf{B}^2\times\mathbf{F} = 0 \tag{2.11b}$$

$$\mathbf{A}^2\times\mathbf{B}^2 = -h(\Theta)(\mathbf{C}^1 - \mathbf{C}^2), \tag{2.11c}$$

$$p(\Theta)(\mathbf{A}^2 - \mathbf{B}^2) - \mathbf{B}^2_\theta = \mathbf{C}^1\times\mathbf{B}^2, \tag{2.12a}$$

$$p(\Theta)(\mathbf{A}^2 - \mathbf{B}^2) + \mathbf{A}^2 = \mathbf{A}^2\times\mathbf{C}^1. \tag{2.12b}$$

It should be noted that when $\lambda_\alpha = \lambda_\beta = 0$, (2·10) becomes the full set of equations to be made equivalent to (2.1), which itself reduces to

$$\Theta_{\alpha\beta} = g(\Theta), \tag{2.13}$$

a case of independent interest.

It is easy to see from (2·10a) and (2·10c) that

$$\mathbf{G}\cdot\mathbf{G} = k_1^2, \quad \mathbf{F}\cdot\mathbf{F} = k_2^2, \tag{2.14}$$

where k_1 and k_2 are constants. Using (2·10b) and (2.10c) and (2.10d) it follows that

$$(\mathbf{F}\cdot\mathbf{G})_\theta = \gamma^2 g(\Theta), \tag{2.15}$$

where $\gamma^2 = (\mathbf{C}^1 - \mathbf{C}^2)\cdot(\mathbf{C}^1 - \mathbf{C}^2)$. It is then not difficult to show, using several vector identities and (2·10a) that

$$g'' + \gamma^2 g = 0, \tag{2.16}$$

where $g' \equiv dg(\Theta)/d\Theta$. The only forms of $g(\Theta)$ that are possible are given by (2·16).

The system (2·10) can now easily be solved since the general form of the solutions of (2·10b) and (2·10c) are immediate. Explicit solutions will be displayed in the next section. For the moment it will simply be assumed that (2·10) are solved and that F and G are known. The problem now is to find what, if any restrictions there are on h and p.

To find these restrictions note that it follows from (2·11a) and (2.11b) that

$$A^2(\Theta) = t(\Theta)G, \tag{2.17a}$$

$$B^2(\Theta) = r(\Theta)F, \tag{2.17b}$$

while (2·11c) implies

$$\mathrm{tr}g = h. \tag{2.18}$$

Now (2·12a) can be written

$$p(tG - rF) - r_\Theta F - rF \times C^2 = rC^1 \times F. \tag{2.19}$$

Taking the dot product with F yields

$$p(t\ F\cdot G - r\ k_2^2) - r_\Theta k_2^2 = 0, \tag{2.20}$$

hence

$$r_\Theta + pr = \frac{p}{k_2^2}\ F\cdot G\ t, \tag{2.21}$$

or

$$(r^2)_\Theta + 2pr^2 = \frac{2p}{k_2^2}\ F\cdot G\ \frac{h}{g}. \tag{2.22}$$

Likewise

$$(t^2)_\Theta + 2pt^2 = \frac{2p}{k_1^2}\ F\cdot G\frac{h}{g}. \tag{2.23}$$

Thus

$$k_2^2\ r^2 = k_1^2\ t^2 + C\ \exp\ (-2\int^\theta p\ d\Theta'). \tag{2.24}$$

It suffices to take the constant C equal to zero so that

$$t = \left(\frac{k_2^2}{k_1^2}\right)^{1/2} r, \tag{2.25}$$

hence

$$r^2 = \left(\frac{k_1^2}{k_2^2}\right)^{1/2} \frac{h}{g}. \tag{2.26}$$

Using this result in (2·22) it follows that

$$\left(\frac{h}{g}\right)_\Theta = -2p\left(1 - \frac{F\cdot G}{(k_1^2k_2^2)^{1/2}}\right)\frac{h}{g}. \tag{2.27}$$

Clearly either h or p can be taken independently, the remaining function can be computed by (2.27). Here p will be treated as independent; thus

$$\frac{h}{g} = C\ \exp\left[-2\int^\theta p\left(1 - \frac{1}{(k_1^2k_2^2)}F\cdot G\right)d\Theta'\right]. \tag{2.28}$$

Notice that the constant C can be absorbed in a simple equal, change of scale of λ_α and λ_β and is not essential.

It has been shown that (2.1) can be written in the form (2.2) with $C^n_{i\beta} = \epsilon_{ni\beta}$, provided (2.16) is satisfied and h and p are related by (2.27). In the next section various examples are discussed: A and B are explicitly computed so that subsequently associated eigenvalue problems and isospectral flows for (2.1) can be written down. These associated structures are, as follows from the general theory,[4] the differential form of the linear group action given by the bilocally parameterized Lie group defined (locally) by (2.2).

3. EXAMPLES

In this section various examples of the general solution to the problem of writing (2.1) in the form (2.2) will be presented. In particular the vectors A and B will be explicitly computed for several representative cases. These will be used in the next section to obtain the associated eigenvalue problem and isospectral flow for (2.1) as a direct application of the general theory presented in Ref. 4.

Due to (2.10a) it is possible to introduce a constant vector C such that $C^1 = aC$ and $C^2 = bC$. With this notation the general solution to (2.10b) and (2.10c) is given by

$$F = F^1(\Theta) + c_1C, \tag{3.1a}$$

$$G = G^1(\Theta) + c_2C, \tag{3.1b}$$

where F^1 and G^1 are orthogonal to C. It is convenient to introduce a coordinate system at this point and sufficient to let $c_1 = c_2 = 0$.

Let

$$C = (0, 1, 0), \tag{3.2}$$

and write $g(\Theta)$ in the form

$$g(\Theta) = g_1 \exp(i\gamma\Theta) + g_2 \exp(-i\gamma\Theta). \tag{3.3}$$

The appropriate solution of (2.10b) and (2.10c) is

$$F = (b_1 \exp(ib\Theta) + b_2 \exp(-ib\Theta),\ 0,\ -ib_1 \exp(ib\Theta) + ib_2 \exp(-ib\Theta)), \tag{3.4a}$$

$$G = (a_1 \exp(ia\Theta) + a_2 \exp(-ia\Theta),\ 0,\ -ia_1 \exp(ia\Theta) + ia_2 \exp(-ia\Theta)). \tag{3.4b}$$

Due to (2.10c)

$$a_1b_2 = -\frac{i}{2}\gamma g_1, \tag{3.5a}$$

$$a_2b_1 = \frac{i}{2}\gamma g_2, \tag{3.5b}$$

where, now, $\gamma = a - b$. Clearly

$$F\cdot F = k_2^2 = 4b_1b_2, \tag{3.6a}$$

$$G\cdot G = k_1^2 = 4a_1a_2, \tag{3.6b}$$

$$k_1^2k_2^2 = 4\gamma^2 g_1g_2, \tag{3.7}$$

$$\frac{k_2^2}{k_1^2} = \frac{4b_1^2b_2^2}{\gamma^2 g_1g_2}. \tag{3.8}$$

Further,

$$F\cdot G = -g'(\Theta). \tag{3.9}$$

Notice that $k_1^2k_2^2$ is independent of the integration constants a_1, a_2, b_1, b_2 due to the constraint (2.10d). Equation (2.28) now becomes

$$\frac{h}{g} = c\ \exp\ -2\int^\Theta p(\Theta')\ 1 + \frac{1}{2\gamma\sqrt{g_1g_2}}g'(\Theta')\ d\Theta'\ . \tag{3.10}$$

It is now possible to write A and B explicitly, using

(2.9), (2.16), (2.17), (2.25), (2.26), (3.3)–(3.5), and (3.8). In particular the components of **A** and **B** are:

$$A^1 = b_1 \exp(ib\Theta) + b_2 \exp(-ib\Theta) - i\lambda_\alpha \left(\frac{\gamma b_1 b_2 h}{2g}\right)^{1/2} (g_1 g_2)^{-1/4} \times \left(\frac{g_1}{b_2} \exp(ia\Theta) - \frac{g_2}{b_1} \exp(-ia\Theta)\right), \tag{3.11a}$$

$$A^2 = a\Theta_\alpha, \tag{3.11b}$$

$$A^3 = -i(b_1 \exp(ib\Theta) - b_2 \exp(-ib\Theta)) - \lambda_\alpha \left(\frac{\gamma b_1 b_2 h}{2g}\right)^{1/2} \times (g_1 g_3)^{-1/4} \left(\frac{g_1}{b_2} \exp(ia\Theta) + \frac{g_2}{b_1} \exp(-ia\Theta)\right), \tag{3.11c}$$

$$B^1 = -i\frac{\gamma}{2}\left(\frac{g_1}{b_2} \exp(ia\Theta) - \frac{g_2}{b_1} \exp(-ia\Theta)\right) + \lambda_\beta \left(\frac{\gamma h}{2g b_1 b_2}\right)^{1/2} \times (g_1 g_2)^{1/4} (b_1 \exp(ib\Theta) + b_2 \exp(-ib\Theta)), \tag{3.12a}$$

$$B^2 = b\Theta_\beta, \tag{3.12b}$$

$$B^3 = -\frac{\gamma}{2}\left(\frac{g_1}{b_2} \exp(ia\Theta) + \frac{g_2}{b_1} \exp(-ia\Theta)\right) - i\lambda_\beta \left(\frac{\gamma h}{2g b_1 b_2}\right)^{1/2} \times (g_1 g_2)^{1/4} (b_1 \exp(ib\Theta) - b_2 \exp(-ib\Theta)). \tag{3.12c}$$

Notice that up to this point all expressions derived were symmetric in the a's and b's reflecting the symmetry of (2.1) in α and β. In (3.11) and (3.12) an asymmetry is introduced by solving (3.5) for $a_1 a_2$ in terms of b_1, b_2. The reverse could obviously be done. Further, notice that (3.11) and (3.12) depend on *two* free parameters b_1 and b_2 which arose as integration constants of (2.10b) and (2.10c).

Several specializations of (3.11) and (3.12) are of interest. By far the most important, given the current status of inverse scattering-solition theory, is the case when $b=0$, $a=\gamma$, and $b_1=-b_2=\eta$. In this case:

$$A^1 = -\lambda_\alpha \left(\frac{\gamma h}{2g}\right)^{1/2} (g_1 g_2)^{-1/4} g(\Theta), \tag{3.13a}$$

$$A^2 = \gamma\Theta_\alpha \tag{3.13b}$$

$$A^3 = -2i\eta + \lambda_\alpha \left(\frac{h}{2\gamma g}\right)^{1/2} (g_1 g_2)^{-1/4} g^1(\Theta), \tag{3.13c}$$

$$B^1 = \frac{i\gamma}{2}\frac{1}{\eta} g(\Theta), \tag{3.14a}$$

$$B^2 = 0, \tag{3.14b}$$

$$B^3 = -i\frac{1}{2\eta}\, g^1(\Theta) - (\gamma\beta)^2 \left(\frac{\gamma h}{g}\right)^{1/2} (g_1 g_2)^{1/4}. \tag{3.14c}$$

It will be shown in the next section that the linear group action of G defined through A and B given above are the eigenvalue problem and isospectral flow associated with (2.1) subject to (2.16) and (2.27). It is interesting to observe that even when the full two-parameter freedom in (3.11) and (3.12) is not used, i.e., the restriction $b_1=-b_2$ is employed, a tremendous amount of information about (2.1) can be gained from the linear group action through the inverse scattering method. What, if any, additional information about (2.1) might be gained by not relating b_1 and b_2 is an open question.

It should be observed that solving for b_1 and b_2 in (3.5) using the result in (3.11) and (3.12) and specializing to $a=0$, $b=-\gamma$, together with $a_1=-a_2$ would yield a representation which is "isospectral" in the α direction.

The nonlinear group action associated with a symmetric specialization of (3.11) and (3.12) yields an interesting observation about the Bäcklund transformation for the sine-Gordon equation. Suppose in (3.11) and (3.12) that $g(\Theta)=\frac{1}{8}\sin 2\Theta$ and $a=1$, $b=-1$, $b_1=b_2=i\eta$, and $\lambda_\alpha=\lambda_\beta=0$, then:

$$A^1 = 2i\eta \cos\Theta, \tag{3.15a}$$

$$A^2 = \Theta_\alpha, \tag{3.15b}$$

$$A^3 = -2i\eta \sin\Theta, \tag{3.15c}$$

$$B^1 = \frac{i}{8\eta}\cos\Theta, \tag{3.16a}$$

$$B^2 = -\Theta_\beta, \tag{3.16b}$$

$$B^3 = \frac{i}{8\eta}\sin\Theta. \tag{3.16c}$$

The relationship between this representation of the sine-Gordon equation, the nonlinear group action of G and the Bäcklund transformation for sine-Gordon will be discussed in the next section.

4. GROUP ACTIONS

In the previous sections it has been shown which equations of the type (2.1) can be written in the form (2.2). In group theoretic terms (2.2) is the necessary and sufficient condition for the (local) existence of a bilocal parameterization of a Lie group. The next step is to consider linear and nonlinear group actions of the group. This is now done.

In the general theory the infinitesimal form of the group action is given by

$$\frac{\partial q^a(x)}{\partial x^\lambda} = f^k_\lambda(x) X^a_k(q) \tag{4.1}$$

(see Ref. 4 for a detailed derivation), where the q^a are elements of the d-dimensional representation space Q, $a=1,\cdots,d$. The $X^a_k(q)$ satisfy

$$[X_k, X_l]^a \equiv \frac{\partial X^a_k}{\partial q^b} X^b_l - X^b_k \frac{\partial X^a_l}{\partial q^b} = C^m_{kl} X^a_m. \tag{4.2}$$

In the case of a linear group action

$$X^a_k(q) = I^a_{kb} q^b, \tag{4.3}$$

where the matrices I_k, with matrix element I^a_{kb}, form a d-dimension matrix representation of the Lie algebra of G so that

$$I_k I_l - I_l I_k = C^m_{kl} I_m. \tag{4.4}$$

Consider the case when $C^m_{kl}=\epsilon_{mkl}$, $f=3$. Futhermore let $d=2$. Clearly the matrices

$$I_1 = \frac{i}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad I_2 = \frac{1}{2}\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad I_3 = \frac{i}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{4.5}$$

satisfy

$$[I_i, I_j] = \epsilon_{ijl} I_l. \tag{4.6}$$

If $\mathbf{I} = (I_1, I_2, I_3)$ and $\hat{q} = \begin{pmatrix} q^1_{(\alpha,\beta)} \\ q^2_{(\alpha,\beta)} \end{pmatrix}$, (4.1) specializes

$$\hat{q} = -\mathbf{A}\cdot\mathbf{I}\hat{q}, \quad \hat{q}_\beta = -\mathbf{B}\cdot\mathbf{I}\hat{q}, \tag{4.7}$$

when (2.5) is satisfied. [Recall the sign convention of (2.3).]

When (3.11) and (3.12) are specialized to (3.13) and (3.14), (4.7) becomes

$$\hat{q}_\alpha = -\begin{bmatrix} \eta + \frac{i\lambda_\alpha}{2}\left(\frac{h}{2\gamma g}\right)^{1/2}(g_1 g_2)^{-1/4} g'(\Theta), & -\frac{\gamma}{2}\Theta_\alpha - \frac{i}{2}\lambda_\alpha\left(\frac{\gamma h}{2g}\right)^{1/2}(g_1 g_2)^{-1/4} g(\Theta) \\ \frac{\gamma}{2}\Theta_\alpha - \frac{i}{2}\lambda_\alpha\left(\frac{\gamma h}{2g}\right)^{1/2}(g_1 g_2)^{-1/4} g(\Theta), & -\eta - \frac{i\lambda_\alpha}{2}\left(\frac{h}{2\gamma g}\right)^{1/2}(g_1 g_2)^{-1/4} g'(\Theta) \end{bmatrix}\hat{q}, \tag{4.8a}$$

$$\hat{q}_\beta = -\begin{bmatrix} \frac{1}{4\eta} g'(\Theta) - \frac{i\lambda_\beta}{g}\left(\frac{2\gamma h}{g}\right)^{1/2}(g_1 g_2)^{-1/4}, & -\frac{\gamma}{4}\frac{1}{\eta} g(\Theta) \\ -\frac{\gamma}{4}\frac{1}{\eta} g(\Theta) & -\frac{1}{4\eta} g'(\Theta) + \frac{i\lambda_\beta}{2}\left(\frac{2\gamma h}{g}\right)^{1/2}(g_1 g_2)^{1/4} \end{bmatrix}\hat{q}. \tag{4.8b}$$

The free parameter η plays the role of the eigenvalue in (4.8a). When $\lambda_\alpha = \lambda_\beta = 0$ the eigenvalue problem and isospectral flow for (2.13) and (2.16) is recovered; when $g(\Theta) = \frac{1}{8}\sin 2\Theta$ and $p(\Theta) = (\sin\Theta\cos\Theta)^{-1}$, (2.1) becomes the Lund—Regge equations with h given by (3.10), and (4.8) are the eigenvalue problem and isospectral flow derived by them. The eigenvalue problem and isospectral flow for (2.1), subject to (2.16) and (3.10) for $g(\Theta)$, $h(\Theta)$, and $p(\Theta)$, follows by direct substitution. The two "singular" cases $\gamma = 0$ or $g_1 g_2 = 0$ can easily be treated in exactly the same fashion starting with (2.10)—(2.12).

The nonlinear action of G is closely connected with the conservation laws for the system (2.1). To see this consider a nonlinear action of G on a one complex dimensional representation space $\mathcal{Q}$, and let the generator functions be given by, say,

$$X_1(q) = iq, \quad X_2(q) = \tfrac{1}{2}(1+q^2), \quad X_3(q) = \frac{i}{2}(1-q^2). \tag{4.9}$$

Since $d = 1$ the upper index on the X^a_k is suppressed. Notice that when $d = 1$ and $C^i_{jk} = \epsilon_{ijk}$, (4.2) becomes

$$\frac{\partial X_i}{\partial q} X_j - X_i \frac{\partial X_j}{\partial q} = \epsilon_{ijk} X_k, \tag{4.10}$$

and that the X_i specified by (4.9) satisfy (4.10). In accordance with (4.1) the infinitesimal nonlinear group action is given by

$$q_\alpha = -\mathbf{A}\circ\mathbf{X}(q), \quad q_\beta = -\mathbf{B}\circ\mathbf{X}(q), \tag{4.11}$$

where $\mathbf{X} = (X_1, X_3, X_3)$ and $\mathbf{A}$, $\mathbf{B}$ are given by, say (3.13) and (3.14). An asymptotic expansion of (4.11) in powers of η, following Ref. 13, gives (in the by now usual way) conservation laws associated with (2.1). It would be of interest to use the full two-parameter freedom in (3.11) and (3.12) together with the generator functions (4.9) to explore the conservation of (2.1) or even its reduction the sine-Gordon equation.

Another nonlinearaction of G that is of interest is that associated with the generator functions,

$$X_1(q) = i\sin q, \quad X_2(q) = 1, \quad X_3(q) = i\cos q. \tag{4.12}$$

These again satisfy (4.10). If $\lambda_\alpha = \lambda_\beta = 0$ and the representation (3.15) and (3.16) is used, (4.11) gives

$$q_\alpha = -\Theta_\alpha - 2\eta\sin(\Theta - q), \tag{4.12a}$$

$$q_\beta = \Theta_\beta + \frac{1}{8\eta}\sin(\Theta + q). \tag{4.12b}$$

This is the Bäcklund transformation for the sine-Gordon equation. At this time it is not clear how to generalize this construction for (2.1) when λ_α, $\lambda_\beta \neq 0$. It appears that in the general case the surface given by the (naturally coordinatized) nonlinear group action is not again a solution of the integrability conditions for the existence of the bilocal group parameters, i.e., the soliton equation, as in the case for the sine-Gordon equation.

It might be remarked parenthetically that from the Lie group point of view Bäcklund transformations are gauge transformations. Why? First recall that (2.2) can be thought of as $F^k_{uv} = 0$, where F^k_{uv} is the Yang—Mills field strength.[14] Take one solution of (2.1). This defines a vacuum configuration of the gauge field associated with $C^i_{jk} = \epsilon_{ijk}$ via the f^k_λ defined by (2.3) and, say, (3.11) and (3.12). A second solution of (2.1) defines another configuration in the same way. Now all vacuum states are pure gauge terms and hence (to within possible problems of singularities) can be reached, one from another, by a gauge transformation. Indeed, in principal, solutions of two different equations with the same gauge group, i.e., (2.1) with $\lambda_\alpha = \lambda_\beta = 0$ and with λ_α, $\lambda_\beta \neq 0$, can be connected by a gauge transformation. This point of view thus provides at least a theoretical unity for all equations with a given gauge group, i.e., all equations integrable by the generalized Zakharov—Shabat (AKNS) eigenvalue problem and isospectral flow since these have the same gauge group.[10] Whether this point of view has any computational impact remains to be seen.

5. DISCUSSION AND CONCLUSION

It has been shown that (2.1) subject to (2.16) and (3.10) has an associated eigenvalue problem and isospectral flow. The calculations illustrate a recently proposed Lie group framework for soliton equations.[3,4] In particular they illustrate the computational method used to "inject" a given partial differential equation into the group theoretic framework. However, it must be

pointed out that the computations were simplified by assuming a given set of structure constants in Eq. (2.2), i.e., $C^l_{n\rho}=\epsilon_{ln\rho}$. In general part of the computation involves finding these structure constants, a nontrivial task. This problem will be addressed in a subsequent paper.[15] Further it should be pointed out that only non-Abelian groups are of interest, i.e., $C^l_{n\rho}\neq 0$.[12]

The Lie group framework for soliton equations illustrated in this paper was formulated after a detailed study of pseudopotentials and prologation structures.[9–12] It was shown in the Introduction how the Lie and pseudopotential ideas diverge. Various other geometric, as opposed to group theoretic, approaches have recently been compared to the Wahlquist–Estabrook approach.[16] The relationship between these and the Lie approach will be discussed elsewhere.

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Time-reversal noninvariance of the quantum-mechanical kinetic equation of Kadanoff and Baym[a)]

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Applying anticausal Green's function technique, it has been shown that the origin of time-reversal noninvariance of the quantum-mechanical kinetic equation of Kadanoff and Baym lies in the selection of the boundary condition that the system be in thermodynamical equilibrium at time $t = -\infty$.

1. INTRODUCTION

Kadanoff and Baym[1] have developed the Green's function approach to derive the quantum-mechanical kinetic equation which, successfully describes the irreversible phenomena in nonequilibrium quantum systems. But the weak point of the Kadanoff and Baym method is that they tacitly pass over the question of the origin of time-reversal noninvariance of the resulting kinetic equation. However, having the view that this equation is derived starting from the equation of motion for the one-particle causal Green's function (GF) which is invariant under time-reversal operation, this question arises by itself.

In order to provide an answer to this question we have considered a time-reversed situation described by anticausal Green's functions which represent time-reversed solutions of the corresponding equations of motion for the causal GF.

In order to derive the close equation of motion for the real-time one-particle causal GF from the close equation of motion for the complex-time one-particle causal GF Kadanoff and Baym have used the method of analytical continuation, assuming that the system was in thermodynamical equilibrium in the remote past, and that it was taken from it by switching in the external field at time $t = -\infty$.

To investigate whether this assumption violates time-reversal invariance of the initial equation, we have derived, from the equation of motion for the imaginary-time one-particle anticausal GF, by the method of analytical continuation, the closed equation of motion for the real-time one-particle anticausal GF. We had to use the boundary condition that the system lies in thermodynamical equilibrium in the far future, i.e., at time $t = +\infty$.

We have shown that this equation cannot be derived from the equation of motion for the real-time one-particle causal GF upon Wigner time reversal, which proves that the latter is time-reversal noninvariant.

To prove the boundary condition, that the system lies in thermodynamical equilibrium at time $t = -\infty$, predetermines the irreversible motion of the system towards equilibrium in the future, we have shown that the substitution of this boundary condition by the "anti-causal" boundary condition, i.e., the condition that the system is in equilibrium at time $t = +\infty$, yields the "quantum-kinetic equation" with the erroneous sign of the collisions term.

2. DEFINITION, DOMAIN OF ANALYCITY, AND EQUATION OF MOTION FOR THE THERMODYNAMICAL COMPLEX-TIME ONE-PARTICLE ANTICAUSAL GREEN'S FUNCTION

The thermodynamical real-time one-particle anticausal GF will be defined as a thermodynamical average of the antitime ordered product of field operators,

$$\tilde{G}(\mathbf{r}t, \mathbf{r}_0 t_0) = i \frac{\mathrm{Tr}\{\exp[-\beta(H-\mu)]\ [\tilde{T}(\psi_H(\mathbf{r}, t)\psi_H^\dagger(\mathbf{r}_0, t_0)]\}}{\mathrm{Tr}\{\exp[-\beta(H-\mu N)]\}}, \tag{2.1}$$

where $\tilde{T}$ is the antitime ordering operator.

The extension of definition (2.1) to the complex-time domain can be derived by using the same assumptions used by Mills.[2] We get for $\mathrm{Im}t < \mathrm{Im}t_0$

$$\tilde{G}^<(t, t_0) = i \frac{\mathrm{Tr}\{\exp[-\beta\bar{H}_0]\, u(0, t)\psi(t)u(t, t_0)\psi^\dagger(t_0)u(t_0, i\beta)\}}{\mathrm{Tr}\{\exp[-\beta H_0]u(0, i\beta)\}}, \tag{2.2}$$

where the operator u represents the inverse of the corresponding time-development operators.

The so defined anticausal GF is analytical on the imaginary segment $[0, +i\beta]$ and could be written in a shorter form,

$$\tilde{G}(t, t_0) = i \frac{\langle \tilde{T}[\tilde{S}\psi(t)\psi^\dagger(t_0)]\rangle}{\langle \tilde{T}[\tilde{S}]\rangle}, \tag{2.3}$$

where the operator $\tilde{S}$ is defined as

$$\tilde{S} = u(0, i\beta) = \tilde{T}\left\{\exp\left[-i\int_{i\beta}^{0} dt' H_{\mathrm{int}}(t')\right]\right\}. \tag{2.4}$$

Starting from the equations of motion for field operators in the Heisenberg representation we have derived the equation of motion for the one-particle anti-causal GF:

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right)\tilde{G}(1, 1')$$

$$= \delta(1'-1) \mp \int d\mathbf{r}_2\, v(|\mathbf{r}_1 - \mathbf{r}_2|)\, \tilde{G}_2(1\ 2^-;\ 1'\ 2^{--})|_{t_2 = t_1}, \qquad \hbar = 1. \tag{2.5}$$

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3. DEFINITION OF THE ANTICAUSAL GF FOR A SYSTEM IN THE PRESENCE OF THE SCALAR POTENTIAL AND THE CLOSED EQUATION OF MOTION FOR THE IMAGINARY-TIME ONE-PARTICLE ANTICAUSAL GF

Let us consider a time-reversed system in the presence of the scalar potential $U(\mathbf{r}, t)$. The external field can be observed as a time dependent perturbation which starts to act on the system which is in the thermodynamical equilibrium. For that case it can be shown that a nonequilibrium anticausal GF has a form

$$\tilde{G}(1,1';U)=i\frac{\langle\tilde{T}[\tilde{S}\psi(1)\psi^{\dagger}(1')]\rangle}{\langle\tilde{T}[\tilde{S}]\rangle}, \tag{3.1}$$

where the operator $\tilde{S}$ is now defined as

$$\tilde{S}=\exp\left[-i\int_{i\beta}^{0}d2\tilde{n}(2)U(2)\right]. \tag{3.2}$$

In order to get rid of the two-particle anticausal GF in the equation of motion for such a GF we use the functional derivative technique[3,4] and we get

$$\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-U(1)\right]\tilde{G}(1,1';U)+\int_{i\beta}^{0}d\bar{1}\,\tilde{\Sigma}(1,\bar{1};U)\tilde{G}(\bar{1},1';U)=\delta(1'-1). \tag{3.3}$$

Equation (3.3) represents the closed equation of motion for the imaginary-time one-particle anticausal GF because, in principle, anticausal self-energy $\tilde{\Sigma}$ can be expressed by means of the one-particle anticausal GF in the approximation of any order.

4. ANALYTIC CONTINUATION TO REAL TIMES AND DERIVATION OF THE CLOSED EQUATION OF MOTION FOR THE REAL-TIME ONE-PARTICLE ANTICAUSAL GF

In order to get a closed equation of motion for the real-time one-particle anticausal GF from (3.3), we will proceed in the following way:

Let us define the anticausal GF for a system in the external field on a complex segment $[t_0, t_0+i\beta]$ as

$$\tilde{G}(1,1';U;t_0)=i\frac{\langle\tilde{T}[\tilde{S}\psi(1)\psi^{\dagger}(1')]\rangle}{\langle\tilde{T}[\tilde{S}]\rangle}, \tag{4.1}$$

where

$$\tilde{S}=v(t_0,t_0+i\beta)=\tilde{T}\left\{\exp\left[-i\int_{t_0+i\beta}^{t_0}d2\,\tilde{n}(2)U(2)\right]\right\}. \tag{4.2}$$

For the case $\mathrm{Im}t_0>\mathrm{Im}t_{1'}$ (4.1) can be written in the developed form

$$\tilde{G}^{>}(1,1';U;t_0)=\pm i\frac{\langle v(t_0,t_{1'})\psi^{\dagger}(t_{1'})\,v(t_{1'},t_1)\psi(t_1)v(t_1,t_0+i\beta)\rangle}{\langle v(t_0,t_0+i\beta)\rangle}. \tag{4.3}$$

We define the anticausal GF for real-time arguments for the system in an external field as

$$\tilde{g}(1,1';U)=i\langle\tilde{T}[\psi_U(1)\psi_U^{\dagger}(1')]\rangle. \tag{4.4}$$

Let us assume that the observed time-reversed system lies in thermodynamical equilibrium in the future and that the external field starts acting at the moment $t_0=+\infty$. For such a system, for the case $\mathrm{Im}t_1>\mathrm{Im}t_{1'}$, definition (4.4) becomes

$$\tilde{g}^{>}(1,1';U)=\pm i\langle v(\infty,t_{1'})\psi^{\dagger}(t_{1'})v(t_{1'},t_1)\psi(t_1)v(t_1,\infty)\rangle, \tag{4.5}$$

where time-development operators v act in the negative sense of the real-time axis.

The integral path represented by the segment $[t_0, t_0+i\beta]$ can be deformed, because the functions under the inegral sign satisfy the Cauchy theorem, so that arguments t_1 and $t_{1'}$ lie on a negative part of the real-time axis retaining the order they had at the original integral path (Fig. 1).

If we let $t_0\to+\infty$ under the assumption that $\lim_{t_0\to\infty}v(t_0+i\epsilon, t_0+i\beta)\approx 1$, and applying the group property of operators v, we get

$$\lim_{t_0\to\infty}\tilde{G}^{\gtrless}(1,1',U;t_0)=\tilde{g}^{\gtrless}(1,1';U). \tag{4.6}$$

Thereby we have proved that the anticausal GF for negative real-time arguments is an analytical continuation of the anticausal GF with the positive imaginary-time arguments. For the anticausal GF defined on the segment $[t_0, t_0+i\beta]$ in the case when the interchanging term is neglected in the Hartree-Fock term of self-energy, the equation of motion has the form

$$\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-\tilde{U}_{\mathrm{eff}}(1,t_0)\right]\tilde{G}(1,1';U;t_0)=\delta(1'-1)-\int_{t_0+i\beta}^{t_0}d\bar{1}\tilde{\Sigma}_c(1,\bar{1};U;t_0)\tilde{G}(\bar{1},1';U;t_0). \tag{4.7}$$

Let us now seek the limes of (4.7) for the case $t_0\to+\infty$, when the integral path in (4.7) is substituted by the integral path from Fig. 1. In the case $|t_1|>|t_{1'}|$, we get by means of Eq. (4.6) the equation

$$\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-\tilde{U}_{\mathrm{eff}}(1)\right]\tilde{g}^{>}(1,1';U)=\int_{\infty}^{t_1}d\bar{1}[\tilde{\Sigma}^{>}(1,\bar{1};U)-\tilde{\Sigma}^{<}(1,\bar{1};U)]\tilde{g}^{>}(\bar{1},1';U)-\int_{\infty}^{t_{1'}}d\bar{1}\tilde{\Sigma}^{>}(1,\bar{1};U)[\tilde{g}^{>}(\bar{1},1';U)-\tilde{g}^{>}(\bar{1},1';U)] \tag{4.8}$$

which, together with the corresponding equation for $\tilde{g}^{<}$ represents the close equation of motion for the real-time one particle anticausal GF.

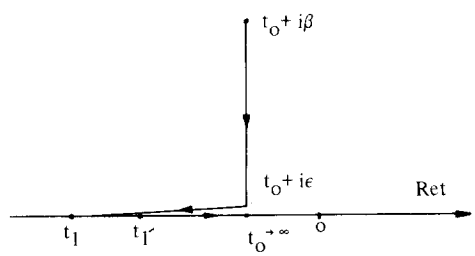

FIG. 1.

5. PROOF THAT THE EQUATION OF MOTION FOR REAL-TIME ONE-PARTICLE CAUSAL GF IS TIME-REVERSAL NONINVARIANT

If Wigner time-reversal[5] is applied to equation KB (3.2b) (the KB denotes that the equation is from Ref. 1), i.e., if we first exchange the arguments $1 \rightleftharpoons 1'$ and afterwards perform the complex conjugation of the equation, we get

$$\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right]\tilde{G}(1,1') = \delta(1'-1)\mp i\int d\mathbf{r}_2 v(|\mathbf{r}_1-\mathbf{r}_2|)\tilde{G}_2(12^-;1'2^{--})|_{t_2=t_1}. \tag{5.1}$$

Equation (5.1) is equivalent to the Eq. (2.5), i.e., to the equation of motion for one-particle anticausal GF which is derived on the basis of the definition of this function. Since we have shown that this equation can be derived from the equation of motion for one-particle causal GF upon the Wigner time-reversal, it could be concluded that the anticausal Green's function defined here represents the time-reversed solution.

In the same way we can derive Eq. (3.3) from KB (5.22) which means that Eq. KB (5.22), i.e., KB (8.16a) is time-reversal invariant.

When we exchange the arguments $1 \rightleftharpoons 1'$ in KB (8.28a) and when we perform the complex conjugation of the equation we get

$$\left(i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-\tilde{U}_{eff}(1)\right)\tilde{g}^{>}(1,1';U) = \int_{-\infty}^{t_1} d\bar{1}[\tilde{\Sigma}^{>}(1,\bar{1};U)-\tilde{\Sigma}^{<}(1,\bar{1};U)]\tilde{g}^{>}(\bar{1},1';U) - \int_{-\infty}^{t_{1'}} \tilde{\Sigma}^{>}(1,\bar{1};U)[\tilde{g}^{>}(1,1';U)-\tilde{g}^{<}(1,1';U)]. \tag{5.2}$$

The comparison of Eqs. (4.8) and (5.2) shows that they are not identical because lower bounds of the integrals over time in them differ. Therefrom it follows that Eq. KB (8.27a, b) is time-reversal noninvariant. The difference in the lower bounds of integrals stems from the different boundary conditions under which these mentioned equations were derived. From the foregoing it follows that the origin of time-reversal noninvariance lies exclusively in the boundary condition.

6. DERIVATION OF THE QUANTUM-MECHANICAL "ANTICAUSAL KINETIC EQUATION" AND THE QUANTUM "ANTICAUSAL BOLTZMANN EQUATION"

Since the quantum-mechanical kinetic equation KB (9.30), describing the irreversible motion of the system tending to the equilibrium in the future, could be derived from Eq. KB (8.27a, b) it could be expected that a similar equation could be derived from (4.8) which would describe the irreversible motion of a time-reversed system towards equilibrium in the past.

When we assume that $U(\mathbf{r},t)$ varies slowly in space and time, $\tilde{g}$ are slowly varying functions of the coordinates $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_{1'})/2$, $T=(t_1+t_{1'})/2$, but are sharply peaked about zero values of $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_{1'}$, $t=t_1-t_{1'}$. By means of these new coordinates we define $\tilde{g}^{>}(\mathbf{p}_-,\omega;\mathbf{R},T_-;U)$ as

$$\tilde{g}^{>}(\mathbf{p}_-,\omega;\mathbf{R},T_-;U) = \int_{-\infty}^{\infty} d\mathbf{r}\int_{-\infty}^{\infty} dt\exp(-i\mathbf{p}_-\cdot\mathbf{r}+i\omega t) \times[\pm(1/i)\tilde{g}^{>}(\mathbf{r},t;R,T_-;U)] \tag{6.1}$$

which can be interpreted as the particle density with the pulse $\mathbf{p}=-\mathbf{p}$ and by energy ω in the space–time point, R, $T_-<0$ of the time reversed system. Therefrom stems the definition of the corresponding distribution function

$$f(\mathbf{p}_-,\mathbf{R},T_-)=\int\frac{d\omega}{2\tilde{\pi}}\,\tilde{g}^{>}(\mathbf{p}_-,\omega;\mathbf{R},T_-). \tag{6.2}$$

If the corresponding adjoint equation of motion is subtracted from (4.8), inserting the new coordinates, and by means of defining (6.1) upon a lengthy transformation, we get the equation

$$\left[\frac{\partial}{\partial T_-}+\frac{\mathbf{p}_-\cdot\nabla_{\mathbf{R}}}{m}-\nabla_{\mathbf{R}}\tilde{U}_{eff}(\mathbf{R},T_-)\cdot\nabla_{\mathbf{p}_-}+\frac{\partial}{\partial T_-}\tilde{U}_{eff}(\mathbf{R},T_-)\frac{\partial}{\partial\omega}\right]\times\tilde{g}^{>}(\mathbf{p}_-,\omega;\mathbf{R},T_-) = \tilde{g}^{>}(\mathbf{p}_-,\omega;\mathbf{R},T_-)\tilde{\Sigma}^{>}(\mathbf{p}_-,\omega;\mathbf{R},T_-) - \tilde{g}^{<}(\mathbf{p}_-,\omega;\mathbf{R},T_-)\tilde{\Sigma}^{<}(\mathbf{p}_-,\omega;\mathbf{R},T_-) \tag{6.3}$$

which describes time reversal of the original process described by Eq. KB (9.7). Therefore, we shall call it the "anticausal kinetic equation."

From this equation, under the same assumption used by Kadanoff and Baym, the "Boltzmann equation" can be derived relevant to the time-reversed system. It has the form

$$\left[\frac{\partial}{\partial T_-}+\frac{\mathbf{p}_-\cdot\nabla_{\mathbf{R}}}{m}-\nabla_{\mathbf{R}}\tilde{V}_{eff}(\mathbf{R},T_-)\cdot\nabla_{\mathbf{p}_-}\right]\tilde{f}(\mathbf{p}_-,\mathbf{R},T_-) = \int\frac{d\mathbf{p}'_-}{(2\tilde{\pi})^3}\frac{d\bar{\mathbf{p}}_-}{(2\tilde{\pi})^3}\frac{d\bar{\mathbf{p}}'_-}{(2\tilde{\pi})^3}(2\tilde{\pi})^4\delta(\mathbf{p}_-+\mathbf{p}'_--\bar{\mathbf{p}}_--\bar{\mathbf{p}}'_-) \delta\left(\frac{p_-^2}{2m}+\frac{p_-'^2}{2m}-\frac{\bar{p}_-^2}{2m}-\frac{\bar{p}_-'^2}{2m}\right)\tfrac{1}{2}[v(\mathbf{p}_--\bar{\mathbf{p}}_-)\mp v(\mathbf{p}_--\bar{\mathbf{p}}'_-)]^2 \times\{\tilde{f}\tilde{f}'[1\pm\bar{\tilde{f}}][1\pm\bar{\tilde{f}}']-[1\pm\tilde{f}][1\pm\tilde{f}']\bar{\tilde{f}}\bar{\tilde{f}}'\}$$

where

$$\tilde{f}'=\tilde{f}(\mathbf{p}'_-,\mathbf{R},T_-),\ \bar{\tilde{f}}=\tilde{f}(\bar{\mathbf{p}}_-,\mathbf{R},T_-),\ \bar{\tilde{f}}'=\tilde{f}(\bar{\mathbf{p}}'_-,\mathbf{R},T_-).$$

Equation (6.4) differs from the quantum-mechanical Boltzmann equation KB (9.16) only in the sign of the collision term.

7. DISCUSSION

Kadanoff and Baym have derived the quantum-mechanical kinetic equation using the boundary condition that the system was in thermodynamical equilibrium at time $t=-\infty$. Through action of the external fields the system is removed from its equilibrium state and brought to some arbitrary state at time t. The distribution function which represents the solution of the quantum-mechanical Boltzmann equation is at moment t determined by the external field which acts on the

system until that moment, i.e., its satisfies the causality condition.[6]

In Sec. 6 we have seen that if the boundary condition was chosen so that the system lies in thermodynamical equilibrium at time $t = +\infty$, then the "time-reversed" situation results, which implies the "Boltzmann equation" with negative collision term. The solution of this equation represents the distribution function of the time-reversed system which at moment t depends on the external field acting on the system upon moment t. This obviously contradicts the causality condition.

Consequently, in the Kadanoff and Baym method the difference between the causal and anticausal behavior of the system can be established only upon the selection of the boundary condition and irreversibility appears as a consequence of the causality condition.

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Tensor spherical harmonics on S^2 and S^3 as eigenvalue problems[a)]

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Tensor spherical harmonics for the 2-sphere and 3-sphere are discussed as eigenfunction problems of the Laplace operators on these manifolds. The scalar, vector, and second-rank tensor harmonics are given explicitly in terms of known functions and their properties summarized.

The analysis of scalar, vector, and tensor wave equations on the manifolds S^2 and S^3 is greatly facilitated by having a set of basis functions that reflect the symmetries and are eigenfunctions of the Laplace operator. The use of scalar S^2 harmonics in multipole expansions of electrostatic fields is probably the most well known example;[1] but cosmological pertubation,[2] stellar pulsations,[3,4] and scattering problems also make use of multipole expansion using the vector and tensor harmonics as well. In this paper the S^2 and S^3 harmonics are approached as eigenfunction problems (based on an analogy with the discussion of S^2 harmonics by Thorne and Compolattaro[4] and the discussion of S^3 harmonics by Lifshitz and Khalatnikov[2]) with an emphasis on explicit solutions, summarized in Tables I and II. These harmonics will

TABLE I. S^2 tensor harmonics.

$\gamma_{\theta\theta}=1,\quad \gamma_{\varphi\varphi}=\sin^2\theta$		$\epsilon_\theta{}^\varphi=\dfrac{1}{\sin\theta},\quad \epsilon_\varphi{}^\theta=-\sin\theta$
Scalar:	$Y^{(lm)}$	$\nabla^2 Y^{(lm)}=-l(l+1)\,Y^{(lm)}$
Vector:	$\psi_a^{(lm)}=Y_{\|a}^{(lm)}$	$\nabla^2\psi_a^{(lm)}=[1-l(l+1)\,]\psi_a{}^{(lm)}$
		$\psi_{a\|b}^{(lm)}\gamma^{ab}=-l(l+1)\,Y^{lm}$
	$\phi_a{}^{(lm)}=\epsilon_a{}^b Y_{\|b}^{(lm)}$	$\nabla^2\phi_a^{(lm)}=[1-l(l+1)\,]\phi_a{}^{(lm)}$
		$\phi_{a\|b}^{(lm)}\gamma^{ab}=0$
Tensor:	$\eta_{ab}^{(lm)}=Y^{(lm)}\gamma_{ab}$	$\nabla^2\eta_{ab}^{(lm)}=-l(l+1)\,\eta_{ab}^{(lm)}$
		$\eta_{ab\|c}^{(lm)}\gamma^{bc}=\psi_a^{(lm)}$
		$\eta_{ab}^{(lm)}\gamma^{ab}=2Y^{(lm)}$
	$\psi_{ab}^{(lm)}=Y_{\|a\|b}^{(lm)}+\frac{1}{2}l(l+1)\,Y^{(lm)}\gamma_{ab}$	
		$\nabla^2\psi_{ab}^{(lm)}=[4-l(l+1)\,]\psi_{ab}^{(lm)}$
		$\psi_{ab\|c}^{(lm)}\gamma^{bc}=\frac{1}{2}[2-l(l+1)\,]\psi_a^{(lm)}$
		$\psi_{ab}^{(lm)}\gamma^{ab}=0$
	$\chi_{ab}^{(lm)}=Y^{(lm)}\epsilon_{ab}$	$\nabla^2\chi_{ab}=-l(l+1)\,\chi_{ab}^{(lm)}$
		$\chi_{ab\|c}^{(lm)}\gamma^{bc}=\phi_a^{(lm)}$
		$\chi_{ab}^{(lm)}\gamma^{ab}=0$
	$\phi_{ab}^{(lm)}=\frac{1}{2}(\phi_{a\|b}^{(lm)}+\phi_{b\|a}^{(lm)})$	
		$\nabla^2\phi_{ab}^{(lm)}=[4-l(l+1)\,]\phi_{ab}^{(lm)}$
		$\phi_{ab\|c}^{(lm)}\gamma^{bc}=\frac{1}{2}[2-l(l+1)\,]\phi_a^{(lm)}$
		$\phi_{ab}^{(lm)}\gamma^{ab}=0$

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Orthogonality relations

$d^2\Omega = \sin\theta\, d\theta\, d\varphi \qquad 0<\theta<\pi, \quad 0<\varphi<2\pi$

$$\int d^2\Omega \;\; Y_{lm} Y^*_{lm'} = \delta_{ll'}\delta_{mm'}$$

$$\int d^2\Omega \;\; \psi^{lm}_a \psi^{*lm'}_b \gamma^{ab} = l(l+1)\delta_{ll'}\delta_{mm'}$$

$$\int d^2\Omega \;\; \phi^{lm}_a \phi^{*lm}_b \gamma^{ab} = l(l+1)\delta_{ll'}\delta_{mm'}$$

$$\int d^2\Omega \;\; \eta^{lm}_{ab} \eta^{*lm'}_{cd} \gamma^{ac}\gamma^{bd} = -2\delta_{ll'}\delta_{mm'}$$

$$\int d^2\Omega \;\; \psi^{lm}_{ab} \psi^{*lm'}_{cd} \gamma^{ac}\gamma^{bd} = l(l+1)\left[\tfrac{1}{2}l(l+1)-1\right]\delta_{ll'}\delta_{mm'}$$

$$\int d^2\Omega \;\; \chi^{lm}_{ab} \chi^{*lm'}_{cd} \gamma^{ac}\gamma^{bd} = 2\delta_{ll'}\delta_{mm'}$$

$$\int d^2\Omega \;\; \phi^{lm}_{ab} \phi^{*lm}_{cd} \gamma^{ac}\gamma^{bd} = l(l+1)\left[\tfrac{1}{2}l(l+1)-1\right]\delta_{ll'}\delta_{mm'}$$

All other products vanish, e.g.,

$$\int d^2\Omega \;\; \psi^*_{ab}\chi^{ab} = 0, \text{ etc.}$$

The completeness of these functions follows from the completeness of the scalar harmonics

$$\sum_{l,m} Y^{(lm)}(\theta,\varphi)\, Y^{*(lm)}(\theta',\varphi') = \delta\;(\cos\theta-\cos\theta')\delta(\varphi-\varphi')$$

TABLE II. S^3 tensor harmonics.

$g_{\chi\chi}=1, \quad g_{\theta\theta}=\sin^2\chi, \qquad g_{\varphi\varphi}=\sin^2\chi\sin^2\theta, \qquad \epsilon_{\chi\theta\varphi}=\sin^2\chi\sin\theta$

Scalar: $Y^{(nlm)}(\chi,\theta,\varphi) \qquad \Delta Y^{(nlm)} = -n(n+1)\,Y^{(nlm)}$

Vector: $A^{(nlm)}_\alpha = \left(0, \sin^{l+1}\chi\, C^{(l+1)}_{n-1}(\cos\chi)\,\phi^{(lm)}_i(\theta,\varphi)\right)$

$$B^{(nlm)}_\alpha = \left(-l(l+1)\sin^{l-1}\chi C^{(l+1)}_{n-l}(\cos\chi)\,Y^{(lm)}(\theta,\varphi) - \partial_\chi\left[\sin^{l+1}\chi\, C^{(l+1)}_{n-l}(\cos\chi)\right]\psi^{(lm)}_i(\theta,\varphi)\right)$$

$$C^{(nlm)}_\alpha = \left(\frac{2^{2l+1}(n+1)(n-l)!(l!)^2}{\pi(n+l+1!)}\right)^{1/2}\left(\partial_\chi\left(\sin^l\chi\, C^{(l+1)}_{n-l}(\cos\chi)\right)Y^{(lm)}(\theta,\varphi),\ \sin^l\chi\, C^{(l+1)}_{n-l}(\cos\chi)\,\psi^{(lm)}_i(\theta,\varphi)\right)$$

$$B^{(nlm)}_\alpha = \epsilon_\alpha{}^{\mu\nu} A^{(nlm)}_{\mu;\nu}$$

$$C^{(nlm)}_\alpha = Y^{(nlm)}{}_{;\alpha}$$

$$\Delta A^{(nlm)}_\alpha = [1-n(n+2)]A^{(nlm)}_\alpha$$

$$\Delta B^{(nlm)}_\alpha = [1-n(n+2)]B^{(nlm)}_\alpha$$

$$\Delta C^{(nlm)}_\alpha = [2-n(n+2)]C^{(nlm)}_\alpha$$

$$A_{\alpha;\beta}g^{\alpha\beta} = B_{\alpha;\beta}g^{\alpha\beta} = 0$$

$$C_{\alpha;\beta}g^{\alpha\beta} = -n(n+2)\,Y^{(nlm)}$$

Tensor: $A^{(nlm)}_{\alpha\beta} = \tfrac{1}{2}(A^{(nlm)}_{\alpha;\beta} + A^{(nlm)}_{\beta;\alpha}), \qquad \bar{A}^{(nlm)}_{[\alpha\beta]} = \tfrac{1}{2}\epsilon^\mu{}_{\alpha\beta}B^{(nlm)}_\mu$

$$B^{(nlm)}_{\alpha\beta} = \tfrac{1}{2}(B_{\alpha;\beta} + B_{\beta;\alpha}), \qquad \bar{B}^{(nlm)}_{[\alpha\beta]} = -\tfrac{1}{2}[1+n(n+2)]\epsilon^\mu{}_{\alpha\beta}A^{(nlm)}_\mu$$

$$C^{(nlm)}_{\alpha\beta} = Y^{(nlm)}_{;\alpha;\beta} + \tfrac{1}{3}n(n+2)\,Y^{(nlm)} g_{\alpha\beta}$$

$$D^{(nlm)}_{\alpha\beta} = Y^{(nlm)} g_{\alpha\beta}$$

$$G^{(nlm)}_{\alpha\beta} = Y^{(nlm)}_{;\mu} \epsilon^{\mu}{}_{\alpha\beta}$$

$$E^{(nlm)}_{\chi\chi} = 0$$

$$E^{(nlm)}_{a\chi} = \sin^{l}\chi\, C^{(l+1)}_{n-1}(\cos\chi)\,\phi^{(lm)}_{a}(\theta,\varphi)$$

$$E^{(nlm)}_{ab} = -\frac{2}{[2-l(l+1)]}\frac{\partial}{\partial\chi}[\sin^{l+2}\chi\, C^{(l+1)}_{n-l}(\cos\chi)]\,\phi^{(lm)}_{ab}(\theta,\varphi)$$

$$F^{(nlm)}_{\chi\chi} = -l(l+1)\sin^{l+1}\chi\, C^{(l-1)}_{n-l}(\cos\chi)\,Y^{(lm)}(\theta,\varphi)$$

$$F^{(nlm)}_{a\chi} = -\csc\chi\frac{\partial}{\partial\chi}[\sin^{l+1}\chi\, C^{(l+1)}_{n-l}(\cos\chi)]\,\psi^{(nlm)}_{a}(\theta,\varphi)$$

$$F^{(nlm)}_{ab} = \tfrac{1}{2}(l+1)\sin^{l}\chi\, C^{(l-1)}_{n-l}(\cos\chi)\,\phi^{(lm)}_{ab}(\theta,\varphi) + \Big[\sin^{l}\chi\, C^{(l-1)}_{n-l}(\cos\chi) + \frac{2}{[2-l(l+1)]}\Big(\frac{\partial^2}{\partial\chi^2}(\sin^{l+2}\chi\, C^{(l-1)}_{n-l}(\cos\chi) - \cot\chi\frac{\partial}{\partial\chi}(\sin^{l+2}\chi\, C^{(l-1)}_{n-l}(\cos\chi))\Big)\Big]\psi^{(lm)}_{ab}(\theta,\varphi)$$

$$F^{(nlm)}_{\alpha\beta} = \tfrac{1}{2}[E_{\alpha\mu;\nu}\epsilon_{\beta}{}^{\mu\nu} + E_{\beta\mu;\nu}\epsilon_{\alpha}{}^{\mu\nu}]$$

Eigenvalues:

$$\Delta A_{\alpha\beta} = [5-n(n+2)]A_{\alpha\beta} \qquad \Delta D_{\alpha\beta} = -n(n+2)D_{\alpha\beta}$$

$$\Delta \widetilde{A}_{[\alpha\beta]} = [1-n(n+2)]\widetilde{A}_{[\alpha\beta]} \qquad \Delta E_{\alpha\beta} = [2-n(n+2)]E_{\alpha\beta}$$

$$\Delta B_{\alpha\beta} = [5-n(n+2)]B_{\alpha\beta} \qquad \Delta F_{\alpha\beta} = [2-n(n+2)]F_{\alpha\beta}$$

$$\Delta \widetilde{B}_{[\alpha\beta]} = [1-n(n+2)]\widetilde{B}_{[\alpha\beta]} \qquad \Delta G_{\alpha\beta} = [2-n(n+2)]G_{\alpha\beta}$$

$$\Delta C_{\alpha\beta} = [6-n(n+2)]C_{\alpha\beta}$$

Divergence conditions:

$$A_{\alpha\beta;\gamma}g^{\beta\gamma} = \tfrac{1}{2}(3-n(n+2))A_{\alpha}$$

$$B_{\alpha\beta;\gamma}g^{\beta\gamma} = \tfrac{1}{2}(3-n(n+2))B_{\alpha}$$

$$C_{\alpha\beta;\gamma}g^{\beta\gamma} = \tfrac{2}{3}(3-n(n+2))C_{\alpha}$$

$$D_{\alpha\beta;\gamma}g^{\beta\gamma} = C_{\alpha}$$

$$E_{\alpha\rho;\gamma}g^{\beta\gamma} = 0$$

$$F_{\alpha\beta;\gamma}g^{\beta\gamma} = 0$$

Trace conditions:

$$A_{\alpha\beta}g^{\alpha\beta} = B_{\alpha\beta}g^{\alpha\beta} = C_{\alpha\beta}g^{\alpha\beta} = E_{\alpha\beta}g^{\alpha\beta} = F_{\alpha\beta}g^{\alpha\beta} = 0$$

$$D_{\alpha\beta}g^{\alpha\beta} = 3Y^{(nlm)}$$

be used in a separate paper to discuss perturbations in space–times with these symmetries.

We use the conventions of Ref. 1 for the scalar S^2 harmonics and the conventions of Ref. 5 for the Gegenbauer polynomials. We denote three-dimensional covariant derivatives by a semicolon, two-sphere covariant derivatives by a vertical line, represent the two-sphere metric by γ_{ab}, the three-sphere metric by $g_{\mu\nu}$, and define the sign of the curvature tensor so that the Ricci identity is given by

$$V_{\alpha;\beta;\gamma} - V_{\alpha;\gamma;\beta} = V_{\mu}R^{\mu}{}_{\alpha\beta\gamma}.$$

Greek indices run from 1 to 3 and denote three-sphere indices, Latin indices run from 2 to 3 and denote two-sphere indices.

The manifold S^3 is characterized by its metric

$$ds^2 = g_{\mu\nu}\,dx^{\mu}\,dx^{\nu} = d\chi^2 + \sin^2\chi(d\theta^2 + \sin^2\theta\,d\varphi^2),$$

where the coordinates $x^{\mu} = (\chi,\theta,\varphi)$ have the domains $0 < \chi < \pi$, $0 \leqslant \theta < \pi$, and $0 < \varphi < 2\pi$ with the usual polar singularities at 0 and π. The sufaces $\chi = \text{const}$ are conformal to S^2 [described as above with the coordinates $x^a = (\theta,\varphi)$]. The S^3 harmonics are the tensorial eigenfunction solutions

$T_{\alpha\beta\cdots\gamma}$ to the equations

$$\Delta T_{\alpha\beta\cdots\gamma} \equiv T_{\alpha\beta\cdots\gamma;\mu;\nu} g^{\mu\nu} = \lambda T_{\alpha\beta\cdots\gamma} \tag{1}$$

that are regular on S^3 and have eigenvalues λ. The S^2 harmonics satisfy the obvious, similar conditions to the above.

At this point it is convenient to restrict consideration to the S^2 harmonics and review the scalar, vector, and second rank tensor solutions of Ref. 4. The scalar harmonics are the well known $Y^{(lm)}(\theta,\varphi)$ listed in Ref. 1 and these form a complete basis for scalars on S^2. The tangent space to a point on S^2 is two-dimensional, to span it we need two linearly independent solutions to the vector form of Eq. (1). These can be obtained from the gradient of the scalar harmonics ($\psi_a^{(lm)}$) and the dual of the gradient ($\phi_a^{(lm)}$) (see Table I for definitions) (since the space is two-dimensional taking a vector's dual gives another vector). That the gradient ψ_a is a solution to the vector form of Eq. (1) follows from Ricci's identity

$$Y_{,a|b|c}\gamma^{bc} = (Y_{,b|c}\gamma^{bc})_{,a} + Y_{,d} R^{d}_{\ bac}\gamma^{bc}$$

$$= [1 - l(l+1)] Y_{,a},$$

where (for S^2)

$$R_{abcd} = \gamma_{ac}\gamma_{bd} - \gamma_{ad}\gamma_{bc}.$$

That the dual vector ϕ_a satisfies the same equation with the same eigenvalues follows from the vanishing of the covariant derivative of the Levi–Civita tensor. Under the improper transformation $\theta' = \pi - \theta, \varphi' = \varphi + \pi$ which corresponds to a coordinate inversion ψ_a transform as a polar vector and ϕ_a transforms as an axial vector, hence they are called even and odd parity vector spherical harmonics, respectively. For second rank tensors the space is four-dimensional and can be spanned by a skew tensor χ_{ab} and three symmetric tensors η_{ab}, ψ_{ab}, and ϕ_{ab} defined in Table I. These satisfy the tensor form of Eq. (1) from arguments analogous to the vector case. The point to be made here is that all the S^2 harmonics can be constructed from a knowledge of the scalar S^2 harmonics, but this is not the case for the S^3 harmonics as will be shown below.

The dimensionalities of the tensor spaces over S^3 complicate the previous analysis as can be seen by a count of the number of independent solutions to Eq. (1) as a function of the rank of the tensor. For scalars there is one set of functions $Y^{(nlm)}(\chi,\theta,\varphi)$. For vectors there are three linearly independent harmonics. In three dimensions we cannot use the trick of using the dual of a vector harmonic as we did on S^2, but we can use a generalization of this idea and use the curl of a vector to generate a linearly independent vector. In three dimensions there are two main types of vectors: divergence and curl free. The latter is exemplified by the gradient of the scalar harmonic

$$C_\alpha^{(nlm)} = Y_{;\alpha}^{(nlm)}. \tag{2}$$

Two other vector harmonics $A_\alpha^{(nlm)}$ and $B_\alpha^{(nlm)}$ can be found by imposing the divergence condition

$$A_{\alpha;\beta} g^{\alpha\beta} = 0, \tag{3}$$

solving for A_α from

$$\Delta A_\alpha = \lambda A_\alpha, \tag{4}$$

and forming the third vector from $B_\alpha = -(\mathrm{curl} A)_\alpha$ (obviously B_α is also divergenceless). The vectors $A_\alpha^{(nlm)}$, $B_\alpha^{(nlm)}$, and $C_\alpha^{(nlm)}$ form an harmonic basis for the three-dimensional space of vectors on S^3. The second rank tensors on S^3 for a nine-dimensional vector space so we need nine independent tensor harmonics to span it. Two candidates come from the scalar harmonics

$$D_{\alpha\beta}^{(nlm)} = Y_{(\chi,\theta,\varphi)}^{(nlm)} g_{\alpha\beta} \tag{5}$$

and

$$C_{\alpha\beta}^{(nlm)} = Y_{;\alpha;\beta}^{(nlm)} + \tfrac{1}{3} n(n+2) Y^{(nlm)} g_{\alpha\beta} \tag{6}$$

[n.b. these are symmetric tensors and $C_{\alpha\beta}^{(nlm)} g^{\alpha\beta} = 0$]. Two more come from the divergenceless vectors

$$\widetilde{A}_{\alpha\beta}^{(nlm)} = A_{\alpha;\beta}^{(nlm)}, \tag{7}$$

$$\widetilde{B}_{\alpha\beta}^{(nlm)} = B_{\alpha;\beta}^{(nlm)}. \tag{8}$$

These can be further decomposed into symmetric and antisymmetric tensors:

$$A_{\alpha\beta}^{(nlm)} = \tfrac{1}{2}(\widetilde{A}_{\alpha\beta}^{(nlm)} + \widetilde{A}_{\beta\alpha}^{(nlm)}), \tag{9}$$

$$B_{\alpha\beta}^{(nlm)} = \tfrac{1}{2}(\widetilde{B}_{\alpha\beta}^{(nlm)} + \widetilde{B}_{\beta\alpha}^{(nlm)}), \tag{10}$$

$$\widetilde{A}_{[\alpha\beta]}^{(nlm)} = \tfrac{1}{2} B_\gamma^{(nlm)} \epsilon^{\gamma}_{\ \alpha\beta}, \tag{11}$$

$$\widetilde{B}_{[\alpha\beta]}^{(nlm)} = -\tfrac{1}{2}[1 + n(n+2)] A_\gamma^{(nlm)} \epsilon^{\gamma}_{\ \alpha\beta}, \tag{12}$$

and

$$G_{\alpha\beta}^{(nlm)} = \epsilon_\beta^{\ \mu\nu} Y_{;\mu}^{(nlm)}, \tag{13}$$

where $\epsilon_{\alpha\beta\gamma}$ is completely antisymmetric,

with

$$\epsilon_{123} = \sin^2\chi\sin\theta \quad \text{and} \quad \epsilon_{1ab} = \sin^2\chi\epsilon_{ab}. \tag{14}$$

The antisymmetric tensors arises algebraically from the vectors while the symmetric tensors come from the covariant derivatives of the vectors. To find two more independent harmonic solutions we impose tracefree and divergenceless conditions on a symmetric tensor $E_{\alpha\beta}$ and solve Eq. (1) with these constraints. The last harmonic $F_{\alpha\beta}$ is then found from $E_{\alpha\beta}$ by taking the symmetrized curl

$$\widetilde{F}_{\alpha\beta} = E_{\alpha\mu;\nu}\epsilon_\beta^{\ \mu\nu}, \tag{15}$$

$$F_{\alpha\beta} = \tfrac{1}{2}(\widetilde{F}_{\alpha\beta} + \widetilde{F}_{\beta\alpha}), \tag{16}$$

(n.b. $\widetilde{F}_{[\alpha\beta]} = 0$ due to the trace and divergence conditions on $E_{\alpha\beta}$).

We now proceed to verify these statements. For the S^3 scalar harmonics we have

$$\csc^2\chi\left\{\frac{\partial}{\partial\chi}\left(\sin^2\chi\frac{\partial Y}{\partial\chi}\right) + \csc\theta\left[\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \csc\theta\frac{\partial^2 Y}{\partial\varphi^2}\right]\right\} = \lambda Y^{(nlm)}. \tag{17}$$

The solutions that are regular at the poles are

$$Y^{(nlm)}(\chi,\theta,\varphi) = \left(\frac{2^{2l+1}(n+1)(n-l)!(l!)^2}{\pi(n+l+1)!}\right)^{1/2}$$

$$\times \sin^l\chi\, C_{n-l}^{(l+1)}(\cos\chi)\, Y^{(lm)}(\theta,\varphi) \tag{18}$$

with eigenvalues given by

$$\lambda = -n(n+2), \quad |m| \leqslant l \leqslant n = 0,1,2,\ldots.$$

The $C_{n-l}^{(l+1)}(x)$ are Gegenbauer polynomials as defined in Ref. 5, the $Y^{(lm)}(\theta,\varphi)$ are the S^2 scalar harmonics, and the coefficient is chosen[6] to normalize the harmonics

$$\int d^3\Omega\; Y^{(nlm)}(\chi,\theta,\varphi)\; Y^{(n'l'm')}(\chi,\theta,\varphi)^* = \delta_{nn'}\delta_{ll'}\delta_{mm'}, \tag{19}$$

where the S^3 volume element is given by

$$d^3\Omega = \sin^2\chi d\chi \sin\theta\, d\theta\, d\varphi.$$

The vector $C_\alpha^{(nlm)}$ satisfies

$$\Delta C_\alpha^{(nlm)} = (\Delta Y^{(nlm)}{}_{;\alpha} + Y^{(nlm)}_{;\beta} R^{\beta}{}_{\mu\alpha\nu} g^{\mu\nu}. \tag{20}$$

On S^3 the curvature tensor is given by

$$R^{\beta}{}_{\mu\alpha\nu} = \delta^{\beta}_{\alpha} g_{\mu\nu} - g^{\beta}_{\nu} g_{\mu\alpha} \tag{21}$$

and hence

$$\Delta C_\alpha^{(nlm)} = [2-n(n+2)]\, C_\alpha^{(nlm)} \tag{22}$$

so $C_\alpha^{(nlm)}$ satisfies Eq. (1) for a vector. It is not divergenceless, but satisfies

$$C^{(nlm)}_{\alpha;\beta} g^{\alpha\beta} = -n(n+2)\, Y^{(nlm)}. \tag{23}$$

To solve Eq. (4) we consider the obviously divergenceless vector (motivated by considering an odd parity split of a divergenceless vector)

$$A_\alpha^{(nlm)} = (o, h(\chi)\phi_a^{(lm)}(\theta,\varphi)) \tag{24}$$

then using the properties of the S^2-harmonics Eq. (4) becomes

$$\frac{d^2h}{d\chi^2} + \{-\lambda + [2-l(l+1)]\csc^2\chi - 2\cot^2\chi\}\, h(\chi) = 0 \tag{25}$$

which has the regular solution

$$h^{(nl)}(\chi) = \sin\chi^{\,l+1} C_{n-l}^{(l+1)}(\cos\chi), \tag{26}$$

with eigenvalue $\lambda = [1-n(n+2)]$.

From Eq. (7) and Eq. (21) we note that the Laplace operator acting on $\widetilde{A}_{\alpha\beta}$ is given by

$$\Delta \widetilde{A}_{\alpha\beta} = [3-n(n+2)]\, \widetilde{A}_{\alpha\beta} + 2\widetilde{A}_{\beta\alpha}. \tag{27}$$

Therefore, the vector $B_\alpha = \epsilon_\alpha{}^{\mu\nu} A_{\mu\nu}$ satisfies the S^3 vector harmonic equation

$$\Delta B_\alpha = \epsilon_\alpha{}^{\mu\nu} \Delta A_{[\mu;\nu]} = [1-n(n+2)]\, B_\alpha \tag{28}$$

and obviously B_α is divergenceless. It has the components

$$B_1^{(nlm)} = -l(l+1)\csc^2\chi\, h^{(nl)}(\chi)\, Y^{(lm)}(\theta,\varphi),$$

$$B_a^{(nlm)} = -\frac{dh^{(nl)}}{d\chi}\psi_a^{(lm)}(\theta,\varphi). \tag{29}$$

The tensor harmonics consist of three antisymmetric tensors and six symmetric tensors. It is easy to verify that $D_{\alpha\beta}^{(nlm)}$ and $C_{\alpha\beta}^{(nlm)}$ satisfy

$$\Delta D_{\alpha\beta}^{(nlm)} = -n(n+2)\, D_{\alpha\beta}^{(nlm)} \tag{30}$$

and

$$\Delta C_{\alpha\beta}^{(nlm)} = [6-n(n+2)]\, C_{\alpha\beta}^{(nlm)}. \tag{31}$$

Using Eqs. (11), (12), and (13), the vanishing of the covariant derivative of the $\epsilon_{\alpha\beta\gamma}$ tensor, and Eqs. (28), (27), and (22), it follows

$$\Delta \widetilde{A}_{[\alpha\beta]}^{(nlm)} = [1-n(n+2)]\, \widetilde{A}_{[\alpha\beta]}^{(nlm)}, \tag{32}$$

$$\Delta \widetilde{B}_{[\alpha\beta]}^{(nlm)} = [1-n(n+2)]\, \widetilde{B}_{[\alpha\beta]}^{(nlm)}, \tag{33}$$

and

$$\Delta G_{\alpha\beta}^{(nlm)} = [2-n(n+2)]\, G_{\alpha\beta}^{(nlm)}. \tag{34}$$

From Eq. (27) and the analogous equation for $\widetilde{B}_{\alpha\beta}$ we find

$$\Delta A_{\alpha\beta}^{(nlm)} = [5-n(n+2)]\, A_{\alpha\beta}^{(nlm)}, \tag{35}$$

$$\Delta B_{\alpha\beta}^{(nlm)} = [5-n(n+2)]\, B_{\alpha\beta}^{(nlm)}. \tag{36}$$

The two remaining tensor harmonics are found by solving Eq. (1) for a symmetric tracefree divergenceless tensor $E_{\alpha\beta}^{(nlm)}$.

The properties of the S^3-harmonics in Table I suggest as a candidate the odd parity traceless tensor

$$(E_{\alpha\beta}^{(nlm)}) = \begin{bmatrix} 0 & H(\chi)\phi_a^{(lm)}(\theta,\varphi) \\ H(\chi)\phi_a{}^{(lm)}(\theta,\varphi) & S(\chi)\phi_{ab}^{(lm)}(\theta,\varphi) \end{bmatrix}. \tag{37}$$

The conditions $E_{\alpha\beta;\gamma} g^{\beta\gamma} = 0$ impose the relation

$$\frac{dH}{d\chi} + 2\cot\chi H(\chi) + \tfrac{1}{2}[2-l(l+1)]\csc^2\chi S(\chi) = 0 \tag{38}$$

which we will use to determine S given H. (In what follows we assume $l > 1$. The $l=1$ case will be treated later.) Using the divergence condition the E_{1a} equation

$$\Delta(E_{1a}) = \frac{\partial^2 E_{1a}}{\partial\chi^2} + \csc^2\chi\, E_{1a|b|c}\gamma^{bc} + [\csc^2\chi - 6\cot^2\chi]E_{1a} - 2\cot\chi\csc^2\chi E_{ab|c}\gamma^{bc} = \lambda E_{1a} \tag{39}$$

decouples and we find

$$\frac{d^2H}{d\chi^2} + 2\cot\chi\frac{dH}{d\chi} + \{[2-l(l+1)]\csc^2\chi - 2\cot^2\chi\}H = \lambda H. \tag{40}$$

The solution regular at the poles for $l > 1$ is given by

$$H^{(nl)}(\chi) = \sin^l\chi\, C_{n-l}^{(l+1)}(\cos\chi) \tag{41}$$

with the eigenvalue given by

$$\lambda = [2-n(n+2)]. \tag{42}$$

The symmetric tensor $F_{\alpha\beta}$ defined by Eq. (16) is obviously traceless, divergenceless, and linearly independent of the eight previously defined tensor harmonics. It is straight-

forward to show from Eq. (1) and Eq. (15) that $F_{\alpha\beta}$ satisfies the same harmonic equation as does $E_{\alpha\beta}$. The properties of the S^3 harmonics are summarized in Table II. The antisymmetric tensor $\widetilde{F}_{[\alpha\beta]}$ is identically zero. This follows from Eq. (15) and the divergenceless and traceless properties of $E_{\alpha\beta}$,

$$\epsilon_{\mu}{}^{\alpha\beta}\widetilde{F}_{[\alpha\beta]}=2E^{\nu}_{\mu;\nu}-2E^{\nu}_{\nu\ ;\mu}=0.$$

For the case in which $l=1$, Eq. (38) implies

$$\frac{dH}{d\chi}+2\cot\chi H=0$$

which integrates to give $H=\csc^2\chi$ and implies $\Delta E_{\alpha\beta}|_{l=1}=2E_{\alpha\beta}|_{l=1}$. But this solution is not regular at the poles. If we consider Eq. (39) with $l=1$, we find it is already decoupled but it is not divergencefree. In fact it is proportional to the $A_{\chi a}|_{l=1}$ tensor harmonic. There are no regular $l=1$ divergenceless tracefree harmonics.

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Conformal two-structure as the gravitational degrees of freedom in general relativity

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In this paper, we suggest that what we shall call the conformal 2-structure may, in an appropriate coordinate system, serve to embody the two gravitational degrees of freedom of the Einstein (vacuum) field equations. The conformal 2-structure essentially gives information concerning the manner in which a family of 2-surfaces is embedded in a 3-surface. We show that, formally at least, this prescription works for the exact plane and cylindrical gravitational wave solutions, for the double-null and null-timelike characteristic initial value problems, and for the usual Cauchy spacelike initial value problem. We conclude with a preliminary consideration of a two-plus-two breakup of the field equations aimed at unifying these and other initial value problems; and a discussion of some aspirations and remaining problems of this approach.

1. INTRODUCTION

The gravitational field, as described by the Einstein field equations, embodies the possibility of gravitational radiation; this has been known in linearized approximation since the early days of the development of the theory.[1] Consideration of plane waves in this approximation showed that they involved *two* degrees of freedom per space—time point.[2] When the linearized theory is interpreted as the theory of a massless spin two field in flat space—time, this is just an exemplification of the general property of massless, integral spin, free fields of having two helicity states.[3] Of course, in the gravitational case we should not interpret the linearized theory as a Poincaré-covariant theory, but rather as (one hopes) the first approximation to a solution of the full (nonlinear) field equations. Thus, it becomes important to know whether this property of having two degrees of freedom per space—time point is also characteristic of the exact theory. A number of arguments to establish that this is indeed the case have been given, probably the earliest being based upon consideration of the spacelike hypersurface initial value or Cauchy problem.[4]

The question of precisely how these two degrees of freedom may best be expressed analytically in terms of the components of the metric tensor and its derivatives (or such combinations of these as the Riemann tensor, notably) for a particular solution to the field equations, in a particular coordinate system, is not a simple one—nor indeed one with a unique answer. Any theory with a gauge group, such as Maxwell theory or general relativity, will allow a wide lattitude in the expression of true degrees of freedom of the field in terms of nongauge invariant quantities such as potentials for the gauge-invariant fields. Thus, it is not a question of finding a uniquely "right" answer to the question: What quantities are the bearers of the gravitational degrees of freedom? But rather, a question of seeing what particularly convenient embodiments of this information can be found when considering various problems of physical or mathematical interest in the study of the theory. Of course, the answer to any physically well-formulated problem within the theory must be the same, whatever method of treatment is employed, and therefore that answer could always be formulated invariantly in principle (that is in such a way that anyone could arrive at it by the use of any coordinate system—or, perhaps better said, by intrinsically geometrical considerations). Clearly, in practice, one may not be able (or willing) to reformulate the problem in such a way; and for actual computational purposes various coordinate choices, explicitly or implicitly adapted to some fully or partially geometrically determined structure, may vastly facilitate the treatment of particular problems.

In this paper, we shall attempt to show that a unified treatment of several important problems in general relativity may be given by adapting a coordinate system, such that the gravitational degrees of freedom are embodied in that portion of the metric tensor which we term the conformal 2-structure. In the next section we shall explain just what we mean by "conformal 2-structure." We shall then review part of the motivation for singling out this entity by looking at some exact and approximate solutions of the Einstein vacuum field equations. More specifically, in Sec. 3 we shall consider exact plane and cylindrical gravitational waves and establish in each case that it is precisely the conformal 2-structure which, in the standard representations of these solutions, embodies the two degrees of freedom of the field. In the following two sections, we shall briefly review the double-null initial value problem, as analyzed by Sachs,[5] and the null-timelike initial value problem as analyzed by Bondi *et al.*,[6] Sachs,[7] and

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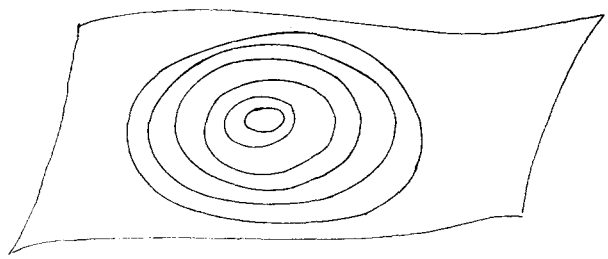
Tamburino and Winicour.[8] In these cases as well, we shall see that it is the conformal 2-structure on two null hypersurfaces, or a null surface and timelike tube (or some appropriate limit of it) respectively, which embodies the two gravitational degrees of freedom. Then, in the following section we shall discuss the spacelike or Cauchy initial value problem, and show (at least formally) how the constraint equations on the initial spacelike hypersurface may be interpreted so that again the conformal 2-structure on the initial hypersurface and its "velocity" play the role of the gravitational degrees of freedom.

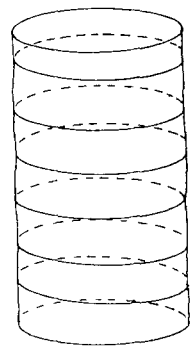
However, we wish to be clear from the beginning about the limitations of what we are attempting in this paper. In general, when considering a question such as the solution of a boundary value problem for a system of partial differential equations we should require that the problem be well posed, mathematically speaking. To be more precise, such problems require a specification of data which lead to the problem having a solution (existence), no more than one solution (uniqueness), and dependence of the solution on the specified data such that small variations in the data ("small" being suitably defined) lead to small variations in the solution (stability). Now, from the physical viewpoint, problems that seem physically reasonable are usually mathematically well posed; conversely, a problem that is ill posed mathematically often has turned out to conceal some physically dubious feature. This rule is by no means infallible. (Some ill-posed problems of physical importance are known.[9]) However, the posing of such problems is a signal for caution, at the very least.

In discussing the double-null and null-timelike type of initial value problems, as well as our approach to the initial value question in the case of the Cauchy (spacelike) problem, we are treading on quite dangerous territory. Very little is known about how such problems may be well posed, if at all; and global problems are known to abound here.[10] Since we have nothing to contribute to the solution of these difficulties, we shall sidestep the issue and adopt the following point of view, provisionally at least. Instead of claiming to construct solutions on the basis of the initial data for these problems, we imagine that we are *given* a solution to the field equations, and ask what data we need to give on our initial hypersurfaces to characterize it uniquely. Thus, we bypass the existence and stability questions, and merely consider the *uniqueness* of the problem. Of course, if in addition the solution we are considering is analytic, then the solution could actually be constructed from our initial data. But in any case, we claim no more than to analyze given solutions (given in the imagination at any rate) in terms of data characterizing them uniquely.

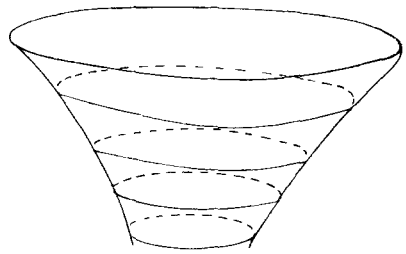
In the penultimate section, we shall consider a formulation which may eventually lead to a unified treatment of all the various initial value problems. In the concluding section we shall mention some of the still unresolved problems connected with this approach. Finally, an Appendix is included which recalls how, in a somewhat analogous manner, the various problems can be formulated in the case of the one-dimensional wave equation. We shall throughout restrict our attention to the Einstein vacuum field equations, and all our considerations will be purely local in character.



(i) Spacelike hypersurface



(ii) Timelike hypersurface



(iii) Null hyperspace

FIG. 1. Hypersurface foliated into topological 2-spheres.

2. CONFORMAL 2-STRUCTURE

We attempt to make precise in this section the meaning to be attached to the term "conformal 2-structure." (We owe this term to B. Carter, whose suggestion we gratefully acknowledge.) If we consider an arbitrary Riemannian 2-geometry, it is a classic theorem that it is conformally flat.[11] In this sense, there is no conformal 2-geometry; or rather only the trivial flat one. However, consider a family of 2-geometries $g_{AB}(x^C, p)$, given as a function of some preferred parameter p (where from now on Greek indices run from 0 to 3, lower case Latin from 1 to 3, and upper case Latin from 2 to 3). Obviously, we may now extract a conformal factor $\lambda^{-1}(x^C, p)$ from g_{AB} so that the determinant of the remaining conformal metric, $\bar{g}_{AB} = \lambda g_{AB}$, is parameter independent, i.e.,

$$|\bar{g}_{AB}| = f(x^C).$$

This property is clearly invariant under all parameter-independent coordinate and conformal transformations. Then, the two remaining independent components of

$\bar{g}_{AB}$, as functions of the two coordinates and of the preferred parameter p, contain the information which we refer to as the conformal 2-structure. [If we were to attempt to transform away this information, by a parameter-dependent family of coordinate and conformal transformations, on each 2-surface $p=\text{const}$ of the three-dimensional (x^A, p)-space, we would need two functions of the original coordinates and of the parameter to make each metric locally flat, and these functions would be equivalent to the original two functions in their information content.]

Note that, since $(|g_{AB}|_{,p})/(|g_{AB}|)=g^{AB}g_{AB,p}$ for any metric, our condition that $|\bar{g}_{AB}|$, $p=0$, is equivalent to the condition that the trace of $\bar{g}_{AB,p}$ vanish. This condition is invariant under the remaining conformal freedom. Namely, if $\bar{\bar{g}}_{AB}=K^2\bar{g}_{AB}$, K^2 must be independent of p to preserve the condition that the determinant of $\bar{g}_{AB}$ be independent of p, so $\bar{\bar{g}}^{AB}\bar{\bar{g}}_{AB,p}=\bar{g}^{AB}\bar{g}_{AB,p}$. Thus, it is really the conformal structure which is important. Indeed, $\bar{g}^{BC}\bar{g}_{AB,p}$ is invariant under any such allowed conformal transformations.

Now we shall translate these results into more geometrical language. Consider a three-dimensional manifold, which is fibered by the trajectories of a vector field V^a $(a=1,2,3,)$, and foliated by a family of 2-surfaces generated from any member of the family by dragging it with the vector field (alternatively, of course, one could start with the foliation and set up a correspondence between points on each 2-surface to generate the vector field). If p is the preferred parameter of the vector field, starting from some value on the initial 2-surface, then it can be used together with two coordinates x^A chosen on the initial 2-surface of the family and dragged with the vector field, to set up a preferred coordinate system for the 3-space. In this coordinate system each 2-surface in the family will be labeled by a value of p, and the vector field will take the form δ^a_p $(a=A,\ p)$. Any member of the family of 2-surfaces is then a rigged hypersurface in the 3-manifold, with V^a as the rigging field. If we introduce a family of 2-metrics g_{ab} on these rigged hypersurfaces $(g_{ab}V^a=0)$, this not only induces an intrinsic Riemannian geometry on each 2-surface, but enables us to define an extrinsic curvature for each 2-surface as embedded in the 3-manifold, namely $-\frac{1}{2}L_V g_{AB}=h_{ab}$, where $L_v\Phi$ stands for the Lie derivative of the geometric object Φ with respect to the vector field v. In the adapted coordinates (x^A, p), g_{ab} will only have components g_{AB} and h_{ab} only components $h_{AB}=-\frac{1}{2}g_{AB,p}$. Thus the family of 2-geometries $g_{AB}(x^C, p)$ enables us to compute h_{AB} and hence also gives information concerning the manner in which this family of 2-surfaces is embedded in (x^C, p) 3-space. (We are grateful to R. Penrose for a discussion on this point.)

We emphasize again that this construction is quite independent of whether the 3-manifold is endowed with any other structure, and depends only on the inner metric of the 2-surfaces and their rigging. Of course, if the 3-manifold itself has a Riemannian metric, and g_{AB} is the induced metric on a 2-surface rigged with a unit normal vector, h_{AB} is the usual second fundamental form of the 2-surface.

Now we can take the 2-surface metric g_{AB}, compute its inverse metric g^{AB}, and project this back into the 3-manifold using the projection operator $E^a_b=\delta^a_b-V^a w_{,b}$, where $w(x^a)$ is the scalar field which reduces in adapted coordinates to $w=p$. (It follows that this projection g^{ab} obeys $g^{ab}w_{,b}=0$.) We now look for a conformal factor $\lambda(x^a)$ such that $\bar{g}_{ab}=\lambda g_{ab}$ obeys the equation $\bar{h}=\bar{g}^{ab}\bar{h}_{ab}=0$. This always exists, since it merely requires that $L_V \ln\lambda = h=g^{ab}h_{ab}$. Thus, the conformal 2-structure can be invariantly characterized by the condition that the trace of the extrinsic curvature vanishes. This condition is clearly invariant under the remaining conformal freedom, which allows us to introduce any conformal factor K^2 such that $L_V K=0$. Thus, the conformal 2-structure essentially gives information about the traceless extrinsic curvature of the family of 2-surfaces, which we shall call the conformal extrinsic curvature.

It is easy to generalize these ideas[12] to a family of 2-surfaces in a 4-manifold generated from an initial 2-surface by dragging with two commuting vector fields. The 2-surfaces will then form two families of 3-surfaces; and each 2-surface will have two extrinsic curvatures: one with respect to each 3-surface in which it is embedded. If one wants to consider the evolution of the gravitational field from the initial data this is the sort of construction that is needed. But in this paper we confine ourselves (except for the next section) to a discussion of the initial value question only, so our treatment here is sufficient.

3. EXACT SOLUTIONS, PLANE AND CYLINDRICAL

Bondi, Pirani, and Robinson[13] have discussed plane gravitational waves, defining them as nonflat solutions to the gravitational field equations possessing at least as much symmetry as electromagnetic plane waves (actually, an additional symmetry will always exist). Locally, it is always possible to put such solutions into the form

$$ds^2=\exp(2\phi)(dt^2-d\xi^2)-u^2\bar{g}_{AB}dx^A dx^B, \tag{3.1}$$

where

$$\bar{g}_{AB}=\begin{pmatrix}\cosh 2\beta+\sinh 2\beta\cos 2\theta & -\sinh 2\beta\sin 2\theta\\ -\sinh 2\beta\sin 2\theta & \cosh 2\beta-\sinh 2\beta\cos 2\theta\end{pmatrix},$$

$$|\bar{g}_{AB}|=1, \tag{3.2}$$

and β, θ, and ϕ are functions of $u=t-\xi$. β and θ are arbitrary functions of u, while ϕ is determined by

$$2\phi'=u(\beta'^2+\theta'^2\sinh^2 2\beta). \tag{3.3}$$

We see that the two gravitational degrees of freedom are here explicitly represented by the functions β and θ. Thus, the conformal 2-structure, as a function of the preferred parameter u, embodies the radiation field in this representation of plane gravitational waves.

The problem of gravitational waves with cylindrical symmetry was first solved in the case when they also possess reflection symmetry (and thus only one degree of freedom) by Beck, and rediscovered by Einstein and Rosen. The cylindrical waves without reflection

symmetry, and thus possessing both degrees of freedom, were discovered by Ehlers, and independently by Kompaneets. A detailed discussion, with references, may be found in a paper by one of us.[14] The metric, in the form given by Ehlers, is

$$ds^2 = \exp(\gamma - \psi)(dt^2 - d\rho^2) - \rho \bar{g}_{AB} dx^A dx^B, \tag{3.4}$$

where

$$\bar{g}_{AB} = \begin{bmatrix} \rho^{-1}\exp(2\Psi) & \rho^{-1}\chi\exp(2\Psi) \\ \rho^{-1}\chi\exp(2\Psi) & \rho^{-1}\chi^2\exp(2\Psi) + \rho\exp(-2\Psi) \end{bmatrix},$$

$$|\bar{g}_{AB}| = 1, \tag{3.5}$$

and Ψ, χ, and γ are functions of ρ, t only. Ψ and χ obey coupled nonlinear cylindrical wave equations

$$\Box\Psi = \tfrac{1}{2}\rho^{-2}\exp(4\Psi)(\chi_{,\rho}^2 - \chi_{,t}^2), \tag{3.6a}$$

$$\Box\chi = 2\rho^{-1}\chi_{,\rho} + 4(\chi_{,t}\Psi_{,t} - \chi_{,\rho}\Psi_{,\rho}), \tag{3.6b}$$

where

$$\Box f = \rho^{-1}(\rho f_{,\rho})_{,\rho} - f_{,tt}$$

is the cylindrical wave operator; γ is determined by Ψ and χ through the equations

$$\gamma_{,\rho} = \rho(\Psi_{,\rho}^2 + \Psi_{,t}^2) + \tfrac{1}{4}\rho^{-1}\exp(4\Psi)(\chi_{,t}^2 + \chi_{,\rho}^2), \tag{3.7a}$$

$$\gamma_{,t} = 2\rho\Psi_{,\rho}\Psi_{,t} + \tfrac{1}{2}\rho^{-1}\exp(4\Psi)\,\chi_{,\rho}\chi_{,t}, \tag{3.7b}$$

whose conditions of integrability are precisely the coupled wave equations (3.6) for Ψ and χ. Thus, once again it is the conformal 2-structure $\bar{g}_{AB}$ which embodies the gravitational degrees of freedom of the cylindrical waves. Note that while Eqs. (3.6) have been given in a form appropriate for discussion of the usual Cauchy problem, i.e., using one spacelike coordinate ρ and one timelike coordinate t, by introduction of coordinates $u = t - \rho$ and $v = t + \rho$ we can cast these equations into a form appropriate for consideration of a double-null initial value problem, a Bondi—Sachs problem, etc. The conformal 2-structure will then be given as a function of the appropriate parameter, depending on whether we look at a spacelike, null or timelike hypersurface. Of course, on a spacelike initial hypersurface, the velocities (or momenta) of the conformal 2-structure must be given as well, in keeping with the usual feature of the spacelike Cauchy problem, i.e., the "doubling" of the data needed on spacelike portions of the initial boundary (see the Appendix).

Thus, we see that in both the known cases where exact radiating solutions can be explicitly given with as much generality as the symmetry conditions imposed will allow, it is indeed the conformal 2-structure, as functions of the appropriate parameter or parameters, which exhibits the gravitational degrees of freedom. It might be argued that these solutions are highly specialized, and that this may not necessarily be the case when considering more general situations.

In linearized gravitation theory, it is well known that it is the transverse traceless part of the linearized deviations from the flat metric which explicitly embody the radiation field in the simplest way.[15] Here, the removal of the trace of the transverse components is the linearized version of the removal of the conformal factor of the 2-metric; so that the standard treatment of linearized theory again uses the conformal 2-structure to embody the two degrees of freedom of the radiation field. This suggests the generality of our results; but we shall not enter into any further details of the linearized theory, since we are able to verify our conclusions for the exact theory by considering several types of initial value problems. In the next section we recall the double-null and Bondi—Sachs type of initial value problems, and show that in both cases the initial data needed to characterize a solution uniquely is again the conformal 2-structure on some 3-hypersurfaces.

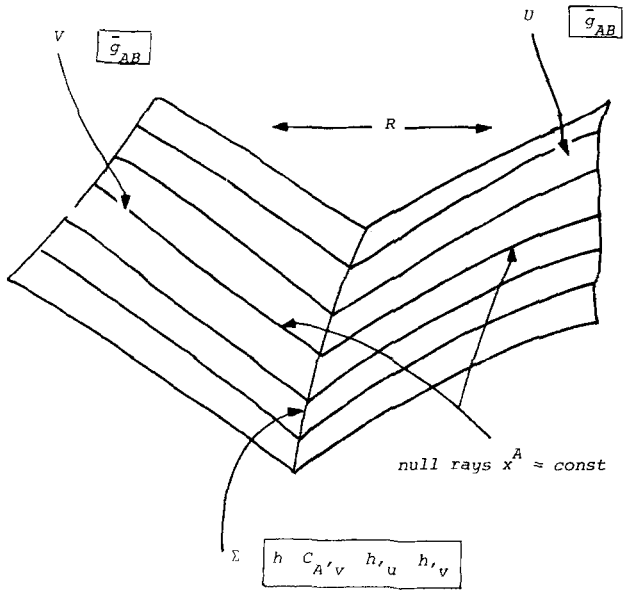


FIG. 2. The initial surfaces and their respective data for the double-null case.

4. DOUBLE-NULL AND NULL-TIMELIKE INITIAL VALUE PROBLEMS

We review first the double-null initial value problem, as formulated by Sachs.[5] The problem, here, is to find a set of functions given on a pair of intersecting null hypersurfaces U and V, together with some lower-dimensional data on their intersection $\sum$ (a two-dimensional spacelike surface), which will serve to completely characterize a solution to the Einstein equations in the region R lying to the future of both null hypersurfaces (see Fig. 2). From the general nature of the double-null initial value problem (see the Appendix), we expect that we shall have to prescribe a pair of functions on each null hypersurface, since the gravitational field has two degrees of freedom.

Sachs shows that one can embed each of the hypersurfaces U and V in a family of null hypersurfaces, $u = \text{const}$, $v = \text{const}$, in such a way that u is a preferred parameter along the null geodesics on V, and v is a preferred parameter along the null geodesics on U (remembering that every null hypersurface is ruled by a family of null geodesics). Two additional coordinates x^A are then chosen on, and continued off, the initial

null hypersurface in such a way that the x^A are constant along each null ray on the null hypersurfaces u = const (it is this latter condition which introduces the asymmetry between u and v in the metric given below). With this choice of coordinates, the general line element takes the form

$$ds^2 = -\exp(2q)du\,dv + \exp(2h)\bar{g}_{AB}(dx^A + C^A\,du)(dx^B + C^B\,du) \tag{4.1}$$

with

$$|\bar{g}_{AB}| = 1, \quad q = 0 \text{ on } U \text{ and } V, \quad C^A = 0 \text{ on } V. \tag{4.2}$$

The conformal flatness of any 2-metric, mentioned in Sec. 2, is used to pick the x^A on $\sum$ so as to make $\bar{g}_{AB}$ take on the form

$$\bar{g}_{AB} = \delta_{AB} \text{ on } \sum. \tag{4.3}$$

Sachs goes on to demonstrate, by means of an analysis of the field equations, that the following data suffice to determine a solution to the field equations in the region R,

$$\bar{g}_{AB} = \bar{g}_{AB}(x^C, u) \text{ on } V, \quad \bar{g}_{AB} = \bar{g}_{AB}(x^C, v) \text{ on } U, \tag{4.4}$$

and the following additional data on Σ

$$h,\ C_{A,v},\ h_{,u}, \text{ and } h_{,v}. \tag{4.5}$$

The data on U and V are again the conformal 2-structure of the family of spacelike 2-surfaces u = const, on V and v = const, on U, as functions of these preferred affine parameters respectively. Of course, as Sachs points out, since these are null hypersurfaces, one may better think of $\exp(2h)\bar{g}_{AB}$ as giving the distance between two null rays at a point, rather than between two points. The data on Σ is also interpreted geometrically by Sachs. For example, giving h on Σ serves to fully determine the inner geometry of Σ, since it is known conformally already; $h_{,u}$ and $h_{,v}$ give the two mean extrinsic curvatures of Σ with respect to its embedding in V and U, respectively. The most important point to note, for our purposes, is that an appropriate choice of coordinates has enabled Sachs to put the information about the two degrees of freedom of the gravitational field into the conformal 2-structure of the two initial null hypersurfaces. In fact, the initial value problem for this double-null case has been solved recently by Müller zum Hagen and Seifert,[16] who have obtained some strong theorems for the existence, uniqueness, and stability of the solutions.

The null-timelike type of initial value problem has been considered in two variants. For our purposes, it will be simpler to consider the second case first, as worked out by Tamburino and Winicour.[8] They consider the initial value problem on a timelike world tube Γ and the initial forward null hypersurface N_0 emanating from some two-dimensional spatial slice S_0 across the timelike tube (see Fig. 3). The initial hypersurfaces thus consist of the future portions of Γ and N_0, both hypersurfaces issuing from their intersection S_0. Coordinates are introduced in the following way: S_0 is coordinatized by a pair of coordinates x^A. The family of timelike curves issuing from S_0 and lying within Γ, which are geodesics with respect to the inner geometry of Γ, are

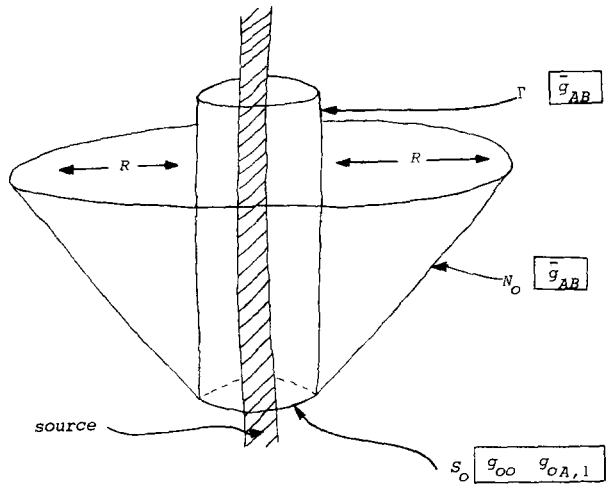


FIG. 3. The initial surfaces and their respective data for the Tamburino—Winicour case.

used to coordinatize Γ. Each geodesic is labeled by the x^A of the point of S_0 from which it issues, and the arc length along each geodesic is taken as a timelike coordinate u ($\equiv x^0$) on Γ. The intrinsic metric of Γ in these geodesic normal coordinates is then given by

$$ds^2(\Gamma) = -du^2 + g_{AB}\,dx^A\,dx^B. \tag{4.6}$$

The family S of geodesically parallel slices to S_0, u = const, are then used to generate a family of forward null hypersurfaces N, of which N_0 is the initial one. These surfaces are labeled by u, and each null ray on such a surface, issuing from a point on S, is also labeled by the x^A of that point. Finally, the fourth coordinate r ($\equiv x^1$) is introduced by choosing it as the luminosity distance along each null ray,

$$|g^{\mu\nu}x^A_{,\mu}x^B_{,\nu}| = [r^4 f(x^A)^2]^{-1}, \tag{4.7}$$

where $f(x^A)$ is some given function, depending on the exact choice of variables x^A used for the spacelike 2-surfaces, u = const, r = const. With this choice of coordinates, the line element of the four-dimensional region between Γ and N_0 is given by

$$ds^2 = g_{00}du^2 + 2[g_{01}du dr + g_{0A}du dx^A] + r^2\bar{g}_{AB}dx^A dx^B, \tag{4.8}$$

where

$$|\bar{g}_{AB}| = [f(x^A)]^2. \tag{4.9}$$

On Γ, r is some given function of u and x^A which is determined by the condition that (4.8) reduces to the form (4.6).

An analysis of the field equations, paralleling that given by Bondi *et al.*,[6] and by Sachs,[7] then shows that a solution to the Einstein field equations in the region between Γ and N_0 is determined by the following initial data:

$$\bar{g}_{AB} \text{ on } N_0, \text{ as a function of } (r, x^A), \tag{4.10a}$$

$$\bar{g}_{AB} \text{ on } \Gamma, \text{ as a function of } (u, x^A), \tag{4.10b}$$

with the lower dimensional data

g_{00}, $g_{0A,1}$ on S_0, as functions of (x^A). (4.11)

Hence, again, we see that in this coordinate system it is the conformal 2-structure on the initial hypersurfaces which embodies the information about the gravitational degrees of freedom.

In fact, Tamburino and Winicour, by analogy to the approach of Bondi *et al.* and Sachs, actually use the time derivative of $\bar{g}_{AB}$ on Γ; this is the analog of the "news functions" of Bondi. In the case when there was no incoming radiation initially present, it bears the news about behavior of sources of the gravitational field inside the timelike tube Γ that can affect the fields outside the tube in the region under consideration. Clearly the two choices are equivalent: The news functions correspond to the conformal extrinsic curvature of the family of 2-surfaces S with respect to Γ, but this amounts to the same thing as giving the intrinsic conformal 2-structure of the family as a function of the parameter that takes us from one member of the family to the (geodesically parallel) next one.

The approach of Tamburino and Winicour also illustrates, in part, the limitations of what we are attempting here. The data (4.10) is not, in fact, specifiable with complete freedom as initial data. For example, the data set on a small region of Γ will, because of the timelike character of Γ, automatically determine the data on a large region of Γ. Tamburino and Winicour suggest that this may in some sense limit the functional form of the data which may be specified on Γ. Thus, although this approach gives us considerable insight into the structure of the field equations, it would appear that this particular initial value problem is not well posed. We now turn to a formulation given by Bondi *et al.*[6] and Sachs,[7] which does not appear to have this same limitation.

The Bondi—Sachs analysis is quite similar to that outlined above (and of course preceded it in time), except that the timelike tube is pushed off to infinity in the null directions defined by the family of null surfaces (see Fig. 4). This results in an asymptotic initial value problem for the hypersurface N_0 and the future null cone at infinity $\mathcal{I}^+$, as defined by Penrose.[17] The form of the line element adopted by Sachs (who treated the case where both gravitational degrees of freedom were present, after Bondi *et al.* has considered the reflection and axially symmetric case with only one degree of freedom) is similar to the form (4.8), but with some specializations of the six nonvanishing components of the metric to facilitate computation. The x^A are picked by analogy with angular polar coordinates, so that $f(x^A) = \sin\theta$, and $\bar{g}_{AB}$ is explicitly parametrized in terms of two functions γ and δ so that

$$\bar{g}_{AB}\,dx^A\,d^B = \exp[2(\gamma+\delta)]d\theta^2 + 4\sin\theta\,\sinh(\gamma-\delta)d\theta\,d\phi + \sin^2\theta\exp[-2(\gamma+\delta)]d\phi^2. \quad (4.12)$$

In addition various boundary *cum* coordinate conditions are imposed as $r\to\infty$ along the null hypersurfaces u = const, partly to ensure the existence of future null infinity. (It was originally hoped that these conditions might also limit the class of systems considered to those representing outgoing radiation only, but it now seems clear that while all outgoing radiation solutions are included in this class, solutions with sufficiently weak incoming radiation fields are also included.)

To summarize the results of their analysis of the field equations under these conditions, the following data are found to be necessary to determine a solution to the field equations in the neighborhood R or $\mathcal{I}^+$ posterior to N_0 (see Fig. 4):

δ and γ on N_0, as functions of (r,θ,ϕ), (4.13a)

c_1 and c_2 on $\mathcal{I}^+$, as functions of (u,θ,ϕ), (4.13b)

where c_1 and c_2 are the "news functions" given by

$$c_1 = \frac{\partial}{\partial u}\lim_{\substack{r\to\infty \\ u=\text{const}}}(r\delta), \quad c_2 = \frac{\partial}{\partial u}\lim_{\substack{r\to\infty \\ u=\text{const}}}(r\gamma).$$

In addition, three functions on the "2-sphere S_0 at infinity" [analogous to (4.11)], which are defined by appropriate limiting processes, must be specified. One of these, $M(u,\theta,\phi)$, was named the "mass aspect" by Bondi, since its integral over S_0 gives the Schwarzschild mass of the solution; while the other two functions $N(u,\theta,\phi)$ and $P(u,\theta,\phi)$ are related to the "dipole aspect" of the field.

So once again, we see that it is essentially the conformal 2-structure on N_0 (in the neighborhood of $\mathcal{I}^+$) and on $\mathcal{I}^+$ that embody the information about the degrees of freedom in the gravitational field. In the next section we shall show that a similar analysis of the spacelike initial value or Cauchy problem is also possible.

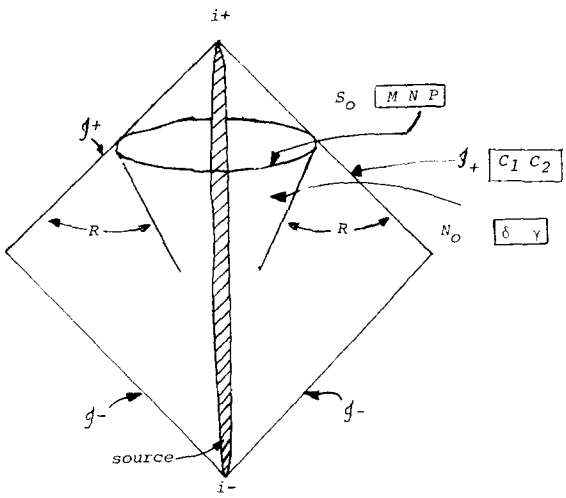


FIG. 4. Penrose diagram indicating the initial surfaces and initial data for the Bondi—Sachs case.

5. CAUCHY INITIAL VALUE PROBLEM

As is well known,[18] when the Einstein equations are analyzed with respect to a family of spacelike hypersurfaces, H, generated from an initial one, H_0, by dragging it with a transvecting vector field, V^μ, they break up into two sets: Those projected once or twice into the normal to the hypersurface—the four constraint equations, and those projected twice into the hypersurface—the six evolution equations. When the metric tensor is similarly decomposed into its com-

ponents with respect to the normal field, it is found that the evolution equations determine the second Lie derivatives with respect to the unit normal, N^μ, to H of the hypersurface components of the metric. This suggests that the Cauchy data on the initial hypersurface H_0 be taken as the metric or first fundamental form of the initial hypersurface: ${}'g_{ab}$ in coordinates adapted to the surface; and its first Lie derivative with respect to N^μ which (up to a factor $-\frac{1}{2}$) is the second fundamental form of the initial hypersurface: h_{ab} in adapted coordinates. However, the four constraint equations then give four relationships between the first and second fundamental forms which this initial data must obey. The contracted Bianchi identities then indicate that the propagation of the initial data off H_0 by the evolution equations guarantees that the propagated data satisfy the constraint equations on any other hypersurface in the family H. The Einstein equations thus form a system in involution.[19]

It might still seem that we have an excessive number of functions to describe the gravitational field: the six ${}'g_{ab}$ and the six h_{ab} ($=-\frac{1}{2}L_N\,{}'g_{ab}$, where L_N denotes the Lie derivative), subject to four constraints. However, the freedom of choice of the coordinates on the initial hypersurface shows that three of these functions contain essentially information about the coordinate system, while the freedom to choose the initial hypersurface, when the characterization of this initial hypersurface is re-expressed in terms of the ${}'g_{ab}$ and h_{ab}, shows that there is an additional relation between them (which again merely represents coordinate information). Thus, we arrive at the need to specify four functions per space—time point on H_0, which in the above formulation are the remaining two "three-metric elements" and the two corresponding "velocities" (or equivalently "momenta"), to characterize a solution to the field equations. This again exhibits the typical "doubling" of the data needed on a spacelike portion of the initial hypersurface (see the Appendix).

We shall restrict our attention in this paper to the four constraint equations. We shall show that the constraint equations can be solved, formally at least, by a two-plus-one breakup of the initial hypersurface H_0 with respect to a family, S, of spacelike 2-surfaces and a transvecting vector field which drags points along from one member of the family to the next (see Fig. 5). Once the "lapse" and "shift" functions[20] fixing the family of 2-surfaces and the relation between points on them has been specified, together with one other function specifying the initial hypersurface, then the conformal 2-structure of the family of 2-surfaces S, as a function of the parameter characterizing the dragging by the transvecting vector field, together with its Lie derivative with respect to N^μ (the "velocities") is the freely specifiable data. The constraint equations may then be solved for the other variables needed to completely specify the first and second fundamental form of the hypersurface. In this way we establish that the initial data characterizing the two gravitational degrees of freedom on a spacelike hypersurface (the Cauchy problem) may be taken as the conformal 2-structure as a function of an appropriate parameter, together with the corresponding velocities. This we now demonstrate in some detail.

Let the initial hypersurface H_0 be given by the equation

$$\Phi(x^\mu) = \text{constant}. \tag{5.1}$$

We adapt coordinates to the initial hypersurface: $\Phi \doteq x^0$, so that the surface H_0 is described by the three coordinates x^a. We now introduce a family, S, of two-dimensional hypersurfaces in H_0: $\phi = \text{const}$. We can always think of this family (at least locally) as generated by dragging an initial 2-surface, S_0, with a transvecting vector field v^a, lying in H_0. As we shall discuss in the final section, this suggests the possibility of taking the initial 2-surface as a closed surface, bounding a region inside of which sources of the gravitational field may be enclosed, which would lead to consideration of mixed Cauchy problems.[21] However, nothing in our analysis (admittedly local and rather formal) prevents the taking of the initial 2-surface as an open surface. Then, adapting coordinates to the family of hypersurfaces,

$$\phi \doteq x^1$$

and to the vector field,

$$v^a \doteq \delta^a_1,$$

the (intrinsic) metric ${}'g_{ab}$ of H_0 takes the form

$${}'g_{ab}\,dx^a\,dx^b = \rho^2(dx^1)^2 + g_{AB}(dx^A + \sigma^A\,dx^1)(dx^B + \sigma^B\,dx^1), \tag{5.2}$$

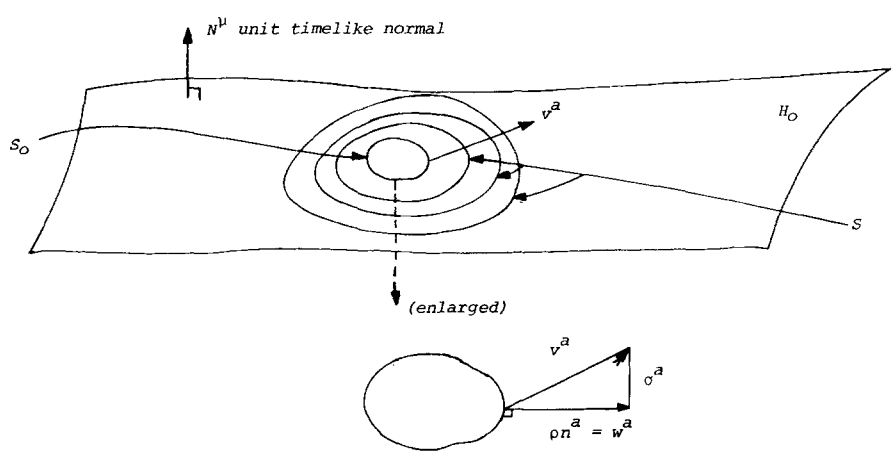


FIG. 5. The initial hypersurface H_0, the initial 2-surface S_0, the family S, and the various vector fields.

where

$$\rho=\rho(x^a),\quad \sigma^A=\sigma^A(x^a),\quad g_{AB}=g_{AB}(x^a).$$

Then the family of 2-surfaces, S, is given by $x^1=$ constant, x^A are coordinates in each 2-surface of S, ρ represents the lapse function (i.e., ρdx^1 is the normal distance between two neighboring 2-surfaces of S), and σ^A represents the shift function (i.e., $\sigma^A dx^1$ is the vector between the point on the neighboring surface reached by v^a and the point reached by going in the normal direction—see Fig. 5). It proves advantageous for our breakup to use Lie derivatives with respect to $w^a\equiv\rho n^a$, where n^a is the unit normal to S in H_0. This choice is merely one of convenience, but it does possess the following advantages: First of all it satisfies the normalizing condition $w^a\,\phi_{,a}=1$, giving the same projection operator as n^a does; thus, applied to the metric it projects out the co- and contravariant 2-metric, i.e., g_{AB} and its inverse. Finally, any rigged hypersurface in an affine manifold has a unique connection induced on it, dependent on the rigging; the induced connection with w^a as the choice of rigging field turns out to be identical to the metric connection of the induced metric g_{AB}.

We use the rigging vector w^a to construct the projection operator B^a_b into S,

$$B^a_b=\delta^a_b-w^a\phi_{,b} \tag{5.3}$$

with which we can decompose $'g_{ab}$ into six parts. Three of these parts, namely the projections twice into S, consist of the family of 2-metrics induced on S, namely g_{AB}; we break this quantity up further by extracting its determinant which we denote by $\exp(\frac{1}{2}\lambda)$. (This choice of conformal factor makes the ensuing equations rather simpler to handle. In general, as indicated earlier in Sec. 2, we may extract any conformal factor for which the determinant of the remaining part is a fixed function of x^A only.) Thus

$$g_{AB}=\exp(\tfrac{1}{2}\lambda)\bar{g}_{AB},\quad \bar{g}_{AB}=1, \tag{5.4}$$

from which it is clear that $\bar{g}_{AB}$ has only two independent components. The remaining projections of $'g_{ab}$: Twice into the normal, and once into the normal and once into S, yield ρ^2 and σ^A respectively. We have now decomposed $'g_{ab}$ into six parts

$$\rho^2,\ \sigma^A,\ \lambda,\ \bar{g}_{AB}, \tag{5.5}$$

where the first three quantities are clearly connected with the choice of a coordinate system (or more geometrically, with the adaptation of a coordinate system to a family of rigged hypersurfaces in H_0). We next break up h_{ab} in an analogous manner. We define the quantities

$$h=h_{ab}w^aw^b,\quad h_A=B^a_A\,w^bh_{ab},\quad h_{AB}=B^a_AB^b_Bh_{ab}, \tag{5.6}$$

where B^a_A is the projection operator of (5.3) with its covariant index restricted to the coordinates on each 2-surface. (Note that h is *not* the trace of h_{ab} in our notation, nor of h_{AB}. We denote the former by h^a_a, the latter by h^A_A.) We then extract the trace of h_{AB}, relative to g_{AB}, and a conformal factor, in order to define the quantity

$$\bar{h}_{AB}=\exp(-\tfrac{1}{2}\lambda)(h_{AB}-\tfrac{1}{2}g_{AB}h^C_C). \tag{5.7}$$

We have now decomposed h_{ab} into six parts which turn out to be just the velocities of the components (5.5) of $'g_{ab}$

$$h=-\tfrac{1}{2}L_N\rho^2,\quad h^A=-\tfrac{1}{2}L_N\sigma^A,\quad h^A_A=-\tfrac{1}{2}L_N\lambda,\quad \bar{h}_{AB}=-\tfrac{1}{2}L_N\bar{g}_{AB}. \tag{5.8}$$

We now insert these decompositions of the first and second fundamental forms into the four constraint equations

$$G_{\mu\nu}N^\mu N^\nu=0,\quad G_{\mu\nu}N^\mu B^\nu_b=0,$$

where B^ν_b is the projection operator into the hypersurface H_0. Written in terms of the first and second fundamental forms of H_0, these take the well-known form

$$\nabla_b(h^{ab}-{}'g^{ab}h^c_c)=0,\quad {}^3R+h^{ab}h_{ab}-(h^c_c)^2=0. \tag{5.9}$$

The resulting equations are

(I) $$L_w(h^A_A)+(\tfrac{1}{4}h^A_A-\rho^{-2}h)L_w\lambda-\rho\bar{H}^{AB}\bar{h}_{AB}-\rho^{-1}\exp(-\tfrac{1}{2}\lambda)\bar{\nabla}_A(\rho h^A)=0,$$

(II) $$L_w(\rho^{-1}h^A)+\tfrac{1}{2}\rho^{-1}h^AL_w\lambda+\exp(-\tfrac{1}{2}\lambda)\bar{\nabla}_B[\rho\exp(\tfrac{1}{2}\lambda)\bar{h}^B_A]-(\rho^{-1}h)_{,A}-\tfrac{1}{2}\rho^{-2}(\rho^{-1}h^B_B)_{,A}=0,$$

(III) $$L^2_w\lambda+\tfrac{3}{8}(L_w\lambda)^2-\rho^{-1}(L_w\rho)(L_w\lambda)-\rho^2\exp(-\tfrac{1}{2}\lambda)[{}^2\bar{R}]+\exp(-\tfrac{1}{2}\lambda)[\tfrac{1}{2}\rho^2\bar{\nabla}^2\lambda+2\rho\bar{\nabla}^2\rho+\rho^2\exp(\tfrac{1}{2}\lambda)\bar{H}^{AB}\bar{H}_{AB}-2h^Ah_A-\rho^2\exp(\tfrac{1}{2}\lambda)\bar{h}^{AB}\bar{h}_{AB}]+2hh^A_A+\tfrac{1}{2}\rho^2h^A_Ah^B_B=0,$$

where

$$\bar{H}_{AB}=-\tfrac{1}{2}\rho^{-1}L_u\bar{g}_{AB},\quad \bar{H}=\bar{g}^{AB}\bar{H}_{AB},\quad \bar{\nabla}^2=\bar{g}^{AB}\bar{\nabla}_A\bar{\nabla}_B, \tag{5.10}$$

and all barred quantities are built out of $\bar{g}_{AB}$ and its inverse $\bar{g}^{AB}$. (Of course, we could equally well formulate these equations in terms of Lie derivatives with respect to v^a or n^a.)

We then consider the following as initial data:

$$\bar{g}_{AB}\text{ on }H_0,\quad\text{as a function of }(x^1,x^A), \tag{5.11a}$$

$$\bar{h}_{AB}\text{ on }H_0,\quad\text{as a function of }(x^1,x^A), \tag{5.11b}$$

i.e., the conformal 2-structure of the family S, as a function of the preferred parameter x^1 specifying the family, and the corresponding velocities, also as a function of the preferred parameter. These four pieces of information then embody the two gravitational degrees of freedom for the usual Cauchy problem. As mentioned earlier, we take ρ and σ^A as given in the above equations, since they simply specify the family of 2-surfaces and the relation between them (being the lapse and shift functions) and thus fix the parameter x^1. In addition, one more function must be specified on H_0; this corresponds, however indirectly, to the specification of the initial hypersurface H_0 (and hence is again coordinate information). Restricting attention to a scheme of formal integration in which we assume the solution in question is analytic, three choices for this additional function then suggest themselves, namely λ, h, or h^A_A. Corresponding to each choice, we need also to specify some lower dimensional data on S_0. The three formal integration schemes are outlined in Table I.

TABLE I.

Functions specified on:	Case 1	Case 2	Case 3
H_0 $\bar{g}_{AB}$, $\bar{h}_{AB}$, ρ, σ^A and (functions of 3 variables)	λ	h	h^A_A
S_0 (functions of 2 variables)	$h^A_A(\neq 0)$, h_A	h^A_A, h_A, λ, $L_w\lambda(\neq 0)$	h_A, λ, $L_w\lambda(\neq 0)$
Formal integration by iteration proceeds by:	III$\rightarrow h$ (algebraically) I$\rightarrow L_w h^A_A$ II$\rightarrow L_w h_A$	I$\rightarrow L_w h^A_A$ II$\rightarrow L_w h_A$ III$\rightarrow L^2_w\lambda$	I$\rightarrow h$ (algebraically) II$\rightarrow L_w h_A$ III$\rightarrow L^2_w\lambda$

Let us consider the scheme in more detail in Case 1, for example. Equation III serves to determine h algebraically on S_0. Then I determines $L_w h^A_A$ on S_0, which is equivalent to knowing h^A_A on the "next neighboring" surface to S_0, S_1 say. Similarly II determines $L_w h_A$ on S_0 and hence h_A on S_1. Thus $h^A{}_A$ and h_A are known on S_1 and assuming $h^A{}_A \neq 0$ we can repeat the above procedure on S_1. Continuing in this way we can formally generate a solution of the constraint equations. The other cases are similar. These are not the only ways in which the equations may be viewed as formally generating a solution, but they do provide examples of the possibility of regarding the conformal 2-structure as the freely specifiable dynamical information. If we now assume that such an integration scheme leads to a knowledge of all the unknown quantities on H_0, then we can construct the first and second fundamental forms by using

$$'g_{ab} = \exp(\tfrac{1}{2}\lambda)B^A_a B^B_b \bar{g}_{AB} + \rho^2 \phi_{,a}\phi_{,b} \tag{5.12}$$

and

$$h_{ab} = h\phi_{,a}\phi_{,b} + (B^A_a\phi_{,b} + B^A_b\phi_{,b})h_A + \exp(\tfrac{1}{2}\lambda)B^A_a B^B_b(\bar{h}_{AB} + \tfrac{1}{2}\bar{g}_{AB}h^C_C). \tag{5.13}$$

The use of the evolution equations to construct a four-dimensional solution into the future (or past) of H_0 then proceeds as usual.

Finally, we mention the way in which some particular simple choices for the nondynamical initial data on H_0 are equivalent to particular coordinate conditions.

$\rho = 1$: In this case $w^a = n^a$, the unit normal vector field, and hence S_0 is dragged into geodesically parallel surfaces.

$\sigma^A = 0$: Points on the surface of any member of S are dragged normally into the neighboring surface of S, i.e., no "shear."

(I) $\lambda = \lambda(x^1)$: This means that λ will in general be a function of x^0 and x^1 only in the four-dimensional manifold. We cannot in general impose a simpler condition on λ, since $\lambda = 0$ leads to $h^A_A = 0$ and the integration scheme (for Case 1) breaks down: Similarly $\lambda = \lambda(x^0)$ only, leads to $L_w\lambda = L_w h^A_A = 0$ which turns I into a constraint between $\bar{h}_{AB}$ and h_A. An example of the occurence of condition (I) is found in the standard treatment of plane waves (see Sec. 3 or Ref. 13).

(II) $h = 0$: This is equivalent to $L_N\rho = 0$, and if this condition can be propagated in time it means that ρ will be time independent.

(III) $h^A_A = 0$: This is equivalent to $L_N\lambda = 0$. The surface area of each S_i in S is given by $\int_{S_i} \exp(\frac{1}{2}\lambda)d^2x$, and hence if this condition can be propagated in time it means that the surface area of each S_i will remain constant in time. An example of the occurence of this condition is found in the standard treatment of cylindrical waves (see Sec. 3 or Ref. 14). It might be termed a "Bondi-type" coordinate condition, since it includes the determinant condition (4.7).

6. A POSSIBLE UNIFYING APPROACH

It is well known from the variational principle formulation of the "Newtonian" approach to the usual Cauchy problem[18] that there is an intrinsic connection between the dynamical equations and the dynamical variables. More precisely, we start by using N^μ to construct a projection operator into H_0 so that, in particular,

$$g^{\mu\nu} = {}'g^{\mu\nu} + N^\mu N^\nu, \tag{6.1}$$

where $'g^{\mu\nu}$, the projection of the contravariant metric twice into H_0, is the induced (contravariant) 3-metric on H_0. Then variation of the Einstein Lagrangian, $\sqrt{-g^4}R$, with respect to $'g^{\mu\nu}$ leads to the equations.

$$B^\mu_\alpha B^\nu_\beta G_{\mu\nu} = 0, \tag{6.2}$$

i.e., the six evolution equations; and variation with respect to N^μ leads to the equations

$$N^\mu B^\nu_\alpha G_{\mu\nu} = N^\mu N^\nu G_{\mu\nu} = 0, \tag{6.3}$$

i.e., the four constraint equations. Thus, in this formulation, the dynamical variables generate their dynamical or evolution equations. However, since there are only two independent dynamical degrees of freedom we should only expect two independent dynamical equations. In fact, investigations by one of us[22] of the Bondi—Sachs

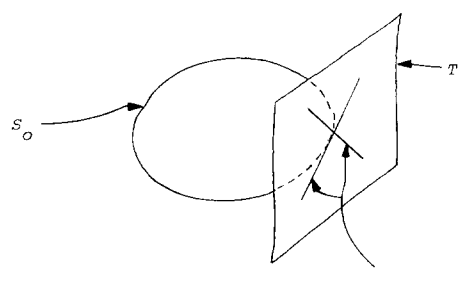


FIG. 6. The spacelike 2-surface S_0, and an orthogonal 2-plane element T.

characteristic initial-value problem demonstrated that in this case it is precisely the conformal 2-structure that generates the true dynamical equations. This suggests that instead of considering the three-plus-one breakup of the field equations, as above, we consider a two-plus-two breakup,[23] in the hope that we may be able to cope with all the various initial value problems simultaneously.

We therefore consider a spacelike 2-surface S_0 and a field of timelike 2-plane elements orthogonal to S_0 at each point of it (see Fig. 6), spanned by two vector fields

$$\underset{\hat{X}}{e^{\mu}} \quad (X=0,1)$$

whose character depends on the type of initial value problem under consideration. We can then continue these vector fields off S_0 and use the resulting four-dimensional family of vector fields to drag the initial 2-surface and fill out some four-dimensional region. If the two vector fields are chosen so that their Lie bracket vanishes, the order of the dragging will be immaterial. We now project the metric $g^{\mu\nu}$ into S_0 to obtain

$$g^{\mu\nu} = {}''g^{\mu\nu} + g^{\hat{X}\hat{Y}} \underset{\hat{X}}{e^{\mu}} \underset{\hat{Y}}{e^{\nu}} \quad (\hat{X},\ \hat{Y}=0,1), \tag{6.4}$$

where $''g^{\mu\nu}$ is the 2-metric induced on S_0. Then variation of the Einstein Lagrangian with respect to $''g^{\mu\nu}$ will generate three equations and variation with respect to $\underset{\hat{X}}{e^{\mu}}$ will generate seven linearly independent equations. We next separate out a conformal factor γ from $''g^{\mu\nu}$,

$$''g^{\mu\nu} = \gamma \bar{g}^{\mu\nu}, \quad |\bar{g}^{AB}| = 1 \tag{6.5}$$

such that the resulting $\bar{g}^{\mu\nu}$ is the conformal 2-structure. If we now consider variations with respect to $\bar{g}^{\mu\nu}$ and γ separately, then, in adapted coordinates, we find

$$\delta\bar{g}^{AB} \rightarrow G_{AB} - \tfrac{1}{2}\bar{g}_{AB}\bar{g}^{CD}G_{CD} = 0, \tag{6.6}$$

$$\delta\gamma \rightarrow \bar{g}^{AB}G_{AB} = 0. \tag{6.7}$$

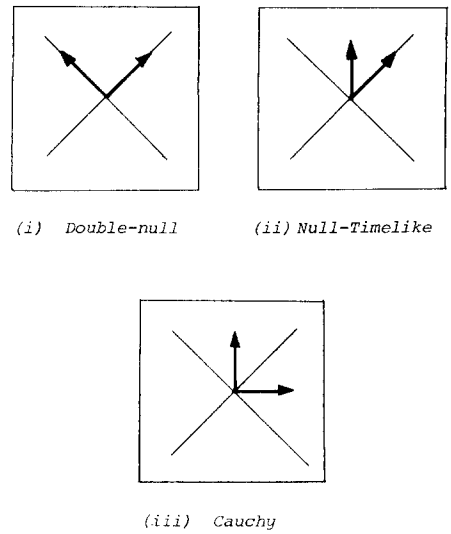
Of course, (6.6) only consists of two independent equations, as contraction with $\bar{g}^{AB}$ reveals. Then in each of the three types of initial value problems we have considered in this paper, we find that the equations (6.6) are precisely the dynamical equations for the evolution of the conformal 2-structure. That is, the only terms involving second derivations in the $e^{\mu}_{\hat{0}}, e^{\mu}_{\hat{1}}$ directions which occur in (6.6) are of the form

$$g^{\hat{X}\hat{Y}} L_{\underset{\hat{X}}{e}} L_{\underset{\hat{Y}}{e}} \bar{g}_{AB}.$$

Indeed, for the appropriate choice of vector fields (see Fig. 7) we find, in adapted (possibly anholonomic) coordinates at any point that the only terms involving second derivatives with respect to 0, 1 coordinates which occur in (6.6) in the three cases are

(1) Double-Null: In this case $\underset{\hat{X}}{e^{\mu}}$ are both null vectors, and

$$g^{\hat{X}\hat{Y}} \overset{*}{=} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$



(i) Double-null (ii) Null-Timelike

(iii) Cauchy

FIG. 7. The two dragging fields e^{μ} for each of the three initial value problems.

where $\overset{*}{=}$ means that an equation holds in adapted coordinates; the only second derivative with respect to 0, 1 which occurs in (6.6) is $\bar{g}_{AB,01}$.

(2) Null-timelike: In this case, $\underset{\hat{0}}{e^{\mu}}$ is timelike and $\underset{\hat{1}}{e^{\mu}}$ is null, and

$$g^{\hat{X}\hat{Y}} \overset{*}{=} \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix};$$

the combination of second derivatives with respect to 0, 1 which occurs in (6.6) is $2\bar{g}_{AB,01} - \bar{g}_{AB,11}$.

(3) Cauchy: In this case, $\underset{\hat{0}}{e^{\mu}}$ is timelike and $\underset{\hat{1}}{e^{\mu}}$ spacelike, and

$$g^{\hat{X}\hat{Y}} \overset{*}{=} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

the only combination of second derivatives with respect to 0, 1 which occur in (6.6) is $\bar{g}_{AB,00} - \bar{g}_{AB,11}$. Reference to the Appendix will show that this is just the form the two-dimensional wave operator should take in each case.

These preliminary results suggest that it is possible to pursue this two-plus-two breakup further and eventually unify all the various approaches to the initial value problem. One of us (J.S.), with another collaborator (Mr. Ben Rosen), has pursued this approach further, and investigated the full two-plus-two breakup of the ten field equations. The results of this study will be published elsewhere.

7. CONCLUSION

General relativity is a gauge theory and hence, in common with other gauge theories, it possesses the property that the potentials (or various concomitants of them) are not uniquely determined by the physical

field but rather, by virtue of the gauge group, the information about this field may reside in the potentials in a variety of ways. Our thesis, in this paper, is that by an appropriate choice of coordinate system, the minimal information which determines a solution of the Einstein (vacuum) field equations, that is the gravitational degrees of freedom, may be cast into that part of the metric tensor which we have termed the conformal 2-structure. We have shown, at least formally, that this prescription works in the cases of the exact solutions for plane and cylindrical gravitational waves, the Sachs investigation of the double-null characteristic initial value problem, the Bondi—Sachs and Tamburino—Winicour investigations of the null-timelike characteristic initial value problems, and the usual spacelike Cauchy problem. We have also suggested that this may herald a new unifying approach to all the various initial value problems, namely by considering a two-plus-two breakup of the field equations.

There are, however, considerable limitations to that which we have undertaken so far. As we have discussed before, our analysis is purely formal and, apart from the rather restricted case of analytic solutions, we have really only considered the question of uniqueness. The deeper, and more difficult, questions of existence and stability remain yet to be investigated and indeed further analysis may reveal that this approach does not in fact lead to a well-posed problem (at least in all cases). For example, as we have already pointed out, there appear to be considerable problems attached to the Tamburino —Winicour type of analysis. Nonetheless, our work so far suggests, at the very least, that this approach may well be worth pursuing further. One major task then would be to investigate the equations (I), (II), and (III) of Sec. 5 to determine, for example, whether or not they can be cast into an elliptic form and thereby attack the questions of existence and stability for the case of the Cauchy problem. Closely related to this are problems of a global topological nature: For example, do we require a global foliation or can we proceed with anholonomic 2-surface elements? In the case of the three-plus-one decomposition for the formulation of the Cauchy problem it is known that anholonomic three-surface elements and a vector field with nonvanishing curl may be used (see work of Ó Murchadha and Kulhanek).[24,25] There is every reason to expect that similar anholonomic extensions of the two-plus-two approach will be possible. This subject is under study. Another interesting global problem would be the consideration of solutions with closed spatial 3-surfaces, to see whether our approach could succeed there.

There are also interesting possibilities for considering other types of initial value problems. Our consideration of the Cauchy problem has been purely local, of course, and confined to consideration of a purely spatial bounding hypersurface. Yet the singling out of an initial 2-surface on such a hypersurface in our approach suggests a very natural extension of our approach to the consideration of a mixed problem, in which data would be given on the spacelike exterior of the initial 2-surface as well as a timelike tube of which the initial 2-surface was a cross section (see Fig. 8). One would conjecture, on the basis of the discussion of the Cauchy and null-like initial value problems in this paper (as well as the mixed problem for the one-dimensional wave equation discussed in the Appendix), that the conformal 2-structure and its Lie derivative in the normal direction would have to be given on the spacelike portion of the boundary, as well as the conformal two structure on the timelike tube, to uniquely determine a solution in the region they bound (see Fig. 8).[21]

There is also the question of how this work relates to other approaches, notably the "conformal 3-geometry" approach, first suggested by Lichnerowicz[26] and Choquet,[27] and brought to considerable fruition by York and Ó Murchadha[28] among others. There is no doubt that their approach is both very elegant and successful; for example, they have some very powerful theorems governing existence and stability. However, we feel that the conformal 2-structure approach is still worth pursuing because of its possible unifying property; more specifically, because it appears to also apply to (indeed is perhaps better suited to them) characteristic initial

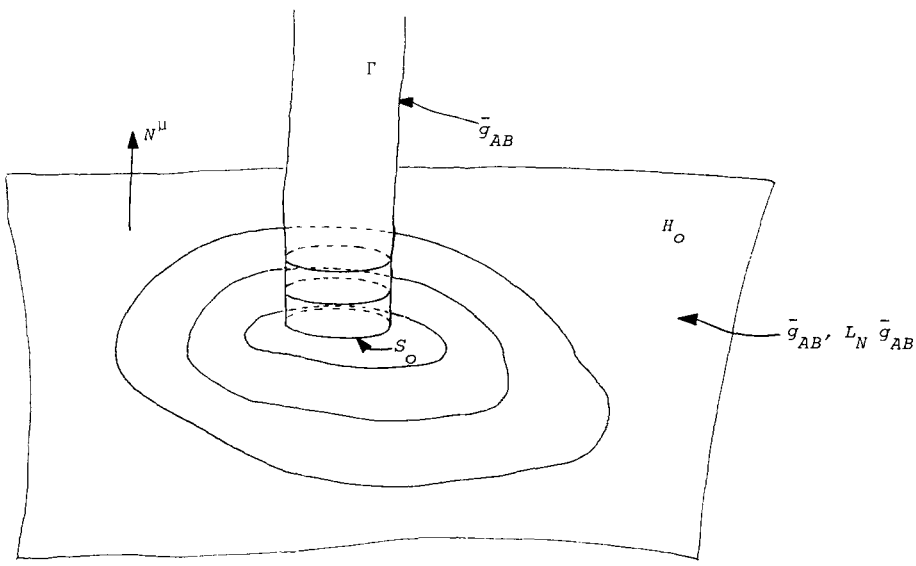


FIG. 8. Conjectured initial data for the mixed initial value problem.

value problems; whereas the conformal 3-geometry approach does not seem capable of such an extension, since there is no Riemannian 3-geometry or conformal 3-geometry on a null hypersurface. There is certainly nothing wrong with the conformal 3-geometry approach, but it does fix attention on a feature which is more reminiscent of nonrelativistic theories, i.e., Galilean-type theories with naturally preferred spacelike hypersurfaces. We would suggest that null hypersurfaces are more characteristic (pun intended) of relativistic theories than spacelike hypersurfaces; and therefore there may be some advantage to an approach which can handle null surfaces. Another lesser point is the practical one that, for some classes of solutions, one may often readily identify the conformal 2-structure but not be able to solve the partial differential equations needed to isolate the two degrees of freedom of the conformal three-geometry approach.

Perhaps the biggest outstanding problem relates to the question of the possible quantization of general relativity. Opinions differ as to the physical significance of such a step, but presumably, to achieve this mathematically, one needs to formulate the problem correctly. Conformal 3-geometry seems to suggest the use of superspace (or some restriction of it), which is once more a generalization of the quantum approach to special relativistic field theories in which the evolution of waves from one spacelike hypersurface to another is singled out—which again seems to stress the features of the theory more closely related to those of nonrelativistic theories. More recently, a good deal of attention has been focused on approaches to quantum field theory which single out families of null hypersurfaces and examine the dynamics with respect to these hypersurfaces. Again, this suggests the possible advantage of an approach to general relativity which enables one to consider null hypersurfaces naturally. Moreover, scattering experiments, which are our main source of information about elementary particles, can be idealized by imagining the target to be surrounded with detectors, which then count for some period of time. This means, of course, that in the relativistic theory they give us data on a timelike world tube (and even in the nonrelativistic theory not on a spacelike hypersurface). Thus, a formalism which can readily handle data on timelike hypersurfaces might be expected to be generally useful in quantum theory.

In at least one approach to quantization one needs the two degrees of freedom of the gravitational field isolated (i.e., with the constraints eleminated); and, as Ashtekar and Geroch have emphasized,[29] it is not enough to have the phase space of the classical canonical variables. One needs to have this phase space as a cotangent bundle over a configuration space in order to apply the canonical quantization procedure. It is natural to hope that in general relativity that "properly" chosen variables (assuming that such variables exist) will have a simple geometrical meaning even in this case. It seems worth investigating whether the conformal 2-structure, and their Lie derivatives or "velocities," can provide such a natural configuration space for the gravitational field, since they have such a local geometrical significance.

ACKNOWLEDGMENTS

This paper has had a long history, which began when one of us (J.S.) was on sabbatical leave at King's College, London, where the other was a doctoral student. The basic ideas were worked out then (1970—71), and each of us has since given talks based on the material. A first draft was written while one of us (J.S.) was guest of the Département de Mécanique Théorique of Paris VI in 1974; a second during the sabbatical of the other (1977). We have thus incurred numerous obligations for which we here express our thanks, notably to Professor Felix Pirani and Professor Yvonne Choquet as hosts, and to the Relativity Seminars they conduct where earlier versions of this work were reported.

APPENDIX

We shall consider briefly in this Appendix the one-dimensional scalar wave equation, which serves as a simple prototype for illustrating various types of initial value problems.[30] The one-dimensional wave equation ($c=1$) is

$$\phi_{,tt}-\phi_{,xx}=0, \tag{A1}$$

where $\phi=\phi(t,x)$, and it admits as general solution the *d'*Alembert solution

$$\phi=f(u)+g(v), \tag{A2}$$

where

$$u=t-x, \tag{A3}$$

$$v=t+x, \tag{A4}$$

and f and g are arbitrary functions. Using this result we can write down the general solution in a two-dimensional region R (see Fig. 9), in terms of the initial data, for the three sorts of initial value problem considered in this paper, as follows:

(1) Double-null: $\phi_{,uv}=0$,

Initial data:

$\phi=\psi(u)$ on $v=v_0$ $(u\geq u_0)$

$\phi=\chi(v)$ on $u=u_0$ $(v\geq v_0)$ with $\chi(v_0)=\psi(u_0)$.

General solution:

$\phi(u,v)=\psi(u)+\chi(v)-\psi(u_0)$ $(u\geq u_0,\ v\geq v_0)$.

(2) Winicour—Tamburino (null-timelike): $2\phi_{,ux}-\phi_{,xx}=0$

Initial data:

$\phi=\psi(u)$ on $x=x_0$ $(u\geq u_0)$

$\phi=\chi(x)$ on $u=u_0$ $(x\geq x_0)$ with $\chi(x_0)=\psi(u_0)$

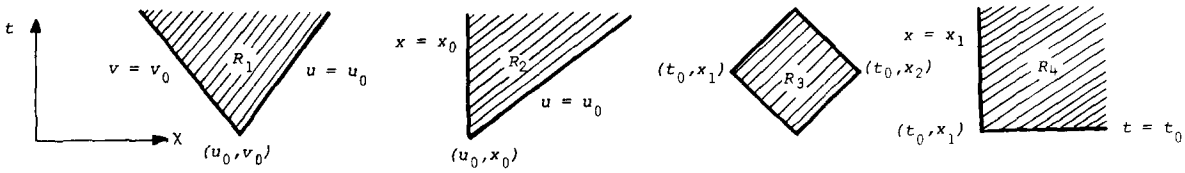
General solution:

$$\phi(u,x)=\chi[x+\tfrac{1}{2}(u-u_0)]-\chi[x_0+\tfrac{1}{2}(u-u_0)]+\psi(u)$$
$$(u\geq u_0,\ x\geq x_0).$$

(3) Cauchy: $\phi_{tt}-\phi_{,xx}=0$ We first consider the finite Cauchy problem.

Initial data:

$\phi=\psi(x)$ on $t=t_0$ $(x_1\leq x\leq x_2)$



(i) Double-Null (ii) Null-Timelike (iii) Finite Cauchy (iv) Mixed Problem

FIG. 9. The region R for each of the four initial value problems.

$\phi_{,t} = \chi(x)$ on $t = t_0$ $(x_1 \leq x \leq x_2)$.

General solution:

$$\phi(x,t) = \tfrac{1}{2}[\psi(x+t-t_0) + \psi(x-t+t_0)] + \tfrac{1}{2}\int_{x-t+t_0}^{x+t-t_0} \chi(x)dx$$

$$(t_0 - x_1 \leq t - x \leq t_0 - x_2,\ t_0 + x_1 \leq t + x \leq t_0 + x_2).$$

The solution is only determined by the data in the region shown in Fig. 9(iii). The infinite Cauchy problem follows by taking the limits $x_1 \to -\infty$, $x_2 \to +\infty$. Note the way in which the initial data "doubles" in the Cauchy problem as compared to characteristic initial value problems.

Thus, appart from the fact that the scalar wave equation has only one degree of freedom, the number of functions which may be specified freely as initial data for each of the problems considered is entirely analogous to the number required for the Einstein vacuum field equations.

We may also consider a fourth type of problem, not discussed so far for the Einstein equations as far as we know

(4) Mixed Cauchy and timelike boundary problem

Initial data on spacelike part of boundary:

$\phi = \psi(x)$ on $t = t_0$ $(x_1 \leq x \leq \infty)$,

$\phi_{,t} = \chi(x)$ on $t = t_0$ $(x_1 \leq x \leq \infty)$,

Data on timelike part of boundary:

$\phi = \lambda(t)$ on $x = x_1$ $(t_0 \leq t \leq \infty)$.

This is seen to break up into a semi-infinite Cauchy problem plus a Winicour—Tamburino type problem [see Fig. 9(iv)]. In this sense it offers nothing new; but physically it is clearly a well-posed problem, as the example of a half-infinite string shows: To determine the future behavior of such a string, its initial position and velocity must be given, as well as the motion of the end point for all times after the initial time.

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Effective Lagrangian in spontaneously broken gauge theories

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In gauge theories of weak and electromagnetic interactions, it is generally assumed that the addition of extra groups [simple or U(1)] commuting with the standard Weinberg–Salam SU(2)⊗U(1) group, generates new degrees of freedom for the model, simply because there are new coupling constants in the game. This assertion is not true in general. When looking at the effective Lagrangian of the physical system ($-q^2$ much smaller than any mass of the massive vector bosons), we see that a coupling constant completely disappears if the generators of its corresponding group do not enter in any surviving unbroken subgroup [U(1) for Weinberg–Salam model]. In those cases, the novelties are provided only by the quantum numbers of the fields and especially by the arbitrariness on the choice of "unphysical" Higgs fields. This effective Lagrangian is defined and constructed in the case where the initial and final symmetry groups are direct products of simple groups and U(1) groups. Some of its remarkable properties are investigated.

INTRODUCTION

The mechanism leading to the spontaneous breakdown of a gauge symmetry in a field theory[1] is well known by most of the theoreticians working in elementary particles. In particular, everyone knows the form of the fundamental Lagrangian of the gauge theories and the procedure to obtain the Lagrangian for the broken theory. But at present state of experiments, this fundamental Lagrangian has no direct use for phenomenologists who need what we will call an effective Lagrangian.

This effective Lagrangian has a part of the type current×current which is constructed by taking the second-order processes occuring with the exchange of a massive vector boson and by supposing that we always make experiments where the transferred momentum $-q^2$ is much smaller than any of the masses of those massive vectors.

In this work, we apply ourselves to construct this effective Lagrangian.

In a first stage, we shall give the definitions of the coupling constants of the broken theory constructed with the old ones. There are two types of new coupling constants (Sec. VI, §14). They couple the conserved currents to the zero mass vector bosons. Those of the second type are all in the form $\cos^2\Psi$(Sec. VI, §15). They appear only in the part of L_{eff} which is due to the massive vector bosons.

In a second stage we construct the currents which are coupled to the massive vector bosons (Sec. VIII). They are combinations of well-known quantities (initial generators): The coefficients of the combinations are the $\cos^2\Psi$'s which were constructed previously.

Finally (Sec. IX) we give the effective Lagrangian: It is obtained by the diagonalization of a matrix constructed with the "unconserved" currents defined in Sec. VIII. In Sec. X we draw the conclusions which are based on the properties of this effective Lagrangian:

(a) the electromagnetic-like coupling constants appear only in the part of L_{eff} due to the zero mass vector bosons.

(b) In the other part of L_{eff}, all coupling constants have disappeared except the $\cos^2\Psi$'s.

(c) Some initial coupling constants have completely disappeared from the game.

(d) There is a kind of scaling for L_{eff}: The physical results are dependent only on the ratios of quantum numbers of the fields [or the matrix elements of the generators].

I. NOTATIONS

We are interested in a spontaneously broken gauge theory based on the symmetry group G which is a direct product of n simple groups $S_{(i)}$ and r groups $U(1)$; we shall denote them $U_{(j)}$:

$$G = S_{(1)} \otimes S_{(2)} \otimes \cdots \otimes S_{(n)} \otimes U_{(1)} \otimes \cdots \otimes U_{(r)}.$$

The physical problem is described by a basic interaction Lagrangian constructed with multiplets of physical fields—(a) the Dirac spinors $\Psi_{(\alpha)}(x)$ transforming under a global gauge transformation under irreducible representation of G (generally the lowest faithful one);

(b) one multiplet of vector bosons transforming under the adjoint representation of G. The number of its constituents is equal to the dimension of G—
and multiplets of "unphysical" fields—

(c) the scalar Higgs fields $\phi_\beta(x)$ grouped into one big multiplet $\phi(x)$ transforming under a generally reducible representation of G. We list here the mathematical quantities which will be used in the text.

For each simple group $S_{(a)}$:

d_a is the dimension of the group;

$G^{i}_{(a)}$ are the infinitesimal generators ($i=1,\ldots,d_a$);

$g^{(a)}_{ijk}$ are the completely antisymmetric structure constants (the metric of the group is proportional to the unit matrix);

$A^{i}_{(a)\mu}$ are the vector bosons;

$g_{(a)}$ is a coupling constant.

In the same manner, we define for $U_{(a)}$:

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$G_{(a)}$ the infinitesimal generator,

$A_{(a)\mu}$ the vector boson,

$g'_{(a)}$ the coupling constant.

The symmetry of the Lagrangian under the local gauge transformations of G will be broken by a Higgs–Brout–Englert mechanism[2] in such a way that the Lagrangian will still be invariant under local gauge transformations of a gubgroup H of G.

We will restrict ourselves to a subgroup H of G which has the same structure as G, a direct product of m simple groups $S'_{(i)}$ and of s groups $U(1)$ noted $U'_{(j)}$.[3]

$$H = S'_{(1)} \otimes \cdots \otimes S'_{(m)} \otimes U'_{(1)} \otimes \cdots \otimes U'_{(s)}$$

We list here the notations which will be useful: for $S'_{(a)}$,

d'_a is the dimension of the group;

$H^i_{(a)}$ are the infinitesimal generators $(i=1,\ldots,d'_a)$;

$h^{(a)}_{ijk}$ are the completely antisymmetric structure constants (the metric is again taken as proportional to the unit matrix);

$B^i_{(a)\mu}$ are the vector bosons;

$h_{(a)}$ is the coupling constant;

while for $U'_{(a)}$,

$H_{(a)}$ is the infinitesimal generator;

$B_{(a)\mu}$ is the vector boson;

$h'_{(a)}$ is the coupling constant.

II. REVIEW OF GAUGE THEORIES

We start with the basic interaction Langrangian L. It is invariant under local gauge transformations of G:

$$L = -\frac{1}{4}\sum_{a\mu\nu} \mathrm{Tr}\{A^{(a)}_{\mu\nu}, A^{(a)\mu\nu}\} - \frac{1}{4}\sum_{a\mu\nu} A'^{(a)}_{\mu\nu} A'^{(a)\mu\nu} + i\sum_{\alpha\mu} \bar{\Psi}_{(\alpha)}\gamma^\mu D_\mu \Psi_{(\alpha)} + \sum_\mu (D^\mu\phi)^*(D^\mu\phi) + V(\phi),$$

where

$$A^{(a)}_{\mu\nu} = \partial_\mu A^{(a)}_\nu - \partial_\nu A^{(a)}_\mu - i g_{(a)}[A^{(a)}_\mu, A^{(a)}_\nu].$$

The $A^{(a)}_\mu$ are constructed with the adjoint representation of $S_{(a)}$:

$$A^{(a)}_\nu = \sum_i A^i_{(a)\nu} G^i_{(a)}, \quad \mathrm{Tr}(G^i_{(a)})^2 = 1,$$

$$A'^{(a)}_{\mu\nu} = \partial_\mu A_{(a)\nu} - \partial_\nu A_{(a)\mu},$$

$$D_\mu\chi = \partial_\mu\chi + i\sum_a g_{(a)} \sum_i (G^i_{(a)}\chi) A^i_{(a)\mu} + i\sum_a g'_{(a)}(G_{(a)}\chi) A_{(a)\mu}.$$

$V(\phi)$ is a quartic polynomial of ϕ invariant under local gauge transformations of G. We now apply the Higgs mechanism, and we try to rewrite L so as to see the local invariance of L under H. ϕ has a nonvanishing vacuum expectation value $\langle\phi\rangle$: $V(\phi)$ has a minimum for $\phi = \langle\phi\rangle \neq 0$. We want a theory describing fields with a vanishing vacuum expectation value. We define $\eta(x) = \phi(x) - \langle\phi\rangle$. Then $\langle\eta\rangle = 0$.

We write L in terms of $\eta(x)$ instead of $\phi(x)$. The terms $(D^\mu\phi)^*(D_\mu\phi) + V(\phi)$ are replaced by

$$(D^\mu\eta)^*(D_\mu\eta) + (D^\mu\eta)^*(D_\mu\langle\phi\rangle) + (D^\mu\langle\phi\rangle)^*(D^\mu\eta) + (D^\mu\langle\phi\rangle)^*(D_\mu\langle\phi\rangle) + V'(\eta),$$

where $V'(\eta) = V(\eta + \langle\phi\rangle)$.

The fourth term is a mass matrix for the fields $A^i_{(a)\mu}$ and $A_{(a)\mu}$ destroying the local invariance of L under G. It must be diagonalized and the remaining part of the Lagrangian must be rewritten in terms of the eigenstates of the mass matrix.

We obtain then a new Lagrangian which must be proven to be invariant under local gauge transformations of H.

III. DIAGONALIZATION OF THE MASS MATRIX

§1. H is a subgroup of G. The infinitesimal generators of H must be independent linear combinations of the infinitesimal generators of G.

$$H^i_{(a)} = \sum_{jk} G^j_{(k)} \beta^{ji}_{(ka)} + \sum_k G_{(k)} \tilde{\beta}^{\ i}_{(ka)}, \qquad H_{(a)} = \sum_{jk} G^j_{(k)} \beta^j_{(ka)} + \sum_k G_{(k)} \beta_{(ka)}. \tag{1}$$

When we consider a physical problem, the coefficients β are known and given.

§2. H is the little group of invariance of $\langle\phi\rangle$ (generated by all the combinations of the initial generators which annihilate $\langle\phi\rangle$).

$$H^i_{(a)}\langle\phi\rangle = 0, \quad H_{(a)}\langle\phi\rangle = 0. \tag{2}$$

No other independent linear combination of the G's can annihilate $\langle\phi\rangle$. In physical problems, usually G and H are given and in turn ϕ and $\langle\phi\rangle$ constructed in order to have the results (1) and (2).

§3. The vector fields $A^i_{(a)\mu}$ and $A_{(a)\mu}$ are real, thus the mass matrix $\sum_\mu [D^\mu\langle\phi\rangle]^* [D_\mu\langle\phi\rangle]$ is symmetric and its eigenstates are orthogonal combinations of the A's.

§4. Some of the eigenstates of the mass matrix have a null eigenvalue. In order to see this, let us discuss more precisely the mass matrix

$$\sum_\mu (D^\mu\langle\phi\rangle)^* (D_\mu\langle\phi\rangle) = \sum_\mu [A^{i\,\mu}_{(a)}, A_{(a)}{}^\mu] \frac{M^2}{2} \begin{bmatrix} A^i_{(a)\mu} \\ \\ A_{(a)\mu} \end{bmatrix}.$$

Each matrix element of $M^2/2$ is a scalar product of two vectors belonging to the set $\Gamma = \{g_{(a)} G^i_{(a)}\langle\phi\rangle, g'_{(a)} G_{(a)}\langle\phi\rangle\}$.

If we diagonalize $M^2/2$, we have

$$[A]^t \frac{M^2}{2}[A] = ([A]^t O)(O^t \frac{M^2}{2} O)(O^t[A]) = (O^t[A])^t \frac{\tilde{M}^2}{2}(O^t[A])$$

with $\tilde{M}^2/2$ a diagonal matrix. Each of its diagonal elements is the squared norm of a vector belonging to the set Γ'.

$$\Gamma' = \{\sum_j \gamma_j O_{ji} \,|\, \gamma_i \in \Gamma\}$$

Proof:

$$(\tilde{M}^2/2)_{ii} = \sum_{jk} O^t_{ij}(\gamma_j, \gamma_k) O_{ki} = (\sum_j \gamma_j O_{ji}, \sum_k \gamma_k O_{ki})$$
$$= \left|\left| \sum_k \gamma_k O_{ki} \right|\right|^2.$$

One obtains a null eigenvalue if and only if the vector $\sum_j \gamma_j O_{ji}$ is the null vector. This means that $\sum_j \gamma_j O_{ji}$ is a linear combination of the generators of H applied on $\langle\phi\rangle$.

The preceeding points §1 and §2 ensure us that the number of null eigenvalues is exactly the number of generators of H.

Going from the kinetic part of the initial Lagrangian for the fields A to the kinetic part for the vector fields B in the broken Lagrangian, one sees that the B's must be orthogonal combinations of the A's. The eigenstates of the mass matrix being also orthogonal combinations of the A's, we have the result that the eigenstates having an eigenvalue zero are orthogonal combinations of the vectors $B^i_{(a)}$ and $B_{(a)}$.

§5. All other states having an eigenvalue different from zero are noted $C_{(i)}$. We shall use the following notations for the matrix of orthogonalization O:

$$A^i_{(a)} = \sum_{jm} O^{ij}_{(am)} B^j_{(m)} + \sum_m O^i_{(am)} B_{(m)} + \sum_m \tilde{\tilde{O}}^i_{(am)} C_{(m)},$$
$$A_{(a)} = \sum_{jm} \tilde{O}^{\ j}_{(a\,m)} B^j_{(m)} + \sum_m O_{(am)} B_{(m)} + \sum_m \tilde{\tilde{O}}_{(am)} C_{(m)}. \quad (3)$$

IV. THE "BROKEN" LAGRANGIAN

§6. The nonkinetic part of the Lagrangian is constructed with expressions $D_\mu\chi$, where χ is any field $A_\mu, \Psi_{(\alpha)}, \eta$. We have just to look to these expressions written in terms of new vector fields B and C. Using (3)

$$D_\mu\chi = \partial_\mu\chi + i \sum_{iajm} [g_{(a)} G^i_{(a)} O^{ij}_{(am)} + g'_{(a)} G_{(a)} \tilde{O}^{\ j}_{(a\,m)}]\chi\, B^j_{(m)\mu}$$
$$+ i \sum_{iam} [g_{(a)} G^i_{(a)} O^i_{(am)} + g'_{(a)} G_{(a)} O_{(am)}]\chi\, B_{(m)\mu}$$
$$+ i \sum_{iam} [g_{(a)} G_{(a)} \tilde{\tilde{O}}_{(am)} + g'_{(a)} G_{(a)} \tilde{\tilde{O}}_{(am)}]\chi\, C_{(m)\mu}. \quad (4)$$

§7. The part proportional to $C_{(m)}$ is noted

$$i \sum_m K_{(m)}\chi C_{(m)}.$$

Thus we have for $D_\mu\chi$

$$D_\mu\chi = D'_\mu\chi + i \sum_m K_{(m)}\chi\, C_{(m)\mu}.$$

The local invariance under H is achieved by imposing that the two parts separately transform as χ does.

§8. The correct transformation of $D'_\mu\chi$ is obtained if

$$D'_\mu\chi = \partial_\mu\chi + i \sum_{ai} h_{(a)} H^i_{(a)}\chi\, B^i_{(a)\mu} + i \sum_a h'_{(a)} H_{(a)}\chi\, B_{(a)\mu}.$$

By comparing with (4), we have the equalities

$$\sum_{ia} g_{(a)} G^i_{(a)} O^{ij}_{(am)} + \sum_a g'_{(a)} G_{(a)} \tilde{O}_{(a\,m)}^{\ \ j}$$
$$= h_{(m)} H^j_{(m)},$$
$$\sum_{ia} g_{(a)} G^i_{(a)} O^i_{(am)} + \sum_a g'_{(a)} G_{(a)} O_{(am)}$$
$$= h'_{(m)} H_{(m)}. \quad (5)$$

§9. With all these substitutions we obtain for the broken Lagrangian

$$L = -\tfrac{1}{4} \sum_{I\mu\nu} \mathrm{Tr}\{B^{(I)}_{\mu\nu}, B^{(I)\mu\nu}\} - \tfrac{1}{4} \sum_{I\mu\nu} B'_{(I)\mu\nu} B'^{\mu\nu}_{(I)}$$
$$- \tfrac{1}{4} \sum_{i\rho\nu} C_{(i)\rho\nu} C^{\rho\nu}_{(i)} + i \sum_{\alpha\mu} \overline{\Psi}_{(\alpha)} \gamma^\mu D'_\mu \Psi_{(\alpha)}$$
$$- \sum_{\alpha m\mu} \overline{\Psi}_{(\alpha)} \gamma^\mu K_{(m)} \Psi_{(\alpha)} C_{(m)\mu} + \sum_\mu (\partial^\mu\eta)^*(\partial_\mu\eta)$$
$$+ V'(\eta) + I(\eta, B_\mu, C_\mu),$$

where I is a quartic polynomial describing the interaction between η, B_μ and C_μ.

V. THE DIAGONALIZATION MATRIX: "SOME RESTRICTIONS" ON THE DEFINITION OF THE SUBGROUP

§10. In all these developments we are interested in the definitions of the new coupling constants $h_{(m)}$ and $h'_{(m)}$ and also of the matrices $K_{(m)}$, giving the coupling of the massive vector bosons to the currents $\overline{\Psi}_{(\alpha)i}\gamma_\mu\Psi_{(\alpha)j}$.

In order to do this, we exploit the relations (5). By replacing there $H^j_{(m)}$ and $H_{(m)}$ by the expressions (1), we obtain the following identities:

$$O^{ij}_{(am)} = \frac{h_{(m)}}{g_{(a)}} \beta^{ij}_{(am)}, \quad O^i_{(am)} = \frac{h'_{(m)}}{g_{(a)}} \beta^i_{(am)},$$
$$\tilde{O}_{(a\,m)}^{\ \ j} = \frac{h_{(m)}}{g'_{(a)}} \tilde{\beta}_{(a\,m)}^{\ \ j}, \quad O_{(am)} = \frac{h'_{(m)}}{g'_{(a)}} \beta_{(am)} \quad (6)$$

[i, a are indices referring to the groups $S_{(a)}$ $(i = 1, \ldots, d_a)$ [or $U_{(a)}$); j, m are indices referring to the subgroup $S'_{(j)}$ $(j = 1, \ldots, d'_m)$ [or $U'_{(m)}$)].

Those relations can mean some restrictions on the coefficients β defining the subgroup H. We shall see that it is not the case.

§11. We shall prove the following identities in the next paragraph. After each identity, we discuss its meaning:

(a) $\tilde{\beta}_{(a\,m)}^{\ \ j} = 0$: No generators of $U_{(a)}$ can enter in the definition of a generator of $S'_{(m)}$.

(b) $\sum_j \beta^{ji}_{(am)} \beta^{jk}_{(an)} = \delta^n_m\, \delta^i_k\, \lambda^2_{am}$:

—When a generator of one $S_{(a)}$ has been used for the construction of one $S'_{(m)}$, it cannot be used in another $S'_{(n)}$;

—a matrix $\beta_{(an)}$ can be different from zero only if $S'_{(n)}$ is a subgroup of $S_{(a)}$; then by a choice of the generators, $\beta_{(an)}$ is proportional to the unit matrix of dimen-

sion d'_n completed with $(d_a - d'_n)$ lines of zeros; the coefficient of proportionality is λ_{an}.

(c) $\sum_i \beta^i_{(am)} \beta^{ij}_{(ak)} = 0$: When a generator of $S_{(a)}$ has been used in the construction of $S'_{(k)}$ it cannot be used again in the construction of $S'_{(k)}$ it cannot be used again in the construction of $U'_{(m)}$.

(d) By a choice of the generators in the center C_k of $S_{(k)}$ and the generators of $U_{(a)}$ and of $U'_{(m)}$, we claim that it is possible to have

$$\sum_i \beta^i_{(km)} \beta^i_{(kn)} = \lambda^2_{k(m)} \delta^n_m$$

and

$$\beta_{(am)} \beta_{(an)} = \lambda^2_{(a)(m)} \delta^n_m.$$

When a generator of $S_{(k)}$ or $U_{(a)}$ has been used for the construction of $U'_{(m)}$, it cannot be used again for the construction of $U'_{(n)}$.

§12. The proof is made using the commutation relations[4]:

$$[H^i_{(p)}, H^j_{(n)}] = \delta^n_p \sum_k h^{(p)}_{ijk} H^k_{(p)},$$

$$[H^i_{(p)}, H_{(n)}] = 0,$$

$$[H_{(p)}, H_{(n)}] = 0.$$

The three relations lead to

$$\sum_{ab} g^{(m)}_{abc} \beta^{ai}_{(mp)} \beta^{bj}_{(mp)} = \sum_k h^{(p)}_{ijk} \beta^{ck}_{(mp)}, \tag{7}$$

$$\sum_{ab} g_{(m)abc} \beta^{ai}_{(mp)} \beta^{bj}_{(mn)} = 0 \quad (p \neq n), \tag{8}$$

$$\sum_k h^{(p)}_{ijk} \tilde{\beta}^{\ k}_{(mp)} = 0, \tag{9}$$

$$\sum_{ab} g^{(m)}_{abc} \beta^{ai}_{(mp)} \beta^{b}_{(mn)} = 0, \tag{10}$$

$$\sum_{ab} g^{(m)}_{abc} \beta^{ai}_{(mp)} \beta^{b}_{(mn)} = 0. \tag{11}$$

(a) Relation (9) implies $\tilde{\beta}^{\ k}_{(mp)} = 0$.

(b) Multiplying (7) by $\beta^{cd}_{(mn)}$ and using (8) $(n \neq p)$, we have

$$\sum_{ck} h^{(p)}_{ijk} \beta^{ck}_{(mp)} \beta^{cd}_{(mn)} = 0.$$

This implies the first part of §11 (b). Multiplying (7) by $\beta^{cd}_{(mp)}$, we obtain

$$\sum_{abc} g^{(m)}_{abc} \beta^{ai}_{(mp)} \beta^{bj}_{(mp)} \beta^{cd}_{(mp)} = \sum_{kc} h^{(p)}_{ijk} \beta^{ck}_{(mp)} \beta^{cd}_{(mp)}.$$

The first term is a completely antisymmetric tensor in the group $S'_{(p)}$. For a simple group there is only one completely antisymmetric tensor which can be constructed. This means $\sum_c \beta^{ck}_{(mp)} \beta^{cd}_{(mp)} = \lambda^2_{mp} \delta^{kd}$, and we have proven the second part of §11(b). (c) Multiplying (7) by $\beta^{c}_{(mn)}$ and using (10), we have

$$\sum_{ck} h_{ijk} \beta^{ck}_{(mp)} \beta^{c}_{(mn)} = 0,$$

which proves relation §11 (c).

§13. We give in Fig. 1 a symbolic resumé of the conclusions of §11 on the matrix β:

(a) A generator of an initial group $S_{(i)}$ or $U_{(j)}$ can be used at most once in the construction of a subgroup or a line of β has at most one element different from zero.

(b) A generator of a final group $S'_{(i)}$ or $U'_{(j)}$ can originate from at least one initial group and must be constructed with at most one generator in each given initial group.

VI. DEFINITIONS OF THE NEW COUPLING CONSTANTS

§14. The electromagnetic-like coupling constants: We see that the columns of β are orthogonal in a very particular manner [§13 (a)]. Thus the orthogonalization of the columns of O defined in § 10 is automatic. We just must be aware of the normalization of the columns. This leads to the definitions of $h_{(k)}$ and $h'_{(k)}$:

$$\frac{1}{h^2_{(k)}} = \sum_a \frac{1}{g^2_{(a)}} \lambda^2_{ak}$$

$$\frac{1}{h'^2_{(k)}} = \sum_a \frac{1}{g^2_{(a)}} \lambda^2_{a(k)} + \sum_a \frac{1}{g'^2_{(a)}} \lambda^2_{(a)(k)}. \tag{12}$$

The summations are taken over the indices with λ_{ak} different from zero.

§15. Other new coupling constants.

First we attach an index k to a subgroup $S'_{(k)}$ and an index (k) to a subgroup $U'_{(k)}$.

For each k, there is a vector normalized to 1 noted $\hat{x}_k$ with $(\hat{x}_k)_i = (h_{(k)}/g_{(i)})\lambda_{ik}$. This vector belongs to R^{n_k} where n_k is the number of λ_{ik} which are different from zero $(n_k \leq n)$.

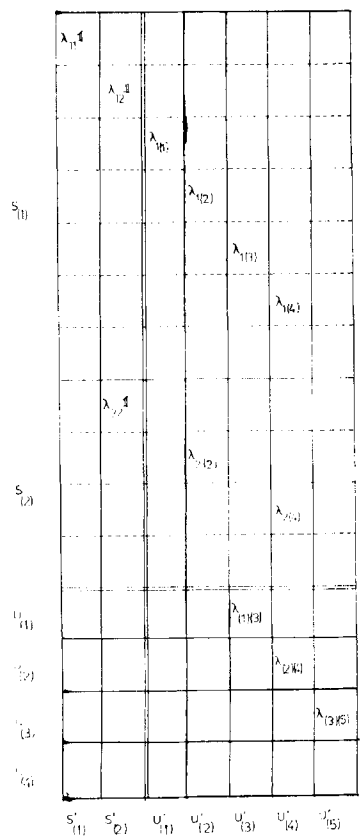

FIG. 1.

We use a recursion procedure to define $n_k - 1$ angles Ψ_{ki} and a system of $n_k - 1$ vectors orthogonal to $\hat{x}_k$ in R^{n_k} [an orthogonal basis of R^{n_k} is $\hat{e}_i$ with $(\hat{e}_i)_j = \delta_{ij}$].

(a) Ψ_{k1} is the angle between $\hat{x}_k$ and $\hat{e}_1$

$$\cos\Psi_{k1} = (\hat{x}_k, \hat{e}_1) = h_{(k)}\lambda_{1k}/g_{(1)}.$$

In the plane $(\hat{x}_k, \hat{e}_1)$ we distinguish two vectors:

—$\hat{x}_k^1$ is the (normalized to 1) projection of $\hat{x}_k$ in the space R^{n_k-1} orthogonal to $\hat{e}_1$:

$$\hat{x}_k^1 = \left(0, \frac{\lambda_{2k}}{g_{(2)}}, \ldots, \frac{\lambda_{nk}}{g_{(n)}}\right) \frac{h_{(k)}}{\sin\Psi_{k1}};$$

—k_1 is the vector (normalized to 1) orthogonal to $\hat{x}_k$ in the plane $(\hat{x}_k, \hat{e}_1)$

$$\hat{k}_1 = -\sin\Psi_{k1}\,\hat{e}_1 + \cos\Psi_{k1}\,\hat{x}_k^1.$$

(b) Knowing Ψ_{ki}, $\hat{k}_i$ and $\hat{x}_k^i$ we define in the plane $(\hat{x}_k^i, \hat{e}_{i+1})$:

$$\Psi_{k,i+1} \text{ by } \cos\Psi_{k,i+1} = (\hat{x}_k^i, \hat{e}_{i+1}),$$

$\hat{k}_{i+1}$ as the (normalized to 1) vector orthogonal to $\hat{x}_k^i$, $\hat{x}_k^{i+1}$ as the (normalized to 1) projection of $\hat{x}_k^i$ on R^{n_k-i-1}, orthogonal to $\hat{e}_1, \hat{e}_2, \ldots, \hat{e}_{i+1}$.

(c) The procedure stops when for $i = n_k$, $\cos\Psi_{ki} = 1$. The procedure is also applied for each index (k). We shall see later that the $\cos\Psi_{ik}$'s play the rôle of new coupling constants.

VII. CONSTRUCTION OF THE ORTHOGONALIZATION MATRIX

§16. We construct an orthogonal matrix V. The first columns of V are the same as those of O. [The matrix $(h/g)\beta$ constructed in §14]. Each of the first columns of O is attached to an index k, with this index we can construct $n_k - 1$ vectors $\hat{k}_i$. For each of the first columns of O, we construct $n_k - 1$ new columns of V by replacing each nonzero element

$$\left(\frac{h}{g}\beta\right)_{jk} = \frac{h_{(k)}}{g_{(j)}}\lambda_{jk}$$

by $(\hat{k}_i)_j$ where $i = 1, \ldots, n_k - 1$ and by keeping zero everywhere else. The same is done for each index (k).

§17. Counting the number of lines of O it is given by $\sum_{k=1}^{n} d_k + r$ But the special form of β says (see §13) that this number is also equal to $\sum_{k=1}^{m} d_k' n_k + \sum_{k=1}^{s} n_{(k)} + n_0$, where n_0 is the number of generators in G which do not contribute to the generators of H. There are $\sum_{k=1}^{m} d_k' + s$ columns in β. We have just constructed with those first columns $\sum_{k=1}^{m} d_k'(n_k - 1) + \sum_{k=1}^{s}(n_{(k)} - 1)$ new columns for V. Thus it remains to define n_0 columns to complete V. For each missing generator of G we construct a column by putting 1 on the line corresponding to this missing generator and by putting zero everywhere else.

§18. Thus we have $p = \sum_{k=1}^{m} d_k'(n_k - 1)\sum_{k=1}^{s}(n_{(k)} - 1) + n_0$ massive vector bosons. The matrix V which has been constructed in §16, 17 is not very different from 0. This last one is obtained by rotating the p last columns of V by an orthogonal matrix of dimension p. We shall note it by $O(p)$.

VIII. CURRENTS COUPLED TO THE MASSIVE VECTOR BOSONS

§19. At this stage we have constructed some orthogonal combinations of the real massive vector bosons $C_{(m)}$. We call them $\tilde{C}_{(i)}$:

$$\tilde{C}_{(m)} = \sum_{i,a} A^i_{(a)}\,\tilde{\tilde{V}}^{\,i}_{(am)} + \sum_a A_{(a)}\,\tilde{\tilde{V}}_{(am)}$$
$$= \sum_k C_{(k)}[O(p)]_{km} \quad [\tilde{\tilde{V}} = \tilde{\tilde{O}}\,O(p)].$$

The matrices V and $O(p)$ were defined in the preceding chapter. They are coupled to the infinitesimal generators of G in the following manner:

$$\sum_m C_{(m)}K_{(m)} = \sum_a \tilde{C}_{(a)}\tilde{K}_{(a)}$$

with

$$\tilde{K}_{(m)} = \sum_{a,i} g_{(a)}\,G^i_{(a)}\,\tilde{\tilde{V}}^{\,i}_{(am)} + \sum_a g'_{(a)}\,G_{(a)}\,\tilde{\tilde{V}}_{(am)}.$$

We are now able to write the elements $\tilde{\tilde{V}}$ in terms of the matrix elements of the matrix β. For each index k referring to a subgroup $S'_{(k)}$ we have the first columns of V given by

$$V^{bj}_{(ak)} = 0^{bj}_{(ak)} = \frac{h_{(k)}}{g_{(a)}}\beta^{bj}_{(ak)} = (\hat{x}_k)_a\,\frac{\beta^{bj}_{(ak)}}{\lambda_{ak}};$$

with each of these columns we find $(n_k - 1)$ new columns of V indicated with i) by

$$\tilde{\tilde{V}}^{\,bj}_{i(ak)} = (k_i)_a\,\frac{\beta^{bj}_{(ak)}}{\lambda_{ak}}, \quad i = 1, \ldots, n_k - 1.$$

This expression leads to the coupling $\tilde{K}^{\,j}_{(ik)}$ for the vector $\tilde{C}^{\,j}_{(ik)}$

$$\tilde{K}^{\,j}_{(ik)} = \sum_{ab} g_{(a)}G^b_{(a)}\,(\hat{k}_i)\,\beta^{bj}_{(ak)}/\lambda_{ak}.$$

Now $(\hat{k}_i)_a = 0$ for $i < a$ (§15). The summation begins at $a = i$. Moreover, this summation is made over the groups $S_{(a)}$ which contribute to $S'_{(k)}$:

$$\tilde{K}^{\,j}_{(ik)} = \frac{g_{(i)}}{\lambda_{ik}}(\hat{k}_i)_i \sum_b G^b_{(i)}\,\beta^{bj}_{(ik)}$$
$$+ \sum_{a=i+1}^{n_k} \frac{g_{(a)}}{\lambda_{ak}}(\hat{k}_i)_a \sum_b G^b_{(a)}\,\beta^{bj}_{(ak)}$$

The construction of $\hat{k}_i$ has been made (§15) such that

$$(\hat{k}_i)_i = -\sin\Psi_{ki},$$

$$(k_i)_a = \cos\Psi_{ki}(\hat{x}_k^i)_a \quad \text{for } n_k \geq a > i.$$

Introducing those definitions and putting in evidence a coupling constant

$$\tilde{K}^{\,j}_{(ik)} = -\frac{g_{(i)}}{\sin\Psi_{ki}\,\lambda_{ik}}\{\sin^2\Psi_{ki}\sum_b G^b_{(i)}\,\beta^{bj}_{(ik)},$$
$$-\sum_{a=i+1}^{n_k}\frac{g_{(a)}}{g_{(i)}}\frac{\lambda_{ik}}{\lambda_{ak}}\sin\Psi_{ki}\cos\Psi_{ki}\,(\hat{x}_k^i)_a\sum_b G^b_{(a)}\,\beta^{bj}_{(ak)}\}$$

But for $i < a \leq n_k$ we can also see that

$$\frac{(\hat{x}_k)_i}{(\hat{x}_k)_a} = \frac{\lambda_{ik} g_{(a)}}{\lambda_{ak} g_{(i)}} = \frac{\cos\Psi_{ki}}{\sin\Psi_{ki}} \frac{1}{(\tilde{x}^i_k)_a}$$

Thus the coupling to $\tilde{C}_{(ik)}^{\ j}$ becomes

$$\tilde{K}_{(ik)}^{\ j} = -\frac{g_{(i)}}{\sin\Psi_{ki}\lambda_{ik}} \{\sin^2\Psi_{ki} \sum_b G^b_{(i)} \beta^{bj}_{(ik)} - \cos^2\Psi_{ki} \sum_{a=i+1}^{n_k} \sum_b G^b_{(a)} \beta^{bj}_{(ak)}\} \tag{13}$$

or

$$\tilde{K}_{(ik)}^{\ j} = -\frac{g_{(i)}}{\sin\Psi_{ki}\lambda_{ik}} \{\sum_b G^b_{(i)} \beta^{bj}_{(ik)} - \cos^2\Psi_{ki} \sum_{a=i}^{n_k} \sum_b G^b_{(a)} \beta^{bj}_{(ak)}\}.$$

For index (k) referring to the subgroup $U'_{(k)}$ we obtain a similar formula,

$$\tilde{K}_{(ik)} = -\frac{g_{(i)}}{\sin\Psi_{(k)i}\lambda_{i(k)}} \{\sum_b G^b_{(i)} \beta^b_{(ik)} - \cos^2\Psi_{(k)i} \times [\sum_{a=i}^{n_k} \sum_b G^b_{(a)} \beta^b_{(ak)} + \sum_a G_{(a)} \beta_{(ak)}]\}, \tag{14}$$

for the coupling to the vector $\tilde{C}_{(ik)} (i = 1, \ldots, n_{(k)} - 1$ is never a U' subgroup index). The n_0 last columns give the couplings to the vectors $\tilde{C}^i_{(a,0)}$ or $\tilde{C}_{(0,a)}$

$$\tilde{K}^i_{(a,0)} = g_{(a)} G^i_{(a)} \text{ or } \tilde{K}_{(0,a)} = g'_{(a)} G_{(a)}. \tag{15}$$

§20. We want to isolate quantities which can play the role of coupling constants, so we write

$$\tilde{K}^{ab}_{(lm)} = k_{(lm)} K'^{ab}_{(lm)} \text{ or, symbolically } \tilde{K}_{(m)} = k_{(m)} K'_{(m)} \tag{16}$$

with the definitions for the four types of couplings given below. When

$$\tilde{K}^{ab}_{(lm)} = \tilde{K}_{(ik)}^{\ j}, \text{ then } k_{(ik)} = -\frac{g_{(i)}}{\sin\Psi_{ki}\lambda_{ik}};$$

$$\tilde{K}^{ab}_{(lm)} = \tilde{K}_{(ik)}, \quad k_{(ik)} = -\frac{g_{(i)}}{\sin\Psi_{(k)i}\lambda_{ik}} \tag{17}$$

$$\tilde{K}^{ab}_{(lm)} = \tilde{K}^j_{(i0)}, \quad k_{(i0)} = g_{(i)};$$

$$\tilde{K}^{ab}_{(lm)} = \tilde{K}_{(0i)}, \quad k_{(0i)} = g'_{(i)}.$$

This leads to a very simple form of the couplings to the massive vector bosons [by comparing (16) and (17) with (13), (14), and (15)]

$$K'_{(ik)}^{\ j} = \sum_b G^b_{(i)} \beta^{bj}_{(ik)} - \cos^2\Psi_{ki} \{\sum_{a=i}^{n} \sum_b G^b_{(a)} \beta^{bj}_{(ak)}\}, \tag{18}$$

$$K'_{(ik)} = \sum_b G^b_{(i)} \beta^b_{(ik)} - \cos^2\Psi_{(k)i} \{\sum_{a=i}^{n} \sum_b G^b_{(a)} \beta^b_{(ak)} + \sum_a G_{(a)} \beta_{(ak)}\}, \tag{19}$$

$$K'^j_{(i0)} = G^j_{(i)} \text{ and } K'_{(0,i)} = G_{(i)}. \tag{20}$$

IX. THE EFFECTIVE LAGRANGIAN

§21. The basic Lagrangian which was written in §9 is of minor interest to phenomenologists. Our final aim is to describe a part of physics which is accessible to the present energies. By this we mean that we restrict ourselves to an effective lagrangian of the type current × current; the massive vector bosons are exchanged with $|q^2|$ negligible with regards to the masses of vector bosons.

The part of the Lagrangian due to the zero mass vector bosons is

$$L^K_{eff} + L^C_{eff} = -\tfrac{1}{4}\sum_l \mathrm{Tr}\{B_{(l)\mu\nu}, B^{\mu\nu}_{(l)}\} - \tfrac{1}{4}\sum_l B'_{(l)\mu\nu} B'^{\mu\nu}_{(l)} + i\bar{\Psi}\gamma^\mu \partial_\mu \Psi - \sum_l h_{(l)} \bar{\Psi}\gamma^\mu H^i_{(l)} \Psi B^i_{(l)\mu} - \sum_l h'_{(l)} \bar{\Psi}\gamma^\mu H_{(l)} \Psi B_{(l)\mu}. \tag{21}$$

By L^K_{eff} we mean the kinetic part of L_{eff} while L^C_{eff} stands for the interaction part with conserved currents. While the interaction part due to the massive vector bosons is defined as

$$L^I_{eff} = (1/\sqrt{2}) \sum_i [\bar{\Psi}\gamma_\mu K(i) \Psi] G_i [\bar{\Psi}\gamma^\mu K_{(i)} \Psi]^+ + \text{h.c.},$$

where $G_i/\sqrt{2} = 1/M_i^2$ is the inverse of the squared mass of $C_{(i)}$

$$M_i^2/2 = [K_{(i)}\langle\phi\rangle]^+ [K_{(i)}\langle\phi\rangle].$$

§22. We claim that this last part of the effective lagrangian can be written

$$L^I_{eff} = (1/2\sqrt{2}) \sum_{il} [\bar{\Psi}\gamma_\mu K'_{(i)} \Psi] (K^2)^{-1}_{il} [\bar{\Psi}\gamma^\mu K'_{(l)} \Psi]^+ + \text{h.c.}, \tag{22}$$

where

$$(K^2)_{il} = [K'_{(i)}\langle\phi\rangle]^+ [K'_{(l)}\langle\phi\rangle].$$

The coupling constants $k_{(i)}$ have completely disappeared from this expression [see (18), (19) and (20)]. We just remember of the old coupling constants g and g' by the expressions $\cos^2\Psi$ which are contained in the definition of $K'_{(i)}$. All generated $\cos^2\Psi$ are included in it.

Proof: The matrix

$$(\tilde{M}^2/2)_{ij} = k_{(i)} k_{(j)} [K'_{(i)}\langle\phi\rangle]^+ [K'_{(j)}\langle\phi\rangle] \equiv k_{(i)} k_{(j)} (K^2)_{ij}$$

is not diagonal. By diagonalization we obtain the eigenstates $C_{(l)}$

$$C_{(l)} = \sum_k O_{lk} \tilde{C}_{(k)}$$

with eigenvalue $M_i^2/2$. The matrix O is the matrix $O(p)$ defined in §19. Then we obtain the following two relations:

$$(O \tilde{M}^2 O^t)_{ij} = M_i^2 \delta_{ij} \text{ and } K_{(l)} = \sum_i k_{(i)} K'_{(i)} O^t_{il}.$$

Remember that

$$\sum_l K_{(l)} C_{(l)} = \sum_i k_{(i)} K'_{(i)} \tilde{C}_{(i)}.$$

Using the definition of $\tilde{M}^2/2$, the first relation is written

$$2\sum_{m,l} O_{im}k_{(m)}(K^2)_{ml}k_{(l)}O^t_{lj} = M_i^2\delta_{ij},$$

which implies by inversion

$$\frac{1}{M_i^2}\delta_{ij} = \tfrac{1}{2}\sum_{m,l} O_{im}\frac{1}{k_{(m)}}(K^2)^{-1}_{ml}\frac{1}{k_{(l)}}O^t_{lj}.$$

And replacing, in L^I_{eff}, G_i by its value,

$$L^I_{eff} = \frac{1}{\sqrt{2}}\sum_{ij}[\bar{\Psi}\gamma_\mu K_{(i)}\Psi]\frac{1}{M_i^2}\delta_{ij}[\bar{\Psi}\gamma^\mu K_{(j)}\Psi]^* + \text{h. c.}$$

$$= \frac{1}{2\sqrt{2}}\sum_{imlj}[\bar{\Psi}\gamma_\mu K_{(i)}\Psi]O_{im}\frac{1}{k_{(m)}}$$

$$\times(K^2)^{-1}_{ml}\frac{1}{k_{(l)}}O^t_{lj}[\bar{\Psi}\gamma^\mu K_{(j)}\Psi]^* + \text{h. c.}$$

and using $K_{(l)} = \sum_i k_{(i)}K'_{(i)}O_{il}$, we obtain

$$L^I_{eff} = \frac{1}{2\sqrt{2}}\sum[\bar{\Psi}\gamma_\mu K'_{(i)}\Psi]k_{(i)}O^t_{il}O_{lm}\frac{1}{k_{(m)}}(K^2)^{-1}_{mn}$$

$$\times\frac{1}{k_{(n)}}O^t_{ns}O_{sr}k_{(r)}[\bar{\Psi}\gamma^\mu K'_{(r)}\Psi]^* + \text{h. c.}$$

$$L^I_{eff} = \frac{1}{2\sqrt{2}}\sum[\bar{\Psi}\gamma_\mu K'_{(i)}\Psi](K^2)^{-1}_{il}$$

$$\times[\bar{\Psi}\gamma^\mu K'_{(l)}\Psi]^* + \text{h. c.}$$

X. GENERAL PROPERTIES OF L_{eff}

§23. Now we count the number of coupling constants which appear in $L^C_{eff} + L^I_{eff}$. Originally we were in possession of n coupling constants of the type $g_{(i)}$ and r coupling constants of the type $g'_{(i)}$. They have been used to redefine new coupling constants: m of the type $h_{(i)}$, s of the type $h'_{(i)}$ (12), and some number of $\cos^2\Psi_{kl}$ (§15). The following possibilities can occur (§13):

(1) A subgroup $S'_{(i)}$ or $U'_{(i)}$ is constructed with only one group $S_{(j)}$ or $U_{(j)}$. Then $g^{(\prime)}_{(j)} = h^{(\prime)}_{(j)}$. The new coupling constants h [or h'] appears only in L^C_{eff} [(21)]. The old coupling constant $g_{(i)}$ can also appear as a "coupling constant" $k_{(i0)}$ (17) but disappears in L^I_{eff} [(22)].

(2) A subgroup $S'_{(i)}$ or $U'_{(i)}$ is constructed with more than a group $S_{(j)}$ or $U_{(j)}$ [n_i groups]. This case gives right to a relation (12) defining a new coupling constant h [or h'] and $(n_i - 1)$ coupling constants of the type $\cos^2\Psi_{ij}$ (§15). An old coupling constant can appear as a k-type coupling constant but disappears in L_{eff} [(17)].

The coupling constants h [or h'] appears only in L^C_{eff} while in L^I_{eff} all $\cos^2\Psi_{ij}$ appear [(21) and (22)].

(3) An initial group $S_{(j)}$ [or $U_{(j)}$] can be "completely broken": There is no subgroup which is constructed with its generators. The old coupling constant $g_{(j)}$ [or $g'_{(j)}$] becomes trivially a "coupling constant" of the type $k_{(i0)}$ or $k_{(0i)}$ [(15), (17)] but disappears in L^I_{eff} [(22)] and it does not appear in L^K nor in L^C. The coupling constant $g_{(j)}$ [$g'_{(j)}$] has completely disappeared from the Lagrangian we constructed in §21.

§24. Looking at the form of L^I_{eff}, we can see a kind of scaling for the physical results. Let us suppose that for each generator $K'_{(i)}$ we have fixed a scale μ_i: This means that all matrix elements of $K'_{(i)}$ are proportional to μ_i. By the same reasoning we did in §21 to suppress the coupling constants $k_{(i)}$ of the Lagrangian, we obtain for L^I_{eff} a result independent of the μ_i.

Thus the physical results for processes of the type current × current will only depend on ratios of matrix elements of each $K'_{(i)}$. Thus we cannot believe that such a theory can provide equivalent processes with cross sections differing by orders of magnitude. Such differences can only naturally proceed from the matrix $(K^2)^{-1}$ defined in §22, but this matrix is, apart from the factors $\cos^2\Psi$, entirely dependent of the Higgs sector.

We thus claim that the really interesting features (the explanation of processes involving same type of physical particles interacting with the exchange of massive vector bosons but with cross sections differing by orders of magnitude) of such theories become almost entirely from the Higgs sector and have very little to do with a choice of the groups G and H.

CONCLUSION

Throughout this work, we have been interested in writing an effective Lagrangian of type current × current for spontaneously broken gauge theories.

We have seen that almost all the old coupling constants which were in the initial symmetric theory are recovered in the broken theory either in the form of an "electromagnetic"-like coupling constant [our $h_{(i)}$ and $h'_{(i)}$], either on the form of a term $\cos^2\Psi$. The "Fermi"-like coupling constants are functions of those $\cos^2\Psi$'s and of an arbitrariness in the theory: the choice of ϕ and its vacuum expectation values.

An old coupling constant disappears in the broken theory if the group corresponding to it is completely broken: None of its generators enters in the definition of the generators of the entire surviving subgroup.

The arbitrariness in the Higgs sector of the theory has very much to do with results of experiments proceeding by the exchange of a massive vector boson: The scaling properties which are exhibited by the effective Lagrangian suggest us that differences of orders of magnitude between the cross sections of "equivalent" experiments come almost entirely from the choice we did in the Higgs sector and not really from the choice of groups.

ACKNOWLEDGMENT

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[1]For a review of spontaneous breakdown of field theories, see the classical work: E.S. Abers and B.W. Lee, Phys. Rep. C **9**, 1 (1973).

[2]F. Englert and R. Brout. Phys. Rev. Lett. **13**, 321 (1964); P.W. Higgs, Phys. Rev. Lett. **13**, 508 (1964).

[3]Here we caution the reader that a more complicated situation could occur with the semidirect product of groups—our analysis does not apply to those more general cases.

[4]The proof which is given here has been suggested to us by Professor Nuyts. An alternative proof can be obtained by considering $h^{(p)}_{ijk}$ as a matrix element of the adjoint representation of $H^i_{(p)}$ and $g^{(m)}_{abc}\beta^{ai}_{(mp)}$ as a matrix element of another representation of $H^i_{(p)}$. Using Schur's lemma in a complicated way leads to the proof.

The retarded Josephson equation

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The retarded Josephson equation, which takes into account, in a simplified form, retardation effects of the Werthamer equation, is a nonlinear, nonsimultaneous, causal integrodifferential equation. It will be solved for kernels which are essentially the asymptotic kernels from BCS theory. Of physical interest are the rotational solutions, especially the characteristics and dynamics, which describe the steady state of a Josephson junction.

I. INTRODUCTION

The Josephson equation can be derived by means of Maxwell's equations together with the frequency relation

$$\dot{\varphi}=\frac{eV}{\hbar}(e=|e|>0), \tag{1.1}$$

and the current phase relation (CPR), which connects the current perpendicular to a planar junction $j(\varphi)$ to the phase difference φ. This CPR is a nonlinear, nonsimultaneous relation, which is invariant by time transformations and obeys causality

$$j[\varphi]=\int_{-\infty}^{t} dt'\, K(t-t';\varphi(t),\varphi(t')). \tag{1.2}$$

The current therefore vanishes as long as the phase difference is zero. If the two sides of the Josephson junction are interchanged, $\varphi \to -\varphi$, the current changes its sign, $j[-\varphi]=-j[\varphi]$. If voltage changes are slow or small, then second- and higher-order derivatives of $\varphi(t)$ are neglected and the CPR becomes

$$j(\varphi)=k(\varphi,\dot{\varphi}). \tag{1.3}$$

This is the first-order adiabatic approximation (AA), since only the first-order term $\dot{\varphi}$ (voltage) is retained. If the voltage itself is small, the linear adiabatic approximation (LAA) is sufficient,

$$j(\varphi)=k_0(\varphi)+\dot{\varphi}k_1(\varphi). \tag{1.4}$$

The Josephson equations for these different approximations (AA, LAA) has been discussed in the literature under various conditions, i.e., for local or extended junctions, for capacitive or inductive loading, and for various inputs. We consider here a capacitive local junction with current input, which will be written in dimensionless units. The classical Josephson equation[1-6]

$$\beta\ddot{\varphi}+\dot{\varphi}(1+\gamma\cos\varphi)+\sin\varphi=\alpha, \tag{1.5}$$

where β is the capacitance parameter, γ the interference term anisotropy, and α the dc current applied, is a result of the LAA. The equation in the adiabatic approximation AA is

$$\beta\ddot{\varphi}+i_0(\dot{\varphi})-i_1(\dot{\varphi})\cos\varphi+j_1(\dot{\varphi})\sin\varphi=\alpha. \tag{1.6}$$

These differential-type Josephson equations have been used predominantly for practical calculations (see, e.g., Ref. 7).

The retarded Josephson equation[8,9] is the simplest integrodifferential equation based on (1.2). It can be considered as a nonsimultaneous generalization of (1.6),

$$\beta\ddot{\varphi}+\dot{\varphi}+\int_0^\infty dt'\, F(t')\sin\varphi(t-t')=\alpha, \tag{1.7}$$

where the retardation in the CPR is given by a memory function (kernel) $F(t)$, which is assumed to be normalized. The most complete equation for a junction has been given by Werthamer,[10]

$$\beta\ddot{\varphi}+\int_0^\infty dt'\left(G(t')\sin\frac{\varphi-\varphi(t-t')}{2}+F(t')\sin\frac{\varphi+\varphi(t-t')}{2}\right)=\alpha. \tag{1.8}$$

It takes the time dependence of the voltage fully into account. The Werthamer equation (WE) has been solved in the zero-temperature case.[11] The kernels F, G can then be given analytically.[12] They are functions oscillating with the gap frequency and decaying very slowly.

The equation (1.7) can also be considered as the special case of (1.8), which neglects the regular part G_1 in $G(t)=G_1(t)+G_0\delta'(t-0^+)$ and instead of a half $[\varphi(t)+\varphi(t-t')]/2$ takes a full retardation $\varphi(t-t')$ for the second integral term into account. The first assumption assumes a linear quasiparticle (dissipative) term, which is well realized for junctions working just below the transition temperature. The second assumption should be considered as a mathematical simplification which is more easily visualizable.

The retarded Josephson equation (RJ) can be transformed into higher-order differential equations, if the kernel is a solution of a linear differential equation of arbitrary (finite) order. Two kernels of this type were investigated earlier.[13] In order to be near to the Werthamer problem, essentially the asymtotic form of the kernel has been used for the present purpose.

The characteristic will be discussed over the whole range of β values, especially the singular frequencies, being submultiples $\omega_n=\omega_g/n$ of the gap frequency $\omega_g=2\Delta/\hbar$ (Δ energy gap), will be investigated in great detail. Together with the characteristic the dynamic of the junction will also be elucidated indicating a special feature not present for the instantaneous case. To support numerical results, limit results, especially for large β, will also be obtained.

II. MATHEMATICAL PRELIMINARIES

The integrodifferential Josephson equations [(1.7)

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and (1.8)] become simple differential equations of higher order, if the kernels $F(t)$ and $G(t)$ are finite Dirichlet series of type

$$F(t)=\sum_{\mu=1}^{I}\sum_{\nu=1}^{n_\mu} a_{\mu\nu}t^{\nu-1}e^{-\lambda_\mu t}, \tag{2.1}$$

where $n=\sum_{\mu=1}^{I}n_\mu$ is finite and related to the order of the differential equation.[8] The kernels entering can, to some extent, be approximated by a Dirichlet series.[13] The major deficiency of such series is their behavior for long times, since the physical kernels oscillate with the gap frequency but decay like $1/t$, i.e., with infinite decay time $\lambda_\mu=0$. The simplest non-Dirichlet kernel for the retarded Josephson equation, which has the properties mentioned and does not generate a singular equation (1.7) is

$$F(t)=\frac{2}{\pi}\cdot\frac{\sin\omega_g t}{t}. \tag{2.2}$$

Apart from general analytical results, the numerical treatment will use the kernel (2.2) with $\omega_g=1$. A more general problem would be the three-parameter case with arbitrary α, β, and ω_g or the equivalent problem with α, β, and an arbitrary coefficient for the first-order term $\dot\varphi$ in (1.7).

The unilateral Fourier transforms of (2.2) are

$$f(\omega)=\int_0^\infty dtF(t)e^{i\omega t}=j(\omega)+ii(\omega), \tag{2.3}$$

$$j(\omega)=\sqcap(\omega_g^2-\omega^2),\quad i(\omega)=\frac{1}{\pi}\ln\left|\frac{\omega+\omega_g}{\omega-\omega_g}\right|, \tag{2.4}$$

where $j(\omega)$ is an even step function and $i(\omega)$ is an odd function with a logarithmic singularity for $\omega=\omega_g$. This is in contrast to the Riedel singularity,[14] which enters in the even tunnel function $j(\omega)$. A model for $F(t)$ consistent with the Riedel singularity will be discussed in Sec. VI.

We want to find rotational solutions $\varphi(t)$ to the RJ equation (1.7), i.e., periodic solutions with a linear time term. Introducing the variable $x=\omega t$ with $\omega=2\pi/T$ and T the period, $\varphi(x)$ fulfills the periodicity

$$\varphi(x+2\pi)=\varphi(x)+2\pi,$$

which as a Fourier series is

$$\varphi(x)=x+\sum_{n=1}^{\infty}a_n(\cos nx-1)+b_n\sin nx, \tag{2.5}$$

where for convenience $\varphi(0)=0$ is assumed, since time origin for the steady state can be freely chosen. Then the Fourier expansion of $\sin\varphi(x)$, which is now a (true) periodic function is

$$\sin\varphi(x)=\sum_{n=0}^{\infty}A_n\cos nx+B_n\sin nx, \tag{2.6}$$

where $A_0=-\sum_{n=1}^{\infty}A_n$ because of $\varphi(0)=0$. This defines the multivariable functions $A_n(a_1,b_1,a_2,b_2,\cdots)$ and $B_n(a_1,b_1,a_2,b_2,\cdots)$, which express the nonlinearity of the problem.

Using these functions, (1.7) can be written as

$$\begin{pmatrix}\beta\omega^2n^2, & -\omega n\\ \omega n & \beta\omega^2n^2\end{pmatrix}\begin{pmatrix}a_n\\ b_n\end{pmatrix}=\begin{pmatrix}j(n\omega), & -i(n\omega)\\ i(n\omega), & j(n\omega)\end{pmatrix}\times\begin{pmatrix}A_n\\ B_n\end{pmatrix},\quad n=1,2,\cdots \tag{2.7}$$

and

$$\omega+A_0=\alpha, \tag{2.8}$$

where the right-hand side of (2.7) is the integral term in (1.7). In order to solve (2.7) and (2.8), the infinite system has to be truncated; introducing the $2N$ component vector $Y=(a_1,b_1,\cdots,a_N,b_N)$, there are two methods to find a solution:

(1) The *iterative method*, which in analogy to the iterative solution of Fredholm integral equations, starts with an initial solution Y_0, puts it into the integral term, i.e., into the right-hand side of the first N equations of (2.7), and finds an improved value Y_1. The solution up to a given precision is found by repeated iteration. N has to be increased until relevant digits no longer change.

(2) The *Newton method* considers (2.7) as a transcendental system of $2N$ equations for the unknown Y. In contrast to the iterative method, it converges fast, but only if initial values Y_0 are near to the solution. For an optimal calculation one starts with the iterative and ends with the Newton method.

On the other hand, there are two procedures possible: either (a) α,β is given and $\omega,a_1,\cdots,b_N$ will be determined, or (b) ω,β is given and $\alpha,a_1,\cdots,b_N$ is calculated. Since the characteristic $\alpha(\omega,\beta)$ is a unique function, procedure (b) has to be preferred; (a) is useful only in regions with positive slope $d\omega/d\alpha>0$. Since in case (a), the characteristic decays into disconnected branches, the solution, which needs a fairly good knowledge of approximate initial values, has to be traced down from large β values, where analytical asymptotic solutions are known, to the β value considered.

III. THE ASYMPTOTICAL SOLUTION

The asymptotical solution for $\beta\gg1$ has been discussed earlier (see Ref. 9) in connection with various (averaged) approximations in the RJ equation. Here the characteristic has been investigated up to an order, where contributions appear that account for $\omega\approx\omega_2=\omega_g/2$,

$$\alpha=\omega-\frac{i(\omega)}{2\omega^2\beta}+\frac{j(\omega)}{2\omega^3\beta^2}+\frac{1}{\beta^3}\left(\frac{3i(\omega)j(\omega)}{8\omega^6}+\frac{i^3(\omega)}{8\omega^6}+\frac{i(\omega)}{2\omega^4}-\frac{i(\omega)j(2\omega)+i(2\omega)j(\omega)}{16\omega^6}\right)+O\left(\frac{1}{\beta^4}\right). \tag{3.1}$$

This expansion is good for large β and ω not too near the singular frequencies ω_n. For $\omega\approx\omega_1$ the first- and third-order terms contribute mainly, whereas for $\omega\approx\omega_2$ the last third-order term becomes singular. In order to extend the validity of (3.1) into the singular frequencies,

certain dominant terms in all orders have to be taken into account (see Appendix A). In the limit $\beta \to \infty$, the characteristic $\alpha(\omega, \beta)$ becomes $\omega = \alpha$ except for $\omega = \omega_1$, where the singularity degenerates to a double lateral peak extending to $\alpha = 0.41813$ ($\omega_g = 1$).

This asymptotical solution for $\beta \gg 1$ can also be extended to the critical current $\alpha_c(\beta)$ which is defined as the limit

$$\alpha_c(\beta) = \lim_{\omega \to 0} \alpha(\omega, \beta). \tag{3.2}$$

The general result has been derived in Appendix B of Ref. 9; it becomes rather involved if $i(\omega)/\omega$ has a logarithmic singularity in $\omega = 0$.

In the case [(2.2)—(2.4)] considered here, the critical current is

$$\alpha_c(\beta) \sim \frac{4}{\pi\sqrt{\beta}} \left(1 - \tfrac{1}{3} i'(0)\right), \tag{3.3}$$

where $i'(0) = 2/\pi$.

IV. THE CHARACTERISTIC

The average voltage $\langle \dot{\psi} \rangle = (1/T)\int_0^{2\pi} dt \dot{\psi} = 2\pi/T = \omega$ versus current α, i.e., $\omega(\alpha, \beta)$, is called the characteristic of the RJ equation. It has the symmetry $\omega(-\alpha, \beta) = -\omega(\alpha, \beta)$, since for $\alpha \to -\alpha$ and $\varphi \to -\varphi$ Eq. (1.7) remains invariant.

The characteristic $\omega(\alpha, \beta)$ will be discussed numerically for the kernel (2.2) with $\omega_g = 1$. It shows a very special behavior for the singular frequencies $\omega_l = 1/l$ where the integral in (1.7), extending over a periodic function, should diverge indicating a self-resonance of the kernel (t period 2π) with the solution $\varphi(t)$ (t period $2\pi l$). Nevertheless, the value $\alpha(\omega_l, \beta) = \bar{\alpha}_l(\beta)$ remains finite, since the lth order Fourier coefficients of $\sin\varphi(t)$ vanish (see Appendix B). The (finite) singularity of $\omega(\alpha, \beta)$ near the singular frequencies ω_l can be dissolved by using the regularizing transformation

$$\eta_l(\omega) = \mathrm{sig}(l\omega - 1)/\ln\left|\frac{l\omega + 1}{l\omega - 1}\right| \tag{4.1}$$

in the vicinity $\omega \approx \omega_l$. For small η_l the characteristic η_l versus α behaves linearly,

$$\alpha(\omega, \beta) \approx \bar{\alpha}_l(\beta) - \bar{A}_l(\beta)\eta_l, \tag{4.2}$$

and the slope $|d\eta_l/d\alpha| = 1/\bar{A}_l(\beta)$ decreases with increasing β.

For $\omega_l = 1$ the regularized characteristic is shown in Fig. 1. α has two minima (lateral points), which become more pronounced and tend to $\omega = 1$ or $\eta_1 = 0$, if β is increased. For smaller β's they approach each other again, flatten out and finally join for $\beta = 0$. The characteristic for $\beta = 0$ and $\omega > 1$ is exactly $\omega = \alpha$ (see Appendix C).

The regularized characteristic for $\beta = 1$ is given in Fig. 2. It shows five curves with five different ordinate regions, which are connected (by dots) in the points, where, between neighboring singular frequencies, the current has a maximum. The upper current minimum lies at $\eta_1 \sim 0.1$, which means $l\omega \approx 1.0001$, whereas the lower is still nearer to $\eta_1 = 0$ and higher in α. There is an absolute current minimum at $\alpha = 0.667$ for $w \approx 0.5001$, which plays an important role for the hysteresis if the current is reduced quasistatically.

Figure 3 shows the characteristics $\omega(\alpha, \beta)$ for β ranging from 0 to ∞ in a plot with displaced origin. As mentioned before, $\beta = \infty$ is $\omega = \alpha$ for $\omega \neq 1$, with an infinitely narrow lateral double peak at $\omega = 1$ extending to $\alpha = 0.41813$. For $\beta = 10$ the curve has a hyperbolic-like shape if one disregards the special behavior of the singular frequencies. This shape is generally explained by simple approximative models to the RJ equation.[9] In this case, β is also large enough for the asymptotic solution (3.1) to give reliable results. Also, the asymptotical critical current (3.3) for $\beta = 10$ becomes

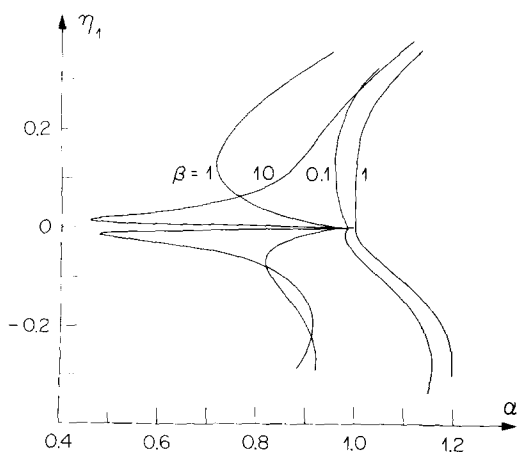

FIG. 1. The regularized characteristic $\eta_1(\alpha)$ near the first singular frequency ω_1 for various β values.

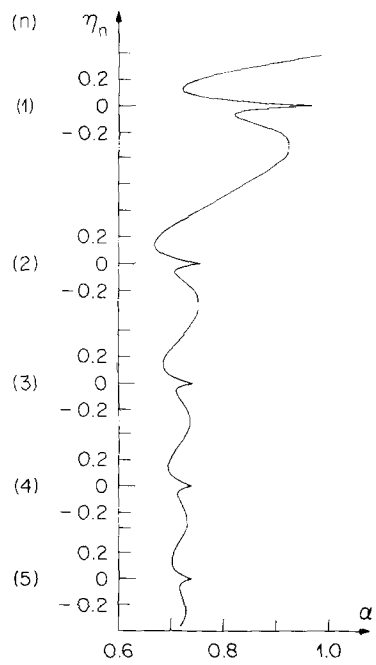

FIG. 2. The regularized characteristic $\eta_n(\alpha)$ for $\beta = 1$. Different regions connected at α maximum (dots).

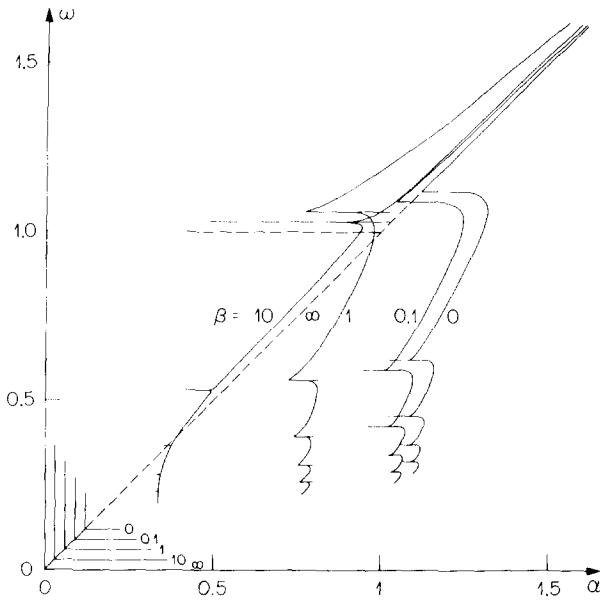

FIG. 3. The (usual) characteristics $\omega(\alpha,\beta)$ for $\beta=0$, 0.1, 1, 10, ∞, and $F(t)=(2/\pi t)\sin t$ with displaced origin (scale belongs to case $\beta=\infty$).

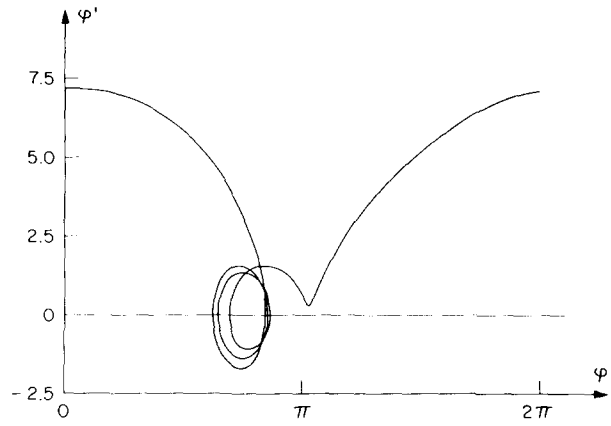

FIG. 4. The phase trajectory $\varphi'(x)=(1/\omega)\,\dot{\varphi}(\omega t)$ versus $\varphi(x)$ for $\beta=1$, $\omega=\frac{1}{4}$ and $\alpha=0.73875$.

$\alpha_c \sim 0.3172$ in agreement with the extrapolated numerical result. The curve $\beta=1$ is identical to Fig. 2. The double-peak structure of the singular frequencies cannot be seen in this conventional plot, in particular the lower $(\omega=\omega_1-0.00\cdots)$ α minimum disappears completely. Nevertheless, all curves $0<\beta<\infty$ show the double-peak structure at ω_1, although the lower peak becomes a small nose for small β. For $\beta=0.1$ even the α maximum $\bar{\alpha}_1(\beta)$ which was clearly visible for $\beta=10$, 1, immerses in the lower branch. For $\beta=0$, $\omega=\alpha$ for $\omega>1$, and for ω_l $(l=2,3,\cdots)$ there are single peaks which seem to diverge numerically.

For technical reasons, the characteristics could not be traced down to $\omega=0$ since, for smaller ω, more and more Fourier coefficients (N large) have to be taken for a certain accuracy. It is therefore difficult to form any conclusions about existence and value of the critical current $\alpha_c(\beta)$. This question has been investigated for some simple Dirichlet kernels,[13] where the RJ equation becomes a differential equation of higher order.

Another problem in connection with the characteristic, is the hysteresis arising when the current is changed quasistatically. If the Josephson junction is at rest, i.e., $\varphi\equiv 0$ and the input current is slowly increased, the solution is stationary and stable at $\varphi=\varphi_\alpha=\arcsin\alpha$ for $\alpha<1$ with $\langle\dot{\varphi}\rangle=\omega=0$. For $\alpha\gtrsim 1$, the solution becomes rotational, i.e., the ω value jumps from $\omega=0$ to the rotational characteristic of Fig. 3, for $\beta=1$ onto the upper $(\omega>1)$ ω_1 branch, where it remains as long as α does not go below the upper α minimum. If it does, the frequency, which is related to the energy of the junction, falls onto the next branch below or down to $\omega=0$, if a rotational solution is no longer possible. This is certainly the case, if α is below the absolute α minimum, which is at $\alpha=0.667$ for $\beta=1$. A similar hysteresis structure holds for other β values; the smallest current, where the junction resets to $\omega=0$ always very near to (but larger than) a singular frequency, because of the general shape of the characteristics.

V. THE DYNAMICS

The dynamics of the solution is contained in the set of Fourier coefficients or in the function $\varphi(x)$ with $x=\omega t$. It is too extensive to give a detailed description of $\varphi(x)$, but there are a few general features which can be stated more easily. As shown earlier[8,13] the voltage $\varphi'(x)$ may become negative in the steady state. An example for $\beta=1$ and $\omega=1/4$ with $\alpha=\bar{\alpha}_4(1)=0.7388$ is demonstrated in Fig. 4. The voltage φ' has then three negative and one positive minima. Therefore, the phase trajectory $\varphi'(\varphi)$ has a triple loop which encloses the unstable equilibrium $\bar{\varphi}_\alpha=2.3104$. A similar behavior has been observed for the other singular frequencies ω_l, where there are l minima in $\varphi'(x)$, only 0 or 1 being positive (up to fifth order). As a measure of higher-order harmonics which enter into the solution, the number M of minima of $\varphi'(x)$ can be used. For large ω down to a little above ω_2, $M=1$; from there down to a little above ω_3, $M=2$, etc. The boundary (a little above ω_l) is almost independent of β, if β is not too large. If β is large, the first harmonic is sufficient to describe $\varphi'(x)$ everywhere except near the singular frequencies.[9] Near ω_l higher harmonics are required, the more the higher l; this again increases M in the vicinity of ω_l with the order of the singular frequency, whereas everywhere else $M=1$ seems to be sufficient.

VI. THE CHARACTERISTIC FOR RIEDEL SINGULARITIES

The problem discussed so far [(2.2), (2.4)] has the logarithmic singularity in the odd function $i(\omega)$, whereas BCS theory predicts it for $j(\omega)$.[14] Assuming

$$j(\omega)=\frac{\omega_g}{2\omega}\ln\left|\frac{\omega+\omega_g}{\omega-\omega_g}\right| \tag{6.1}$$

the corresponding Hilbert transform[15] is

$$i(\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{j(x)dx}{\omega-x}=\frac{\pi\omega_g}{2\omega}\Delta(\omega^2-\omega_g^2), \tag{6.2}$$

where $\int$ means the Cauchy principal value of the integral.

It is easy to verify that these functions, according to (2.3), belong to the kernel

$$F(t)=\omega_g\int_t^\infty ds\,\frac{\sin\omega_g s}{s}=-\omega_g\mathrm{si}(\omega_g t), \tag{6.3}$$

being an integral sine function,[16] which is normalized because of (6.1). The asymptotics for long times,

$$F(t)\sim\frac{\cos\omega_g t}{t}, \tag{6.4}$$

are in agreement with the asymptotics of the BCS theory for $T=0$,[12] and for $T>0$ (see Appendix D). Note that (6.4) taken as $F(t)$ would lead to a singularity in the integral term of (1.7).

The RJ equation will now be solved for the kernel (6.3) with $\omega_g=1$. The characteristics for $\beta=1$, 10 and ∞ are plotted in Fig. 5. The straight line $\omega=\alpha$ is given by $\beta=\infty$ (dashed curve), since similar limits to those derived in Appendix A and Sec. III can be considered. The characteristic for $\beta=10$ is again hyperbolic with cusplike singularities in ω_I. This result can be interpreted by means of the asymptotical formula (3.1), which gives $\alpha\sim\omega-\pi/4\omega^3\beta$ for $\omega>1$ and, since $i(\omega)=0$ for $\omega<1$, $\alpha\sim\omega+j(\omega)/2\omega^3\beta^2$ for $\omega<1$ with the singularities in ω_I pointing to the right. In contrast to Fig. 3, the discontinuity in $\omega=1$ originating from $i(\omega)$ being of order $1/\beta$ is well visible. Again, the asymptotical critical current $\alpha_c(\beta)$ from (3.3), with $i'(0)=0$ giving $\alpha_c=0.4026$, is in good agreement with the value extrapolated. Finally, the characteristic for $\beta=1$ is shown. It has qualitatively the same behavior as Fig. 3, except near the singular frequencies which consist of a cusplike singularity pointing to the left. It would need a more detailed investigation to understand how the direction of the singularities changes by going from $\beta=10$ to $\beta=1$.

VII. FINAL REMARKS

The retarded Josephson equation has been solved for two different non-Dirichlet kernels, which are in asymptotical agreement with the BCS theory. As a result, the characteristics of the rotational solutions, which are essentially hyperbolic, show a very specific structure at the singular frequencies, where the period of the integral kernel is commensurate with the period of the solution. If the tunnel function $i(\omega)$ has a logarithmic singularity and $j(\omega)$ is bound, this structure consists of two lateral peaks, i.e., α minima lying extremely near the singular frequency ω_I. In the opposite case, where $j(\omega)$ is logarithmically singular (Riedel), the structure has one cusplike peak. For small damping, i.e., large β, the solution can be well understood by means of asymptotical expansion. The steady-state solutions again show negative voltage parts, which can be qualitatively understood as a consequence of retardation. The number of negative regions of the voltage and therefore also the number of loops in the phase trajectory is of the order of the nearest singular frequency, if $\omega\approx\omega_I$ and β is not too large.

APPENDIX A. LIMIT BEHAVIOR OF CHARACTERISTICS NEAR $\omega_n = 1/n$ FOR LARGE β

For $\omega\approx 1$ and $\beta\gg 1$, the asymptotic expansion (3.1) gives

$$\alpha=1-\frac{X}{2}+\frac{X^3}{8}+\cdots, \tag{A1}$$

where $X=i_1(\omega)/\beta\approx(1/\pi\beta)\ln 2/|\omega-1|$ is assumed to be of order 1. If X^N is included, $X_N(\alpha)$ with $X_N(1)=0$ follows as a root of the polynomial (A1).

The limit behavior $X(\alpha)$ for $N\to\infty$ can be derived from the RJ equation for the Fourier coefficients (2.7) by taking the limits $\omega\to 1$, $\beta\to\infty$, and X fixed:

$$a_1=-XB_1,\quad b_1=XA_1, \tag{A2}$$

$$a_n=b_n=0,\quad n=2,3,\ldots,\quad \alpha=\omega+A_0.$$

Using $a_1=p\cos\gamma$, $b_1=p\sin\gamma$,

$$A_0=J_1(p)\cos[(p\cos\gamma)-\gamma],$$

$$A_1=J_2(p)\sin[(p\cos\gamma)-2\gamma]-J_0(p)\sin(p\cos\gamma),$$

$$B_1=J_2(p)\cos[(p\cos\gamma)-2\gamma]+J_0(p)\cos(p\cos\gamma),$$

and (A2) gives

(I) $p\cos\gamma=\gamma\Rightarrow$

$$\alpha=1+J_1(p),\quad X=-\frac{p^2}{2J_1(p)},\quad p<0, \tag{A3}$$

(II) $J_2(p)=J_0(p)$, $p=p_0=1.84118\Rightarrow$

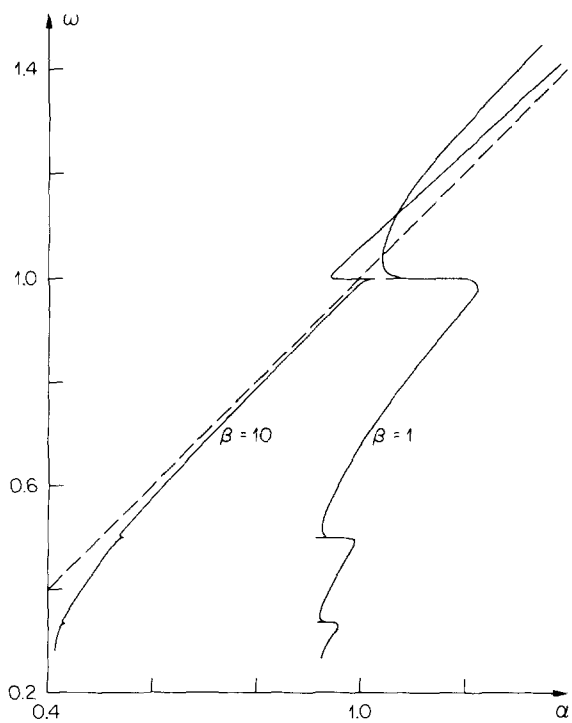

FIG. 5. The characteristic $\omega(\alpha,\beta)$ for $\beta=1$, 10(full), ∞(dashed) for $F(t)=\int_t^\infty dz\,(\sin z)/z\sim(\cos t)/t$.

$$\alpha = 1 - \frac{p_0 J_1(p_0)}{2J_0(p_0)} \frac{1}{X} = 1 - \frac{1.69498}{X}. \tag{A4}$$

An investigation of $X_I(\alpha)$ shows that $X_I(1) = 0$ and $X_I'(1) = -2$; X_I increases with α decreasing until $\alpha_1 = 0.41813$, where $X_I(\alpha_1) = 2.91297$ and $X_I'(\alpha_1) = \infty$. For $\alpha \geq \alpha_1$, $X_{II}(\alpha)$ continues with $X_{II}(\alpha_1) = X_I(\alpha_1)$, $X_{II}'(\alpha_1) = 5.0062$ and being a hyperbola.

The characteristic $\omega(\alpha)$ in the vicinity $\omega \gtrless 1$ is therefore

$$\omega = 1 \underset{(-)}{+} 2\exp[-\pi\beta X(\alpha)], \tag{A5}$$

where $X_I(\alpha)$ holds for $\omega > \omega_1^+(\alpha)$, i.e., beyond the α minimum, and $X_{II}(\alpha)$ for $1 < \omega < \omega_1^+(\alpha)$. For $\omega \lessgtr 1$ the results are analogous.

The solution $X_{II}(\alpha)$ also agrees with the regularization found near the ω_n singularities,

$$\alpha(\omega, \beta) = \bar{\alpha}_n(\beta) - \bar{A}_n(\beta)\left[\ln\left|\frac{n\omega+1}{n\omega-1}\right|\right]^{-1} + O\left(\ln\left|\frac{n\omega+1}{n\omega-1}\right|\right)^{-2}, \tag{A6}$$

since for $\beta \to \infty$, $\bar{\alpha}_1(\beta) \to 1$, and $\bar{A}_1(\beta) \sim 5.34\,\beta$ has been found numerically, whereas (A4) would give $\bar{A}_1(\beta) \sim 1.69498\,\pi\beta$. This proves that, in the limit $\beta \to \infty$, the ω_1 singularity shrinks to an infinitely narrow (in ω) lateral double peak extending to $\alpha = \alpha_1$.

An investigation into the ω_N singularities under similar assumptions is not straightforward; this can also be seen by the $1/\beta$ expansion, where the first term contributing to ω_2 is

$$\alpha = \tfrac{1}{2} - 4j(1/2)\frac{i(2\omega)}{\beta^3} + \cdots,$$

indicating that another quantity X has to be used.

A numerical calculation of (A6) verifies its validity for all ω_n, where $\bar{\alpha}_N(\beta) \to 1/N$ and $\bar{A}_N(\beta) \sim a_N\beta$ for large β. In the same limit, the α minima $\alpha_n^+(\beta)$, $\alpha_n^-(\beta)$ have been investigated. In contrast to $n = 1$ they vanish completely giving rise to $\omega = \alpha$ for $\omega \neq 1$.

APPENDIX B. FINITENESS OF THE CURRENT FOR $\omega = \omega_l = 1/l$

For $\omega = 1/l$, the RJ for the Fourier coefficients (2.7) becomes

$$A_l = 0, \quad E_l = 0,$$

$$\begin{pmatrix} \beta\omega^2 n^2, & -\omega n \\ \omega n & \beta\omega^2 n^2 \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix} = \begin{pmatrix} j(n\omega), & -i(n\omega) \\ i(n\omega), & j(n\omega) \end{pmatrix} \times \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \tag{B1}$$

$$n = 1, 2, \cdots, l-2, l-1, l+1, l+2, \cdots, \quad \alpha = \omega + A_0.$$

Equation (B1) has been calculated numerically for $2N$ equations $n = 1, 2, \cdots, N$ with $2N$ unknowns, a_n, b_n with increasing N. As a numerical result $\alpha, a_1, b_1\ \alpha_2, b_2, \cdots$ exist, and can be calculated to any degree of accuracy if β is not too small (dots in Fig. 3 for $\beta = 0$ characteristic), i.e.,

$$\alpha(\omega = 1/l, \beta) = \bar{\alpha}_l(\beta). \tag{B2}$$

If $\omega \approx \omega_l$, an expansion with respect to $1/i(l\omega)$ or small

$$\eta_l(\omega) = \mathrm{sig}(l\omega - 1)/\ln\left|\frac{l\omega+1}{l\omega-1}\right| \tag{B3}$$

is possible, giving for $X = (\alpha, a_n, b_n, A_n, B_n)$

$$X = X_0 + \eta X_1 + \eta^2 X_2 + \cdots, \tag{B4}$$

where X_0 is the solution resulting from (B1). η is small only when ω is extremely near to ω_n (e.g., $\omega = 1 + 10^{-1000}$ $\eta_1 \approx \perp(\ln 10)1000 \sim 0.434 \times 10^{-3}$), which means that only the first equation of (B1) changes, giving

$$\pi \begin{pmatrix} \beta\omega^2 l^2, & -\omega l \\ \omega l & \beta\omega^2 l^2 \end{pmatrix} \begin{pmatrix} a_l^1 \\ b_l^1 \end{pmatrix} = \begin{pmatrix} -B_l^1 \\ A_l^1 \end{pmatrix} + \begin{pmatrix} \pi j(l\omega), & -1 \\ 1 & \pi j(l\omega) \end{pmatrix} \times \begin{pmatrix} A_l^0 \\ B_l^0 \end{pmatrix}. \tag{B5}$$

If instead of ω, $\eta_l(\omega)$ is used as ordinate for $\omega \approx \omega_l$, the singularity, being a cusp in ω_l, is made regular.

APPENDIX C. THE CHARACTERISTIC FOR $\beta = 0$ AND $\omega > 1$

Because of (2.4), $j(n\omega) = 0$ for $\omega > 1$ and $n = 1, 2, \cdots$; therefore (2.7) for $\beta = 0$ becomes

$$\begin{pmatrix} 0, & -\omega n \\ \omega n, & 0 \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix} = \begin{pmatrix} 0, & -i(n\omega) \\ i(n\omega), & 0 \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} \tag{C1}$$

for $n = 1, 2, \cdots$. This allows for the special solution $a_1 = a_2 = \cdots = 0$, since $\sin\varphi(x)$ is then an odd function with

$$A_n(0, b_1, 0, b_2, \cdots) \equiv 0, \quad n = 0, 1, 2, \cdots. \tag{C2}$$

Therefore, by means of (2.8), $\omega = \alpha$, whereas

$$b_n = \frac{i(n\omega)}{n\omega} B_n(0, b_1, 0, b_2, \cdots), \quad n = 1, 2, \cdots \tag{C3}$$

gives a nontrivial $\varphi(t)$

APPENDIX D. THE ASYMPTOTICS OF THE KERNELS FOR $t \to \infty$ AT TEMPERATURE T

The pair-retardation kernel in the Werthamer equation at temperature T with an energy gap Δ is

$$F(t) = \frac{2G_N}{\pi\hbar e}[\phi'(t, T)\phi''(t, 0) + \phi''(t, T)\phi'(t, 0)], \tag{D1}$$

where

$$\phi(t,T)=\phi'+i\phi''=\int_{\Delta}^{\infty}dE\frac{\Delta}{\sqrt{E^2-\Delta^2}}\tanh\frac{E}{2T}$$

$$\times\exp\left(i\frac{E}{\hbar}t\right). \tag{D2}$$

By means of the method of steepest descent, it is found that for large t

$$\phi(t,T)\sim\tanh\frac{\Delta}{2T}\phi(t,0). \tag{D3}$$

In the case $T=0$ one easily finds

$$\phi(t,0)=\frac{\pi i}{2}H_0^{(1)}\left(\frac{\Delta t}{\hbar}\right),$$

the Hankel function of the first kind, which asymptotically becomes

$$\phi(t,0)\sim\left(\frac{\pi\hbar}{4\Delta t}\right)^{1/2}\exp\left[i\left(\frac{\Delta t}{\hbar}+\frac{\pi}{4}\right)\right]. \tag{D4}$$

Inserting into (D1) finally gives

$$F(t)\sim\frac{2}{\pi}j_m\frac{\cos\omega_g t}{t}, \tag{D5}$$

with $\omega_g=2\Delta/\hbar$ and $j_m=(\pi/2)(\Delta G_N/e)\tanh\Delta/2T$. Analogously for the kernel G:

$$G(t)=\frac{2G_N}{\pi\hbar e}[\Psi'(t,T)\Psi''(t,0)+\Psi''(t,T)\Psi'(t,0)], \tag{D6}$$

$$\Psi(t,T)=\Psi'+i\Psi''=\int_{\Delta}^{\infty}dE\frac{E}{\sqrt{E^2-\Delta^2}}\tanh\frac{E}{2T}\exp\left(i\frac{E}{\hbar}t\right), \tag{D7}$$

$$t\gg\hbar/2\Delta\Rightarrow\Psi(t,T)\sim\tanh\frac{\Delta}{2T}\Psi(t,0), \tag{D8}$$

$$\Psi(t,0)=\frac{\hbar}{i\Delta}\frac{d\phi(t,0)}{dt}\sim\phi(t,0), \tag{D9}$$

$$G(t)\sim\frac{2}{\pi}j_m\frac{\cos\omega_g t}{t}, \tag{D10}$$

i.e., $F(t)$ and $G(t)$ in the Werthamer equation (1.8) have the same asymptotics for large t.

The Werthamer equation would then be

$$\frac{C\hbar}{2e}\ddot{\varphi}+\frac{G_N\hbar}{2e}\dot{\varphi}+\frac{4}{\pi}j_m\sin\frac{\varphi}{2}\int_0^{\infty}dt'\frac{\cos\omega_g t'}{t'}\cos\frac{\varphi(t-t')}{2}$$

$$=I_{in}, \tag{D11}$$

where the linear term comes from the linear quasiparticle characteristic. Also in (D11), the integral would not exist because of a singularity in $t'=0$.

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Evolution of a stable profile for a class of nonlinear diffusion equations. II

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First, explicit formulas are found for all the eigenfunctions and eigenvalues of a Sturm–Liouville problem associated with the class of nonlinear diffusion equations studied previously. The formulas for the eigenfunctions are proportional to Gegenbauer polynomials whose argument depends on the separable solution shape function. Next, rigorous bounds on the asymptotic amplitude are found in terms of integrals of the initial data. These bounds are the best possible bounds of the given type since they produce the exact result for the separable solution. Finally, results of numerical experiments are reported for $D \sim n^{\delta}$ where $\delta = 1, -1/3, -1/2$, and $-2/3$. The rigorous bounds are compared to the perturbation estimates from the earlier work and to the computed values of the asymptotic amplitude.

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I. INTRODUCTION

A previous paper[1] introduced the nonlinear diffusion equation

$$\frac{\partial}{\partial x}\left(D(n)\frac{\partial n}{\partial x}\right) = f(x)\frac{\partial n}{\partial t} \quad \text{for} \quad 0 \leq x \leq 1, \tag{1}$$

where n is a particle density, x is the spatial variable in one dimension, and t is the time. The factor $f(x)$ is a strictly positive function of x. The diffusion coefficient $D(n) \sim n^{\delta}$ where $\delta > -1$. Two regimes of the parameter δ should be distinguished. When $\delta > 0$, the diffusion coefficients, and, hence, the diffusion rate, decreases as $n \to 0$. Therefore, we may call this "decelerating diffusion." When $-1 < \delta < 0$, the diffusion coefficient increases as $n \to 0$ so we may term this "accelerating diffusion." Alternatively, we could label the two regimes as " slow diffusion" and "fast diffusion" respectively.

For convenience, a new dependent variable $m = n^{1+\delta}$ was introduced so (1) becomes

$$m_{xx} = f(x)(m^{q-1})_t, \tag{2}$$

where $q = (2+\delta)/(1+\delta)$. It was shown that the separable solution of (2), $m(x,t) = S(x)T(t)$, was stable against small perturbations when $f(x) = \text{const}$ because all perturbations decay like $T^p(t)$ where $p \geq 4$. Recall that

$$S''(x) + \lambda f(x) S^{q-1}(x) = 0, \tag{3}$$

with $S(0) = S(1) = 0$ and $\sup S(x) = 1$ by definition.

The conjecture that arbitrary initial data evolves toward the separable solution of (2) has now been proven for $f(x)$ a bounded positive function and all $q > 2$. See Ref. 2.

The present paper contains several new results intended to supplement the work of Ref. 1. First, for $f(x) = 1$, we find explicit formulas for all the eigenfunctions and eigenvalues of the Sturm—Liouville problem

$$u_n''(x) + \kappa_n S^{q-2}(x) u_n(x) = 0. \tag{4}$$

The u_n's are the expansion functions of $m(x,t)$ used in the perturbation analysis of Ref. 1. The functions $u_0(x)$ and $u_1(x)$ were known previously. Each $u_n(x)$ is shown to be proportional to a hypergeometric function (or Gegenbauer polynomial) whose argument depends on the separable solution shape function. Next, we find rigorous bounds on the asymptotic amplitude of the separable solution. For fast diffusion ($q > 2$), these bounds give upper and lower bounds on the extinction time t^* (the finite time at which the solution vanishes identically). For slow diffusion ($1 < q < 2$), the results are limited to rigorous upper bounds on the asymptotic amplitude. Next, the results of numerical experiments on various nonlinearities ($q = \frac{3}{2}, \frac{5}{2}, 3, 4$) are presented. The predictions of the perturbation analysis of Ref. 1 are analyzed in light of the new rigorous bounds. Finally, a method of obtaining a high accuracy numerical representation of $S(x)$ when q is an integer and $f(x) = \text{const}$ is presented in the Appendix.

II. EIGENFUNCTIONS AND EIGENVALUES

In Ref. 1, it was recognized that, with $f(x) = 1$, the first two eigenfunctions of (4) are expressible in terms of $S(x)$, the solution of (3). In particular, $u_0(x) = S(x)$ with $\kappa_0 = \lambda$ and $u_1(x) = S(x)S'(x)$ with $\kappa_1 = (q+2)\lambda$. Note that $(S')^2 = \rho^2(1 - S^q)$ where ρ is a known constant.

To obtain the general relation between $u_n(x)$ and $S(x)$, we will change independent variables from x to $y = S^q(x)$. While $0 \leq x \leq 1$, we have $0 \leq y \leq 1$ on the half interval $0 \leq x \leq \frac{1}{2}$. It is straightforward to show that (4) becomes

$$y(1-y)\frac{d^2}{dy^2}u_n(y) + \left[\left(1 - \frac{1}{q}\right) - \left(\frac{3}{2} - \frac{1}{q}\right) y\right] \frac{du_n}{dy} + \epsilon_n u_n = 0, \tag{5}$$

where $\epsilon_n = \kappa_n/\rho^2 q^2$. Note that (5) has the form of the hypergeometric equation. However, the correct boundary conditions for our problem are $u_n(0) = 0$ for all n and $u_n(x = \frac{1}{2}) = 0$ for n odd while $(\partial u_n/\partial x)(x = \frac{1}{2}) = 0$ for n even. The hypergeometric function does not satisfy these boundary conditions. Therefore, we try the following ansatz for u_n,

$$u_n(y) = y^r(1-y)^s F(y). \tag{6}$$

Substituting (6) into (5), we find

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$$y(1-y)F'' + [(\beta+2r) - (\alpha+2r+2s)y]F' + [\epsilon_n - \alpha(r+s) - 2rs - r(r-1) - s(s-1)]F + r(\beta+r-1)y^{-1}F + s(\alpha-\beta+s-1)(1-y)^{-1}F = 0, \quad (7)$$

where $\alpha = \frac{3}{2} - 1/q$ and $\beta = 1 - 1/q$. $F(y)$ will satisfy a new hypergeometric equation if the last two terms vanish. To satisfy $u_n(0) = 0$, we must have $r > 0$. Therefore, $\beta + r - 1 = 0$ or $r = 1/q$. When n is odd, we must have $s > 0$, $\alpha - \beta + s - 1 = 0$ or $s = \frac{1}{2}$. When n is even, we must have $s = 0$.

Now when n is even, F satisfies

$$y(1-y)F'' + \left[\left(1+\frac{1}{q}\right) - \left(\frac{3}{2}+\frac{1}{q}\right)y\right]F' + \left(\epsilon_n - \frac{1}{2q}\right)F = 0. \quad (8)$$

When n is odd, F satisfies

$$y(1-y)F'' + \left[\left(1+\frac{1}{q}\right) - \left(\frac{5}{2}+\frac{1}{q}\right)y\right]F' + \left(\epsilon_n - \frac{1}{2} - \frac{1}{q}\right)F = 0. \quad (9)$$

After transforming back to x, we find that

$$\tilde{u}_n(x) = S(x)F\left(-\frac{n}{2}, \frac{n+1}{2}+\frac{1}{q}; 1+\frac{1}{q}; S^q(x)\right) \quad \text{for } n \text{ even}, \quad (10)$$

$$\tilde{u}_n(x) = \rho^{-1}S(x)S'(x)F\left(-\frac{n-1}{2}, \frac{n}{2}+1+\frac{1}{q}; 1+\frac{1}{q}; S^q(x)\right)$$

for n odd, and (11)

$$\kappa_n = \tfrac{1}{2}(n+1)(qn+2)\lambda \quad \text{for all } n = 0, 1, 2, \cdots. \quad (12)$$

In (10) and (11), $\tilde{u}_n$ has been standardized so that $\tilde{u}_n'(0) = \rho$.

We wish to normalize the u_n's so that $u_0(x) = S(x)$ and

$$\int u_n^2(x)S^{q-2}(x)dx = c \equiv \int S^q(x)dx. \quad (13)$$

In order to compute the normalization, it is helpful to recognize that the particular hypergeometric functions in (10) and (11) are related to Jacobi polynomials. It is well known[3] that

$$F(-n, n+\alpha+1+\beta; \alpha+1; y) = \frac{\Gamma(n+1)\Gamma(\alpha+1)}{\Gamma(n+\alpha+1)} \times P_n^{(\alpha,\beta)}(1-2y), \quad (14)$$

where $\Gamma(\cdot)$ is the gamma function and $P_n^{(\alpha,\beta)}(\cdot)$ is the Jacobi polynomial. Following Bavinck,[4] we define

$$R_n^{(\alpha,\beta)}(\cos\theta) = P_n^{(\alpha,\beta)}(\cos\theta)/P_n^{(\alpha,\beta)}(1) \quad (15)$$

and

$$w^{(\alpha,\beta)}(\theta) = \left(\sin\frac{\theta}{2}\right)^{2\alpha+1}\left(\cos\frac{\theta}{2}\right)^{2\beta+1}. \quad (16)$$

Then it is known[4] that

$$\int_0^\pi d\theta w^{(\alpha,\beta)}(\theta)[R_n^{(\alpha,\beta)}(\cos\theta)]^2 = [\omega_n^{(\alpha,\beta)}]^{-1}, \quad (17)$$

where

$$\omega_n^{(\alpha,\beta)} = \frac{(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)\Gamma(n+\alpha+1)}{\Gamma(n+\beta+1)\Gamma(n+1)\Gamma(\alpha+1)\Gamma(\alpha+1)}. \quad (18)$$

Combining these expressions, we find after some algebra that

$$c_n \equiv \int_0^1 \tilde{u}_n^2(x)S^{q-2}(x)dx = \frac{\Gamma(1/q+\frac{1}{2})\Gamma(1/q+1)}{q\pi^{1/2}}\Gamma\left(\frac{(n+1)}{2}\right)\Gamma\left(\frac{n}{2}+1\right) \times\left[\left(n+\frac{1}{q}+\frac{1}{2}\right)\Gamma\left(\frac{n}{2}+\frac{1}{q}+\frac{1}{2}\right)\Gamma\left(\frac{n}{2}+\frac{1}{q}+1\right)\right]^{-1}. \quad (19)$$

From (19), we obtain the remarkably simple formula

$$c = c_0 = \frac{2}{q+2}. \quad (20)$$

It follows that the u_n's are correctly normalized by taking

$$u_n(x) = \left(\frac{c_0}{c_n}\right)^{1/2}\tilde{u}_n(x). \quad (21)$$

The u_n's are related to the Gegenbauer polynomials as well as to the Jacobi polynomials. In particular,

$$u_n(x) \propto S(x)C_n^{(1/q+1/2)}((1-S^q)^{1/2}) \text{ for all } n, \quad (22)$$

where $C_n^{(\cdot)}(\cdot)$ is the Gegenbauer polynomial. The reader who is interested in studying the general properties of these eigenfunctions (i.e., location of zeros, product formulas, asymptotic behavior for large n, etc.) will find the books of Bavinck[4] and Szëgo[5] to be especially helpful.

The formulas presented here for $u_n(x)$ have been found useful in numerical experiments when a monitor of the nth Fourier coefficient of $m(x,t)$ is desired.

III. RIGOROUS BOUNDS ON THE ASYMPTOTIC AMPLITUDE

In order to establish rigorous bounds on the asymptotic amplitude A_0 for slow diffusion ($1 < q < 2$) and on the extinction time t^* for fast diffusion ($2 < q$), it is useful to consider the following integrals:

$$a_0(t) = c^{-1}\int m(x,t)f(x)S^{q-1}(x)dx, \quad (23)$$

$$\beta(t) = c^{-1}\int m^{q-1}(x,t)f(x)S(x)dx, \quad (24)$$

$$Q(t) = c^{-1}\int m^q(x,t)f(x)dx, \quad (25)$$

$$R(t) = c^{-1}\int m_x^2(x,t)dx, \quad (26)$$

and

$$c = \int f(x)S^q(x)dx. \quad (27)$$

For the formal calculations that follow, we assume only that $f(x)$ is a positive integrable function.

First considering $\beta(t)$, we find

$$\frac{d}{dt}\beta(t) = c^{-1}\int m_{xx}Sdx = c^{-1}\int mS_{xx}dx = -\lambda a_0(t), \quad (28)$$

where we have used Eqs. (2) and (3) and integrated by parts twice. Using Hölder's inequality, it is not difficult to show that

$$a_0(t) \leq [\beta(t)]^{1/(q-1)}. \quad (29)$$

Thus,

$$-\frac{d}{dt}\beta(t) \leq \lambda[\beta(t)]^{1/(q-1)}, \tag{30}$$

from which it follows upon integration that

$$\beta^p(t) \geq \beta^p(0) - \lambda p t, \tag{31}$$

where $p = (q-2)/(q-1)$. Equation (31) is valid for all $1 < q < \infty$ except for $q = 2$ (the linear case) which we need not consider.

For fast diffusion ($2 < q$), the density and therefore $\beta(t)$ will vanish in finite time. Equation (31) shows that the extinction time t^* must satisfy

$$t_L \equiv \beta^p(0)/\lambda p \leq t^*. \tag{32}$$

Equation (32) provides a rigorous lower bound on the extinction time. This argument was first suggested to us by Varadhan.[6]

For slow diffusion ($1 < q < 2$), $p < 0$ and (31) shows that

$$\beta^{|p|}(t) \leq \{\beta^p(0) + \lambda|p|t\}^{-1}. \tag{33}$$

If $m(x,t) \to S(x)T(t)$ asymptotically (this has not yet been proven for $q < 2$ although it is observed in computer experiments) where $T^{q-2}(t) = A_0^{q-2} + \lambda|p|t$, we find easily that (33) implies

$$A_0 \leq [\beta(0)]^{1/(q-1)} \equiv A_u, \tag{34}$$

where A_0 is the asymptotic amplitude.

Another class of inequalities may be derived by first noting that

$$\frac{d}{dt}Q(t) = -\frac{q}{q-1}R(t) \leq 0, \tag{35}$$

$$\frac{d}{dt}R(t) = -\frac{2}{q-1}\int \frac{m_{xx}^2}{m^{q-2}}\frac{dx}{f(x)} \leq 0, \tag{36}$$

and

$$R(t) = -\int m_{xx} m\,dx = -\int \left(\frac{m_{xx}}{m^{q/2-1}f^{1/2}}\right)(m^{q/2}f^{1/2})dx. \tag{37}$$

Applying Schwarz's inequality to (37), we find

$$R^2(t) \leq Q(t)\int \frac{m_{xx}^2}{m^{q-2}}\frac{dx}{f}. \tag{38}$$

From (35), (36), and (38), it is straightforward to show that

$$\frac{d}{dt}[R(t)Q^{-2/q}(t)] \leq 0. \tag{39}$$

Equality occurs in (39) only for the separable solution.

Thus, the quantity in brackets in (39) is always decreasing except for the trivial case. Furthermore, the limiting value as $m(x,t) \to S(x)T(t)$ is

$$R(t)Q^{-2/q}(t) \to \lambda, \tag{40}$$

since

$$\int S_x^2 dx = -\int S_{xx} S dx = \lambda \int f S^q dx = \lambda c. \tag{41}$$

Equations (39) and (40) clearly imply

$$\lambda Q^{2/q}(t) \leq R(t). \tag{42}$$

[Equation (42) also follows easily from a straightforward variational calculation.] Combining (42) and (35) yields

$$-\frac{1}{p}[Q^{(q-2)/q}(t) - Q^{(q-2)/q}(0)] \geq \lambda t. \tag{43}$$

For fast diffusion, $p > 0$ and, since $Q(t^*) = 0$, we have

$$t^* \leq [Q(0)]^{(q-2)/q}/\lambda p \equiv t_u. \tag{44}$$

Thus, we have a rigorous upper bound on the extinction time in terms of an integral of the initial data. For slow diffusion, $p < 0$ and

$$[Q(t)]^{(2-q)/q} \leq \{Q^{(q-2)/q}(0) + \lambda|p|t\}^{-1}. \tag{45}$$

The same ideas used to derive (34) show that

$$A_0 \leq [Q(0)]^{1/q}. \tag{46}$$

However, (34) remains the best bound on the asymptotic amplitude because Hölder's inequality shows that

$$[\beta(t)]^{1/(q-1)} \leq [Q(t)]^{1/q}. \tag{47}$$

The only lower bound known for A_0 is the trivial one $A_0 \geq 0$.

These bounds do not exhaust the possibilities; however, they are the best bounds known to the authors at this time. These bounds are the best possible bounds in terms of $\beta(t)$ and $Q(t)$ since equality is achieved when $m(x,t)$ is the separable solution. These bounds will be compared to the perturbation results of Ref. 1 in the next section.

IV. NUMERICAL EXPERIMENTS

In Ref. 1, a perturbation analysis was used to derive an approximate formula for the asymptotic amplitude A_0 in terms of the initial data. The resulting formula was

$$A_p = a_0(0)\left(1 + \frac{r^2}{2}\frac{B(0) - a_0^2(0)}{a_0^2(0)}\right)^{1/r} \approx A_0, \tag{48}$$

where

$$B(t) \equiv c^{-1}\int m^2(x,t) f(x) S^{q-2}(x)dx \tag{49}$$

and $r = q - 2$. For fast diffusion, (48) may be used to estimate the extinction time. Since t^* is related to A_0 by $t^* = A_0^r/\lambda p$ for the separable solution, we define the perturbation estimate to be

$$t_p \equiv A_p^r/\lambda p. \tag{50}$$

For our numerical experiments, we take $f(x) = 1$. Then, to provide an independent estimate of the asymptotic amplitude and extinction time, we consider the integral

$$N(t) = \int n(x,t)dx = \int m^{q-1}(x,t)dx, \tag{51}$$

which has the physical significance of being the total number of particles. When $m(x,t) = S(x)T(t)$, $N(t) = \gamma T^{q-1}(t)$ where $\gamma = 4/qp$ is a known quantity and $T(t) = (A_0^r - \lambda p t)^{1/r}$. In general, the amplitude A_0 is given by

$$A_0 = \{[N(t)/\gamma]^p + \lambda p t\}^{1/r} \tag{52}$$

for the separable solution. For fast diffusion, we find from (52) that

$$t^* = t + [N(t)/\gamma]^p/\lambda p \tag{53}$$

TABLE I. Values of the rigorous lower bound t_L, perturbation estimate t_p, extinction time t^*, and rigorous upper bound t_u for numerical experiments on (2) with $q=3$ and $f(x)=1$. The formulas appear in Eqs. (32), (50), (53), and (44), respectively. The initial data for the first four cases is given by $m(x,0)=\sum a_l \sin(l+1)\pi x$, where (a_1, a_2, a_3, a_4) equal: (i) (1, 0.4, 0, 0), (ii) (1, 0, 0.3, 0), (iii) (1, 0, −0.3, 0), and (iv) (1, 0, 0, 0.225). For the fifth case, $m(x,0)=1$.

Case	t_L	t_p	t^*	t_u
(i)	0.1834	0.1837[9]	0.1847	0.1927
(ii)	0.1673	0.1675	0.1677	0.1750
(iii)	0.1894	0.1894[9]	0.1895	0.1925
(iv)	0.1761	0.1762	0.1762	0.1793
(v)	0.2102	0.2104	0.2107	0.2301

for the separable solution. For arbitrary initial data, we expect (52) and (53) to approach limiting values as $m(x,t) \to S(x)T(t)$. We will use these formulas to obtain our numerical estimate of the asymptotic amplitude and extinction time.

We decided to study four values of the nonlinearity: $q=\frac{3}{2}$, $\frac{5}{2}$, 3, and 4. For slow diffusion, we have $q=\frac{3}{2}$ which is the midpoint of the interval $1<q<2$ and also corresponds to the physically interesting case of classical diffusion in a plasma[7] ($\delta=1$). For fast diffusion, these values of q correspond to $\delta=-\frac{1}{3}$, $-\frac{1}{2}$, and $-\frac{2}{3}$. Okuda–Dawson diffusion[8] scales like $\delta=-\frac{1}{2}$. The cases $\delta=-\frac{1}{3}$ and $-\frac{2}{3}$ have no known physical significance. However, an interesting qualitative difference exists among these last three cases. As $t \to t^*$, we find $m_t(x,t) \to 0$ for $0>\delta>-\frac{1}{2}$, $m_t(x,t) \to -(\lambda/2)S(x)$ for $\delta=-\frac{1}{2}$, and $m_t(x,t) \to -\infty$ for $-\frac{1}{2}>\delta>-1$.

In Table I, the results for $q=3$ are presented. We immediately observe the empirical relation $t_L \le t_p \le t^* \le t_u$. It turns out we can prove $t_L \le t_p$ for $q=3$. The formulas for t_L and t_p in this case are

$$t_L = 2\beta^{1/2}(0)/\lambda = 2B^{1/2}(0)/\lambda, \tag{54}$$

whereas

$$t_p = [B(0) + a_0^2(0)]/\lambda a_0(0). \tag{55}$$

Recalling that $2 \le y + y^{-1}$ with $y = B^{1/2}/a_0$, we easily find that $t_L \le t_p$. By expanding $m(x,t)$ in terms of its eigenfunctions, we can also show that

$$\begin{aligned} Q^{1/3}(t) &= \{a_0^3(t) + 3a_0(t)[B(t) - a_0^2(t)] + \cdots\}^{1/3} \\ &\cong a_0(t) + \frac{B(t) - a_0^2(t)}{a_0(t)} = B(t)/a_0(t), \end{aligned} \tag{56}$$

so that $t_u \cong 2B(0)/\lambda a_0(0) \ge t_p$ since $B(0) \ge a_0^2(0)$ by Schwarz' inequality. The remarkable agreement of the perturbation estimate t_p with the true extinction time t^* may be partially explained by the fact that t_p always lies between the rigorous upper and lower bounds.

TABLE II. Same as Table I with $q=4$.

Case	t_L	t_p	t^*	t_u
(i)	0.1382	0.1384	0.1409	0.1493
(ii)	0.1040	0.1024	0.1047	0.1138
(iii)	0.1515	0.1523	0.1516	0.1539
(iv)	0.1231	0.1231	0.1234	0.1270
(v)	0.1612	0.1563	0.1622	0.1880

TABLE III. Same as Table I with $q=\frac{5}{2}$. Note that $\lambda=10.8286$, $\rho=2.9433$, and $\gamma=0.5436$ for this case.

Case	t_L	t_p	t^*	t_u
(i)	0.2835	0.2835	0.2842	0.2921
(ii)	0.2761	0.2762	0.2762	0.2823
(iii)	0.2863	0.2862	0.2865	0.2901
(iv)	0.2801	0.2801	0.2802	0.2830
(v)	0.3104	0.3115	0.3106	0.3252

The results for $q=4$ in Table II do not show any simple relationship between t_p and t_L or t_p and t^*. The perturbation estimate is, however, observed to obey $t_p \le t_u$. Again this follows from the fact that

$$\begin{aligned} Q^{1/2}(t) &= \{a_0^4(t) + 6a_0^2(t)[B(t) - a_0^2(t)] + \cdots\}^{1/2} \\ &\cong a_0^2(0) + 3[B(0) - a_0^2(0)], \end{aligned} \tag{57}$$

so

$$t_u \cong 3\{a_0^2(0) + 3[B(0) - a_0^2(0)]\}/2\lambda, \tag{58}$$

whereas

$$t_p = 3\{a_0^2(0) + 2[B(0) - a_0^2(0)]\}/2\lambda \le t_u. \tag{59}$$

In general the perturbation estimate is not as good at predicting t^* for $q=4$ as it is for $q=3$.

For $q=\frac{5}{2}$ in Table III, the perturbation estimate is again remarkably accurate for all cases. However, we also see that the lower bound t_L is a more reliable predictor of t^* since it is often as close as t_p but always remains a lower bound.

Our one case of slow diffusion is $q=\frac{3}{2}$, presented in Table IV. One important difference between results for this case and the previous ones is accuracy. Because computing A_0 from (52) involves taking the difference of two large numbers as $t \to \infty$, we cannot expect a high accuracy estimate of A_0 from a short-duration computer experiment. The values presented were taken at $t=0.1$ in the numerical experiment (as were the values in the fast diffusion experiments) and can be trusted to two significant figures. Practically speaking, the value of A_0 does not possess as much inherent interest as the extinction time does for fast diffusion. As $t \to \infty$,

$$T(t) = [A_0^r + \lambda |p|t]^{1/r} \to 1/(\lambda |p| t)^{1/|r|}, \tag{60}$$

which is completely independent of the initial conditions.

TABLE IV. Values of the asymptotic amplitude A_0, the perturbation estimate A_p, and the rigorous upper bound A_u for numerical experiments on (2) with $q=\frac{3}{2}$ and $f(x)=1$. The formulas appear in Eqs. (52), (48), and (34), respectively. The initial data for the five cases was the same as for Table I.

Case	A_0	A_p	A_u
(i)	0.917	0.941	0.935
(ii)	1.001	1.009	1.013
(iii)	0.889	0.909	0.901
(iv)	0.959	0.969	0.970
(v)	1.277	1.227	1.302

The lack of dependence of the asymptotic state on the initial data is a general characteristic of slow diffusion.

We may conclude from the results of these numerical experiments that the perturbation estimates A_p and t_p are valid approximations to the asymptotic amplitude A_0 and the extinction time t^* for a wide range of nonlinearities. However, still better estimates may exist. In fact, it was found here that the rigorous bounds were occasionally better estimates.

In conclusion, we remark that one of the most interesting questions which remains to be answered is just how the initial data determine the extinction time for fast diffusion. We conjecture that it may be possible to derive a formula for t^*. The rigorous upper and lower bounds on t^* presented here are a first step in that direction.

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APPENDIX

In order to use the formulas for the u_n's derived in Sec. II, we need an accurate numerical representation of the shape function $S(x)$. A general method of successive approximation for arbitrary q was presented in Ref. 1. When q is an integer, another method has been found to be more convenient.

Consider the power series

$$S(x)=\rho x\sum_{n=0}^{\infty}(-1)^n\alpha_n x^{qn}, \tag{61}$$

where $\rho^2=2\lambda/q$ and $\alpha_0=1$. Substituting (61) into (3) when $f(x)=1$ and q is an integer yields a recursion formula for the α_n's. For example, when $q=3$,

$$\alpha_{n+1}=\frac{\lambda\rho}{3(n+1)(3n+4)}\sum_{p=0}^{n}\alpha_p\alpha_{n-p}, \tag{62}$$

and, when $q=4$,

$$\alpha_{n+p}=\frac{\lambda\rho^2}{4(n+1)(4n+5)}\sum_{mp}\alpha_{n-m-p}\alpha_m\alpha_p. \tag{63}$$

The resulting representations of $S(x)$ were used in the numerical experiments of Sec. IV. By computing the first fifty α_n's and using the ratio test, we found that the expected radius of convergence of the power series, with $q=3$, was for all $x<1$ and, with $q=4$, for all $x<0.707$. Since $S(x)=S(1-x)$, we only need to compute $S(x)$ for $0\leq x\leq\frac{1}{2}$, which is well within the radius of convergence of the series in both cases.

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$$I(S)=\frac{1}{q}B_{S^q}\left(\frac{1}{q},\frac{1}{2}\right)=S\,{}_2F_1\left(\frac{1}{q},\frac{1}{2};1+\frac{1}{q};S^q\right).$$

On the exact scattering solution of the Schrödinger and Dirac equations with a short range potential

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The total and partial wave scattering amplitudes in the Schrödinger equation with a short range potential have been derived. The Dirac equation for a short range potential has been exactly solved analytically for all partial waves for positive energies, and an expression for the $S_{1/2}$ wave phase shift has been explicitly deduced.

I. INTRODUCTION

We know that the Schrödinger equation undergoes analytical treatment in all partial waves for the Coulomb and square-well potentials. The short-range nuclear interaction $V(r) = -V_0(1/r - 1/a)$ for $r \leq a$ and $V(r) = 0$ for $r > a$ for which one gets exact analytical solution for all partial waves was analyzed by the authors[1a] for positive energies in the context of the neutron proton scattering. In the present work, we have derived the total scattering amplitude $f(\theta)$ and the partial wave T matrix in momentum variables for the above short-range potential having a sharp cutoff at $r = a$. The separable representation of the T matrix for negative energies is also suggested through numerical solution of the Lippmann–Schwinger equation.

As is well known, the Dirac equation in the Coulomb field of a point charge can be solved exactly.[2] Further, for nuclear charge $Z > 137$, the corresponding solutions of the Dirac equation are not well behaved as they oscillate near the origin. Popov[3] has studied the Dirac equation for an electron in a Coulomb field with $Z > 137$, which results in a collapse to the center in the point charge approximation. Here we have solved the Dirac equation analytically for the scattering of a spin 1/2 particle moving in a centrally symmetric force field, $V(r) = -V_0(1/r - 1/a)$ for $r \leq a$ and $V(r) = 0$ for $r > a$.

II. SCHRODINGER EQUATION WITH SHORT-RANGE INTERACTION

The Schrödinger wave equation with the above-mentioned potential becomes for $r < a$

$$\nabla^2\psi + (K'^2 - \beta/r)\psi = 0, \tag{1}$$

where $\beta = -(2m/\hbar^2)V_0$, $K'^2 = K^2 - \gamma^2$, $\gamma^2 = (2m/\hbar^2)(V_0/a)$; all other symbols have their usual meanings. Substituting $\psi = \exp(iK'z)\,G$ we get

$$\nabla^2 G + 2iK'\frac{\partial G}{\partial z} - \beta\frac{G}{r} = 0, \text{ where } z = r\cos\theta.$$

A solution of the type $G = G(r - z)$ satisfies the above equation and we get (with $P = r - z$)

$$2\left(1 - \frac{z}{r}\right)\frac{d^2G}{dr^2} + \frac{2}{r}\frac{dG}{dr} + 2iK'\left(\frac{z}{r} - 1\right)\frac{dG}{dr} - \frac{\beta}{r}G = 0. \tag{2}$$

Here

$$\rho\frac{d^2G}{d\rho^2} + \frac{dG}{d\rho} - iK'\rho\frac{dG}{d\rho} - \frac{\beta}{2}G = 0. \tag{3}$$

Following Mott and Massey,[2] we $G = {}_1F_1(-i\alpha, 1; iK'\rho)$ for $r < a$, where $\alpha = \beta/2K'$. Since we require an incident wave of unit amplitude, we take for the total wavefunction representing the scattering as

$$\psi(r, \theta) = e^{-\pi\alpha/2}\Gamma(1 + i\alpha)\,e^{iK'z}\,{}_1F_1(-i\alpha, 1; iK'\rho). \tag{4}$$

In the limit $a \to \infty$, $\psi(r, \theta)$ represents the exact wavefunction for pure Coulomb scattering. At $r \geq a$, $\psi(r, \theta)$ should behave as an incident plane wave and a spherically outgoing scattered wave; that is, $\psi(r, \theta) = \exp(iKz) + f(\theta)\exp(iKr)/r$, for $r \geq a$, where $f(\theta)$ is the total scattering amplitude. Matching the two solutions at the boundary $r = a$, we get

$$f(\theta) = [\exp(-\pi\alpha/2)\Gamma(1 + i\alpha)\exp(iK'a\cos\theta) \times {}_1F_1(-i\alpha, 1; iK'a(1 - \cos\theta)) - \exp(iKa\cos\theta)]a\exp(iKa). \tag{5}$$

In the high energy limit, we get

$$f(\theta) = [\exp(-\pi\alpha/2)\Gamma(1 + i\alpha) \times \exp(-i\gamma^2 a\cos\theta/2K)\,{}_1F_1(-i\alpha, 1; iK'a(1 - \cos\theta)) - 1].$$

In the extreme high energy limit,

$$f(\theta) \simeq [\exp(-i\gamma^2 a\cos\theta) - 1]a\exp[-iKa(1 - \cos\theta)].$$

It is worth mentioning that in the limit $a \to \infty$, $f(\theta)$ does not go over to that for the Coulomb scattering amplitude since the distortions of the incident plane wave and the spherically outgoing scattered wave which are the characteristic features of the long-range Coulomb interaction, are not reproduced in the amplitude in the above limiting case. For forward scattering, we have $f(0)$ as

$$f(0) = \exp(-\pi\alpha/2)\Gamma(1 + i\alpha)\exp[i(K' - K)a] - a. \tag{6}$$

Consequently, unlike the pure Coulomb interaction case for $\theta = 0$, it is not singular. Using the optical theorem, we get the total cross section Q as

$$Q = (4\pi/K)\,\mathrm{Im}f(0)$$

 0022-2488/78/1912-2481$1.00

$$= \frac{4\pi a\alpha}{K} \exp(-\pi\alpha/2) \left(\frac{\pi}{\alpha \sinh \pi\alpha}\right)^{1/2}$$

$$\times \cos\{(K' - K)a + \arg\Gamma(i\alpha)\} \tag{7}$$

which is not divergent for $a < \infty$.

From the well-known relation of $f(\theta)$ to the total on shell T matrix, we can calculate the partial wave T matrix elements by partial wave analysis as

$$T(\mathbf{K}_1, \mathbf{K}_2; K^2) = \sum_{l=0}^{\infty} (2l+1) T_l(K_1, K_2; K^2) P_l(\cos\theta).$$

Hence

$$T_l(K_1, K_2; K^2)$$

$$= \frac{1}{2} \int_{-1}^{+1} T(\mathbf{K}_1, \mathbf{K}_2; K^2) P_l(\cos\theta) d(\cos\theta) = A_l - B_l,$$

where

$$A_l = -\frac{\pi a \hbar^2}{m} \Gamma(1 + i\alpha) \exp(-iKa - \pi\alpha/2)$$

$$\times \int_{-1}^{+1} \exp(iK'a\mu)\, {}_1F_1(-i\alpha, 1; iK'a(1-\mu)) P_l(\mu)\, d\mu$$

and

$$B_l = -\frac{\pi a \hbar^2}{m} i^l \exp(-iKa) \int_{-1}^{+1} \exp(iKa\mu) P_l(\mu)\, d\mu.$$

Further,

$$A_l = -\frac{\pi\hbar^2}{m} \frac{\Gamma(1+i\alpha)}{l!} 2^{-l} \exp(iKa - \pi\alpha/2)$$

$$\times \int_{-1}^{+1} (1-\mu^2) \frac{d^l}{d\mu^l}$$

$$\times \{\exp[-iKa(1-\mu)]\, {}_1F_1(-i\alpha, 1; -iKa(1-\mu))\}\, d\mu.$$

Using the Kummer transformation $\exp(-x)\, {}_1F_1(a, c; x) = {}_1F_1(c-a, c; -x)$, we are finally led to the on-shell partial wave T matrix as

$$T_l(K_1, K_2; K^2)$$

$$= -2^{l+1} \exp(-\pi\alpha/2) \Gamma(l+1+i\alpha) i^l (K'a)^l$$

$$\times \exp(iK'a)\, {}_1F_1(l+1+i\alpha, 2l+2; -2iK'a) \frac{\pi\hbar^2 a}{m}$$

$$\times \frac{\exp(-iKa)}{(2l+1)!} + \frac{4\pi a \hbar^2 i^l}{m(2l+1)!} j_l(Ka) \exp(-iKa). \tag{8}$$

In the limit $a \to \infty$ so as to correspond to the Coulomb case, our partial wave on-shell T matrix, however, does not approach a well-defined limit.[3] For the investigation of the binding energies of the three-particle systems by the Faddeev equations, one needs the partial wave two-body T matrix for negative energies, as an input. Hence it will be interesting and useful to study the partial wave T matrix of such short-range potentials, in separable form, which are used as inputs in the Faddeev equations. To derive a partial wave T matrix in the form of a separable expansion in momentum variables K_1 and K_2 for two-particle negative energies, we may use the normalization

$$T_l(K_1, K_2; E)$$

$$= \frac{\exp(i\delta_l)\sin\delta_l}{K_1^2}, \quad \text{where } E = K_1^2 = K_2^2$$

is the two-body center of mass energy and δ_l is the lth partial wave phase shift.[4] Consequently, the partial wave Lippmann–Schwinger equation off the energy shell runs as $(K_1^2 \neq K_2^2 \neq E)$

$$T_l(K_1, K_2; E) = V_l(K_1, K_2) + \frac{1}{\pi} \int_0^{\infty} \frac{V_l(K_1, K') T_l(K', K_2; E)}{K'^2 - E} K'\, dK'^2 \tag{9}$$

for negative energies E, the kernel is nonsingular. We can now write

$$T_l(K_1, K_2; E) = \sum b_{nl}(K_2, E) \phi_{nl}(K_1, E),$$

where b_{nl}'s are the coefficients in the expansion and $\phi_{nl}(K_1, E)$ are the solutions (eigenfunctions) of the homogeneous Lippmann–Schwinger equation with eigenvalues $\lambda_{nl}(E)$ such that

$$\lambda_{n_l}(E)\, \phi_{n_l}(E)$$

$$= \pi^{-1} \int_0^{\infty} \frac{V_l(K_1, K'') \phi_{nl}(K'', E) K''\, dK''^2}{K''^2 - E}. \tag{10}$$

Using the orthonormal property

$$\frac{1}{\pi} \int_0^{\infty} \phi_{m_l}(K'', E) \phi_{n_l}(K'', E) K''\, dK''^2 \frac{1}{K''^2 E} = \delta_{nm}$$

we get

$$T_l(K_1, K_2; E)$$

$$= \sum_n \frac{\lambda_{n_l}(E)}{1 - \lambda_{n_l}(E)}\, \phi_{n_l}(K_1, E)\, \phi_{n_l}(K_2, E).$$

It is to be noted, however, that the Schrödinger equation does not undergo exact analytical solution for negative energies with our short-range potential because of the finite cutoff in our potential at $r = a$ as discussed in our previous work.[1b] Consequently, to obtain exact analytical solutions $\phi_{nl}(K, E)$, one has to solve Eq. (10) numerically. However, an approximate analytic form of $\phi_{n_l}(K, E)$ may be obtained from the Fourier transforms of the corresponding approximate bound state solution $\psi_l(r)$ of the Schrödinger equation where $\psi_l(r)$ represents approximately (neglecting terms $\sim 1/a^2$) the hydrogen-like bound state eigenfunctions. Hence the corresponding approximate momentum space eigen function can be represented through the Gegenbauer polynomials

$$C_{q-1}^{l+1}(x)$$

where

$$C_{q-1}^{l+1}(x) = [\Gamma(q+2l+1)/\Gamma(q)\Gamma(2l+2)]$$

$$\times F(q+2l+1, 1-q, l+3/2; \tfrac{1}{2}(1-x))$$

as

$$\lambda_{nl}(E) \approx \frac{V_0 m^{1/2}}{n\sqrt{-2(E-V_0/a)}},$$

$$\phi_{nl}(K,E) \approx \frac{B_{nl}(E)K^l}{K^2-(E-V_0/a)} \times C^{l+1}_{n-l+1}\left(\frac{K^2+E-V_0/a}{K^2-E+V_0/a}\right), \quad n>l \quad E<0,$$

$$B_{nl}(E) = \left[2^{4l+3}\frac{n(n-l-1)!}{\Gamma(n+l+1)}\right]^{1/2} l!\left(-E+\frac{V_0}{a}\right)^{(2l+3)/4}$$

III. DIRAC EQUATION WITH SHORT-RANGE INTERACTION

The Dirac equation[5,6] for a spin 1/2 particle with mass m and (relativistic) energy E is $H\psi=[\beta m+\alpha\cdot p+V(r)]\psi=E\psi$, where all other symbols have their usual meanings. Since the angular momentum and the parity (relative to the centre of the field, taken as the origin) are conserved in a central field, we have to seek solution of the Dirac equation in the form

$$\psi(r) = \begin{pmatrix} f(r)\xi_{jlm} \\ g(r)\eta_{jl'm}(-1)^{(l-l'+1)/2} \end{pmatrix},$$

$$\eta_{jl'm} = i^{l-l'}\frac{\sigma\cdot r}{r}\xi_{jlm}$$

and

$$\int_0^{2\pi}\int_0^{\pi}\xi^*_{jlm}\xi_{jlm}\sin\theta\,d\theta\,d\varphi = 1,$$

where $l=j\pm\frac{1}{2}$, $l'=2j-l$. Using the orthogonality of ξ_{jlm} and η_{jlm} since they belong to different eigenvalues of β, we arrive at

$$\frac{df}{dr}+\frac{1+K}{r}f-(E+m-V)g=0 \tag{11}$$

and

$$\frac{dg}{dr}+\frac{1-K}{r}f+(E-m-V)f=0 \tag{12}$$

for $r<a$, where $K=-(l+1)$ for $j=l+\frac{1}{2}$ and $K=l$ for $j=l-\frac{1}{2}$. Equations (11) and (12) will yield scattering state solutions so long as $E>m$.

Similarly, for $r\geq a$, we have

$$\frac{df}{dr}+\frac{1+K}{r}f-(E+m)g=0, \tag{13}$$

$$\frac{dg}{dr}+\frac{1-K}{r}g+(E-m)f=0. \tag{14}$$

Defining the new quantity E' as $E'=E-V_0/a$, Eqs. (11) and (12) may be recast into the Dirac equation for the pure Coulomb field with the reduced energy E' as

$$\frac{df}{dr}+\left(\frac{1+K}{r}\right)f-(E'+m+V_0/r)g=0, \tag{15}$$

$$\frac{dg}{dr}+\left(\frac{1-K}{r}\right)g+(E'-m+V_0/r)f=0, \tag{16}$$

for $r<a$. For small r, the terms in $(E'\pm m)$ may be ignored leaving

$$(fr)'+\frac{K}{r}f-\frac{V_0}{r}g=0, \tag{17}$$

$$(gr)'-\frac{K}{r}g+\frac{V_0}{r}f=0. \tag{18}$$

As the functions f and g occur in an equivalent manner in (17) and (18), we write $f(r)\cdot r=a\eta^\gamma$ and $g(r)\cdot r=l\eta^\gamma$, where a and b are now two constants and $\gamma^2=K^2-V_0^2$. If $V_0^2<K^2$, γ is real and for the well-behaved solution at $r=0$, we take γ to be positive. The corresponding solution either does not diverge at $r=0$ or does so less rapidly than the other. It should be noted, however, that if $V_0^2>K^2$, γ becomes purely imaginary; the corresponding solutions oscillate violently near the origin and the subsequent steps in the calculation carry no meaning, similar to the corresponding Coulomb problem with the Dirac equation.[7,8] Now, $a(\gamma+K)=lV_0$ and $aV_0+l(\gamma-K)=0$, whence $f(r)=[V_0/(\gamma+K)]g(r)\sim r^{\gamma-1}$.

With

$$\eta=2\lambda r,\quad \lambda=-ip',\ p'=+\sqrt{E'^2-m^2},$$

$$f=\sqrt{E'+m}\exp(-\eta/2)\eta^{\gamma-1}\{h_1(\eta)+h_2(\eta)\}\equiv u_1, \tag{19}$$

$$g=-i\sqrt{E'-m}\exp(-\eta/2)\eta^{\gamma-1}\{h_1(\eta)-h_2(\eta)\}\equiv v_1, \tag{20}$$

for $r\ll a$. These forms of f and g are justified because of their behavior near the origin and that they switch over exactly to the corresponding solutions of the pure Coulomb scattering problem when $E'=E$. Hence from (15) and (16), we are finally led to

$$\eta h_1'+\left(\gamma-\frac{V_0E'}{\lambda}\right)h_1+\left(K-\frac{V_0m}{\lambda}\right)h_2=0, \tag{21}$$

$$\eta h_2'+\left(\gamma+\frac{V_0E'}{\lambda}-\eta\right)h_2+\left(K+\frac{V_0m}{\lambda}\right)h_1=0, \tag{22}$$

for $r<a$. The solutions of these equations which are finite when $\eta=0$ are given by

$$h_1(\eta)=AF\left(1-\frac{V_0E'}{\lambda},\ 2\gamma+1;\ \eta\right)$$

$$h_2(\eta)=BF(\gamma+1-V_0E'/\lambda,\ 2\gamma+1;\eta).$$

Substituting $\eta=0$ in (21) or (22), we get

$$B=-\left(\frac{\gamma+V_0E'/ip'}{K+V_0m/ip'}\right)A$$

for $r>a$, we have

$$f=\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{r}\left(\frac{E+m}{2E}\right)^{1/2}\sin\left(pr-\frac{l\pi}{2}+\delta_K\right) \tag{23}$$

$$g=-\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{r}\left(\frac{E-m}{2E}\right)^{1/2}\sin\left(pr-\frac{l'\pi}{2}+\delta_K\right), \tag{24}$$

where δ_K is the phase shift and $p=+(E^2-m^2)^{1/2}$. It is interesting to observe that the potential having a sharp cutoff at $r=a$ precludes that both f and dg/dr or g and df/dr can be continuous at such a point. That is, the required conditions for matching the functions on the two sides of the discontinuity is the continuity of the functions $f(r)$ and $g(r)$ themselves. Matching the solution $f(r)$ or $g(r)$ at $r=a$ from the two sides, we have

$$u_1|_{r=a} = u_2|_{r=a}, \tag{25}$$

$$v_1|_{r=a} = v_2|_{r=a}. \tag{26}$$

Combining (25) and (26), we get for $j = 1/2$, $l = 0$, i.e., for $K = -1$, the $S_{1/2}$ wave phase shift as

$$i\left(\frac{E'-m}{E'+m}\right)^{1/2}\left[\left(\frac{V_0 m}{p'}-K\right){}_1F_1(\gamma - i\nu', 2\gamma+1; -2ip'a) - \left(\frac{iV_0E'}{p'}-\gamma\right){}_1F_1(\gamma+1+i\nu', 2\gamma+1; -2ip'a)\right] \tag{27}$$

$$\times \left[\left(\frac{iV_0 m}{p'}-K\right){}_1F_1(\gamma - i\nu', 2\gamma+1; -2ip'a) + \left(\frac{iV_0E'}{p'}-\gamma\right){}_1F_1(\gamma+1-i\nu', 2\gamma+1; -2ip'a)\right]^{-1}$$

$$= \left(\frac{E-m}{E+m}\right)^{1/2} \cot(pa+\delta_{-1}), \quad \text{where } \nu' = V_0E'/p'.$$

IV. CONCLUSION

The exact scattering solution of the Schrödinger equation with such a short range potential yields the scattering amplitude which serves to study and compare it with the corresponding Coulomb problem when $a \to \infty$ for which exact solution is also known. The short range interaction we have investigated, which is an approximation to the Yukawa potential, [1a] may be used to simulate the effect of screened Coulomb type interaction and as such it may be used to investigate analytically the high energy scattering of electrons and the polarization of electrons by heavy atoms like mercury, gold, etc., through Dirac equation.

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Analytic continuations of the Lauricella function

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The Laplace transform of the product of three confluent hypergeometric functions is expressed in terms of Lauricella's function $F_A(\alpha,a_1,a_2,a_3;\ b_1,b_2,b_3;\ x,y,z)$. Two analytic continuation relations of the F_A function are obtained by making use of its Barnes integral representation. One analytic continuation leads to a set of one term transformation relations and in the second, F_A is expressed in terms of eight Lauricella F_B series. Analytic continuations are given for the F_B series, thereby allowing one to obtain a new analytic continuation for the F_A series. Our result is useful for calculating the F_A function when $|x|+|y|+|z|=2$, which occurs in the analysis of the electron scattering from the nucleus.

I. INTRODUCTION

Radial matrix elements of the radiative transitions between the states of a relativistic electron in a Coulomb field can be expressed as a Laplace transform of the product of three confluent hypergeometric functions:

$$I=\int_0^\infty dr\exp(-\Delta r)r^{\alpha-1}{}_1F_1(a_1,b_1,k_1r)$$

$$\times{}_1F_1(a_2,b_2,k_2r){}_1F_1(a_3,b_3,k_3r). \tag{1}$$

This integral can be expressed in terms of the hypergeometric function of Lauricella[1,2] by integrating the power of the integrand term-by-term to obtain

$$I=\Gamma(\alpha)\Delta^{-\alpha}F_A(\alpha,a_1,a_2,a_3,b_1,b_2,b_3;k_1/\Delta,k_2/\Delta,k_3/\Delta), \tag{2}$$

where F_A is the Lauricella's hypergeometric series which is defined as

$$F_A(\alpha,a_1,a_2,a_3,b_1,b_2,b_3;x,y,z)$$

$$=\sum_{m,n,l=0}^{\infty}\frac{(\alpha)_{m+n+l}(a_1)_m(a_2)_n(a_3)_l}{(b_1)_m(b_2)_n(b_3)_l m!n!l!}(x)^m(y)^n(z)^l. \tag{3}$$

The Lauricella F_A series is absolutely convergent if $|x|+|y|+|z|<1$.

Rozics and Johnson[3] have given analytic continuations of the Lauricella function F_A when one of its variables (say x) is greater than one and the remaining two are less than one. Also, the integral [Eq. (1)] can be expressed as infinite series of Appell's F_2 functions which are double infinite series. For problem of electron-nucleus scattering this integral [Eq. (1)] can be reduced in terms of a finite series[4,5] of Appell functions. Analytic continuations, as given in Refs. 5 and 6, for Appell's F_2 series have been used to compute the Lauricella function F_A, and Sud *et al.*[7] have developed a technique to evaluate the radial matrix elements of the radiative transitions. In this method the integrals are expressed in terms of a matrix generalization of the gamma function.[7,8] By making use of the recurrence relations satisfied by the matrix gamma function, the number of basic integrals that are required for the various electron scattering process are reduced to a minimum. This results in considerable saving of calculation time. The elements of such a 8×8 matrix gamma function are Lauricella function F_A. This has led us to investigate in details the analytic properties of the Lauricella function. We give in this paper two analytic continuations for the F_A function. In Sec. II we shall obtain eight one-term transformation relations for the F_A function and with the help of such relations we can continue F_A to a different region of x, y, and z space. A second continuation relation (given in Sec. IV) expresses the F_A series in terms of eight Lauricella's F_B series which have non-overlapping convergence domains. The Lauricella hypergeometric series F_B is defined as,[2]

$$F_B(a_1,a_2,a_3,b_1,b_2,b_3;c;x,y,z)$$

$$=\sum_{m,n,l}\frac{(a_1)_m(a_2)_n(a_3)_l(b_1)_m(b_2)_n(b_3)_l x^m y^n z^l}{(c)_{m+n+l}m!n!l!} \tag{4}$$

which is absolutely convergent for $|x|<1$, $|y|<1$, and $|z|<1$. Analytic continuations of the F_B series are given in Sec. V, which combined with the above result gives a new analytic continuation of the F_A function. In Sec. III we give an analytic continuation of the F_B function which has been used to derive the second analytic continuation relation for the F_A type of function. Finally in Sec VI we present a summary and our conclusion.

II. ONE-TERM CONTINUATION RELATION FOR F_A SERIES:

We shall obtain one-term continuation relations[9] for the F_A series by using the Barnes integral representation which is explicitly given as,

$$F_A(\alpha,a_1,a_2,a_3,b_1,b_2,b_3;x,y,z)$$

$$=\frac{1}{(2\pi i)^3}\frac{\Gamma(b_1)\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)\Gamma(\alpha)}$$

$$\times\iiint_{-i\infty}^{i\infty}ds\,dt\,du\,\frac{\Gamma(\alpha+s+t+u)\Gamma(a_1+s)\Gamma(a_2+t)\Gamma(a_3+u)}{\Gamma(b_1+s)\Gamma(b_2+t)\Gamma(b_3+u)}$$

$$\times\Gamma(-s)\Gamma(-t)\Gamma(-u)(-x)^s(-y)^t(-z)^u. \tag{5}$$

The integrand has the following sequences of poles: the increasing sequences of poles

$$s=n,\quad t=n,\quad \text{and}\quad u=n,\quad \text{where } n=0,1,2,\cdots;$$

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the decreasing sequences of poles

$s=-a_1-n$, $t=-a_2-n$, and $u=-a_3-n$, where

$n=0,1,2,\cdots$.

The F_A series is obtained by closing the contours in the t, u, and s planes on the right-hand side of the imaginary axis, and integrating by making use of the residue theorem. The Barnes integral representation for the F_2 series is given as[10]

$$F_2(\alpha,a_1,a_2,b_1,b_2;x,y)$$
$$=\frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(\alpha)}\frac{1}{(2\pi i)^2}\iint_{-i\infty}^{i\infty} ds\,dt$$
$$\times\frac{\Gamma(\alpha+s+t)\Gamma(a_1+s)\Gamma(a_2+t)\Gamma(-s)\Gamma(-t)(-x)^s(-y)^t}{\Gamma(b_1+s)\Gamma(b_2+t)}. \tag{6}$$

Thus by using the relation (6) we can express the integral representation for the Lauricella function F_A as a single integral which is explicitly given by

$$F_A(\alpha,a_1,a_2,a_3,b_1,b_2,b_3;x,y,z)$$
$$=\frac{\Gamma(b_3)}{2\pi i\Gamma(\alpha)\Gamma(a_3)}\int_{-i\infty}^{i\infty} du\,\frac{\Gamma(\alpha+u)\Gamma(a_3+u)\Gamma(-u)(-z)^u}{\Gamma(b_3+u)}$$
$$\times F_2(\alpha+u,\ a_1,a_2,b_1,b_2;x,y) \tag{7}$$

We will use the following transformation relations for the F_2 series[10]:

$$F_2(\alpha,a_1,a_2,b_1,b_2;\ x,y)$$
$$=(1-x)^{-\alpha}F_2\left(\alpha,b_1-a_1,\ a_2,b_1,b_2;\frac{x}{x-1},\frac{y}{1-x}\right)$$
$$=(1-y)^{-\alpha}F_2\left(\alpha,a_1,b_2-a_2,b_1,b_2;\frac{x}{1-y},\frac{y}{y-1}\right)$$
$$=(1-x-y)^{-\alpha}F_2\left(\alpha,b_1-a_1,\ b_2-a_2,\ b_1,b_2;\frac{x}{x+y-1},\right.$$
$$\left.\frac{y}{x+y-1}\right). \tag{8}$$

Substitution of the above transformation relation in Eq. (7) and integrating the resulting expression by closing the contour on the right-hand side of the imaginary axis with the help of the residue theorem, we obtain the following one-term relations for the F_A type of Lauricella function:

$$F_A(\alpha,a_1,a_2,a_3,b_1,b_2,b_3;\ x,y,z)$$
$$=(1-x)^{-\alpha}F_A\left(\alpha,b_1-a_1,\ a_2,a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{x-1},\frac{y}{1-x},\frac{z}{1-x}\right)$$
$$=(1-y)^{-\alpha}F_A\left(\alpha,a_1,b_2-a_2,a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{1-y},\frac{y}{y-1},\frac{z}{1-y}\right)$$
$$=(1-z)^{-\alpha}F_A\left(\alpha,a_1,a_2,b_3-a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{1-z},\frac{y}{1-z},\frac{z}{z-1}\right)$$
$$=(1-x-y)^{-\alpha}F_A\left(\alpha,b_1-a_1,\ b_2-a_2,\ a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{x+y-1},\frac{y}{x+y-1},\frac{z}{1-x-y}\right)$$
$$=(1-z-x)^{-\alpha}F_A\left(\alpha,b_1-a_1,\ a_2,b_3-a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{z+x-1},\frac{y}{1-z-x},\frac{z}{z+x-1}\right)$$
$$=(1-y-z)^{-\alpha}F_A\left(\alpha,a_1,b_2-a_2,\ b_3-a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{1-y-z},\frac{y}{y+z-1},\frac{z}{y+z-1}\right)$$
$$=(1-x-y-z)^{-\alpha}F_A\left(\alpha,b_1-a_1,\ b_2-a_2,\ b_3-a_3;b_1,b_2,b_3;\right.$$
$$\left.\frac{x}{x+y+z-1},\frac{y}{x+y+z-1},\frac{z}{x+y+z-1}\right). \tag{9}$$

III. AN ANALYTIC CONTINUATION OF THE F_B FUNCTION

In this section we will obtain an analytic continuation of the F_B type of Lauricella function in terms of eight F_A series where the variables of the F_A series are the reciprocals of the corresponding variables of the F_B series. The integral representation for the F_B function is given as

$$F_B(a_1,a_2,a_3,b_1,b_2,b_3;c;x,y,z)=\frac{1}{(2\pi i)^3}$$
$$\frac{\Gamma(c)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)\Gamma(b_1)\Gamma(b_2)\Gamma(b_3)}\iiint_{-i\infty}^{i\infty} ds\,dt\,du$$
$$\times\frac{\Gamma(a_1+s)\Gamma(a_2+t)\Gamma(a_3+u)\Gamma(b_1+s)\Gamma(b_2+t)\Gamma(b_3+u)}{\Gamma(c+s+t+u)}$$
$$\times\Gamma(-s)\Gamma(-t)\Gamma(-u)(-x)^s(-y)^t(-z)^u. \tag{10}$$

The integrand has the following sequences of poles:

(a) an increasing sequences of poles: $s=n$, $t=n$, and $u=n$, where $n=0,1,2,\cdots$; (b) a decreasing sequences of poles: $s=-a_1-n$, $t=-a_2-n$, $u=-a_3-n$, $s=-b_1-n$, $t=-b_2-n$, $u=-b_3-n$, where $n=0,1,2,\cdots$. The analytic continuation of the F_B function is obtained by closing the contours in the t, u, and s planes on the left-hand side of the imaginary axis, and integrating by making use of the residue theorem. The expression so obtained is given by

$$F_B\left(a_1, a_2, a_3, b_1, b_2, b_3; c; \frac{1}{x}, \frac{1}{y}, \frac{1}{z}\right)$$

$$= f(a_1, a_2, a_3, b_1, b_2, b_3)(-x)^{a_1}(-y)^{a_2}(-z)^{a_3} F_A[(1 + a_1 + a_2 + a_3 - c), a_1, a_2, a_3, 1 + a_1 - b_1, 1 + a_2 - b_2, 1 + a_3 - b_3; x, y, z]$$
$$+ f(a_1, a_2, b_3, b_1, b_2, a_3)(-x)^{a_1}(-y)^{a_2}(-z)^{b_3} F_A[(1 + a_1 + a_2 + b_3 - c), a_1, a_2, b_3, 1 + a_1 - b_1, 1 + a_2 - b_2, 1 + b_3 - a_3; x, y, z]$$
$$+ f(a_1, b_2, a_3, b_1, a_2, b_3)(-x)^{a_1}(-y)^{b_2}(-z)^{a_3} F_A[(1 + a_1 + b_2 + a_3 - c), a_1, b_2, a_3, 1 + a_1 - b_1, 1 + b_2 - a_2, 1 + a_3 - b_3; x, y, z]$$
$$+ f(a_1, b_2, b_3, b_1, a_2, a_3)(-x)^{a_1}(-y)^{b_2}(-z)^{b_3} F_A[(1 + a_1 + b_2 + b_3 - c), a_1, b_2, b_3, 1 + a_1 - b_1, 1 + b_2 - a_2, 1 + b_3 - a_3; x, y, z]$$
$$+ f(b_1, a_2, a_3, a_1, b_2, b_3)(-x)^{b_1}(-y)^{a_2}(-z)^{a_3} F_A[(1 + b_1 + a_2 + a_3 - c), b_1, a_2, a_3, 1 + b_1 - a_1, 1 + a_2 - b_2, 1 + a_3 - b_3; x, y, z]$$
$$+ f(b_1, a_2, b_3, a_1, b_2, a_3)(-x)^{b_1}(-y)^{a_2}(-z)^{b_3} F_A[(1 + b_1 + a_2 + b_3 - c), b_1, a_2, b_3, 1 + b_1 - a_1, 1 + a_2 - b_2, 1 + b_3 - a_3; x, y, z]$$
$$+ f(b_1, b_2, a_3, a_1, a_2, b_3)(-x)^{b_1}(-y)^{b_2}(-z)^{a_3} F_A[(1 + b_1 + b_2 + a_3 - c), b_1, b_2, a_3, 1 + b_1 - a_1, 1 + b_2 - a_2, 1 + a_3 - b_3; x, y, z]$$
$$+ f(b_1, b_2, b_3, a_1, a_2, a_3)(-x)^{b_1}(-y)^{b_2}(-z)^{b_3} F_A[(1 + b_1 + b_2 + b_3 - c), b_1, b_2, b_3, 1 + b_1 - a_1, 1 + b_2 - a_2, 1 + b_3 - a_3; x, y, z], \tag{11}$$

where

$$f(\lambda, \mu, \nu, \rho, \sigma, \tau) = \frac{\Gamma(c)\Gamma(\rho - \lambda)\Gamma(\sigma - \mu)\Gamma(\tau - \nu)}{\Gamma(\rho)\Gamma(\sigma)\Gamma(\tau)\Gamma(c - \lambda - \mu - \nu)}$$

and $[|\arg(-1/x)| < \pi,\ |\arg(-1/y)| < \pi,\ |\arg(-1/z)| < \pi]$.

IV. THE F_A FUNCTION EXPRESSED IN TERMS OF F_B FUNCTIONS

We can apply Eq. (11) to the following eight F_B series which have special relations among their variables and parameters:

$$F_B\left(a_1, a_2, a_3, b_1, b_2, b_3; 1 + a_1 + a_2 + a_3 - c; \frac{1}{x}, \frac{1}{y}, \frac{1}{z}\right),\quad F_B\left(1 - b_1, a_2, a_3, 1 - a_1, b_2, b_3; 2 - b_1 + a_2 + a_3 - c; \frac{x-1}{x}, \frac{1-x}{y}, \frac{1-x}{z}\right),$$

$$F_B\left(a_1, 1 - b_2, a_3, b_1, 1 - a_2, b_3; 2 + a_1 - b_2 + a_3 - c; \frac{1-y}{x}, \frac{y-1}{y}, \frac{1-y}{z}\right),\ F_B\left(a_1, a_2, 1 - b_3, b_1, b_2, 1 - a_3; 2 + a_1 + a_2 - b_3 - c; \frac{1-z}{x}, \frac{1-z}{y}, \frac{z-1}{z}\right),$$

$$F_B\left(1 - b_1, 1 - b_2, a_3, 1 - a_1, 1 - a_2, b_3; 3 - b_1 - b_2 + a_3 - c; \frac{x+y-1}{x}, \frac{x+y-1}{y}, \frac{1-x-y}{z}\right),$$

$$F_B\left(a_1, 1 - b_2, 1 - b_3, b_1, 1 - a_2, 1 - a_3; 3 + a_1 - b_2 - b_3 - c; \frac{1-y-z}{x}, \frac{y+z-1}{y}, \frac{y+z-1}{z}\right),$$

$$F_B\left(1 - b_1, a_2, 1 - b_3, 1 - a_1, b_2, 1 - a_3; 3 - b_1 + a_2 - b_3 - c; \frac{z+x-1}{x}, \frac{1-z-x}{y}, \frac{z+x-1}{z}\right),$$

$$F_B\left(1 - b_1, 1 - b_2, 1 - b_3, 1 - a_1, 1 - a_2, 1 - a_3; 4 - b_1 - b_2 - b_3 - c; \frac{x+y+z-1}{x}, \frac{x+y+z-1}{y}, \frac{x+y+z-1}{z}\right). \tag{12}$$

By making use of the one-term continuation relations for the F_A series, as given in Eq. (9), the eight F_A series obtained from use of Eq. (11) for each of the F_B series in Eq. (12) can be written in terms of eight F_A series explicitly appearing in Eq. (11). That is, we have a 8×8 matrix connecting eight F_A series and eight F_B series. This matrix can be inverted to give the following results:

$$F_A(1 + a_1 + a_2 + a_3 - \alpha, a_1, a_2, a_3, b_1, b_2, b_3; x, y, z) = AF_B\left(a_1, a_2, a_3, 1 + a_1 - b_1, 1 + a_2 - b_2, 1 + a_3 - b_3; \alpha; \frac{1}{x}, \frac{1}{y}, \frac{1}{z}\right)$$
$$+ BF_B\left(b_1 - a_1, a_2, a_3, 1 - a_1, 1 + a_2 - b_2, 1 + a_3 - b_3; b_1 - 2a_1 + \alpha; \frac{x-1}{x}, \frac{1-x}{y}, \frac{1-x}{z}\right)$$
$$+ CF_B\left(a_1, b_2 - a_2, a_3, 1 + a_1 - b_1, 1 - a_2, 1 + a_3 - b_3; b_2 - 2a_2 + \alpha; \frac{1-y}{x}, \frac{y-1}{y}, \frac{1-y}{z}\right)$$
$$+ DF_B\left(a_1, a_2, b_3 - a_3, 1 + a_1 - b_1, 1 + a_2 - b_2, 1 - a_3; b_3 - 2a_3 + \alpha; \frac{1-z}{x}, \frac{1-z}{y}, \frac{z-1}{z}\right)$$
$$+ EF_B\left(b_1 - a_1, b_2 - a_2, a_3, 1 - a_1, 1 - a_2, 1 + a_3 - b_3; b_1 - 2a_1 + b_2 - 2a_2 + \alpha; \frac{x+y-1}{x}, \frac{x+y-1}{y}, \frac{1-x-y}{z}\right)$$
$$+ FF_B\left(a_1, b_2 - a_2, b_3 - a_3, 1 + a_1 - b_1, 1 - a_2, 1 - a_3; b_2 - 2a_2 + b_3 - 2a_3 + \alpha; \frac{1-y-z}{x}, \frac{y+z-1}{y}, \frac{y+z-1}{z}\right)$$
$$+ GF_B\left(b_1 - a_1, a_2, b_3 - a_3, 1 - a_1, 1 + a_2 - b_2, 1 - a_3; b_1 - 2a_1 + b_3 - 2a_3 + \alpha; \frac{z+x-1}{x}, \frac{1-z-x}{y}, \frac{z+x-1}{z}\right)$$

$$+HF_B\left(b_1-a_1,b_2-a_2,b_3-a_3,1-a_1,1-a_2,1-a_3;b_1-2a_1+b_2-2a_2+b_3-2a_3+\alpha;\frac{x+y+z-1}{x},\frac{x+y+z-1}{y},\frac{x+y+z-1}{z}\right),\tag{13}$$

where

$$A=\frac{(x)^{-a_1}(y)^{-a_2}(z)^{-a_3}}{\Gamma(b_1-a_1)\Gamma(b_2-a_2)\Gamma(b_3-a_3)\Gamma(\alpha)},\quad B=\frac{(-x)^{a_1-b_1}(y)^{-a_2}(z)^{-a_3}(1-x)^{b_1-2a_1+\alpha-1}}{\Gamma(a_1)\Gamma(b_2-a_2)\Gamma(b_3-a_3)\Gamma(b_1-2a_1+\alpha)},$$

$$C=\frac{(x)^{-a_1}(-y)^{a_2-b_2}(z)^{-a_3}(1-y)^{b_2-2a_2+\alpha-1}}{\Gamma(b_1-a_1)\Gamma(a_2)\Gamma(b_3-a_3)\Gamma(b_2-2a_2+\alpha)},\quad D=\frac{(x)^{-a_1}(y)^{-a_2}(-z)^{a_3-b_3}(1-z)^{b_3-2a_3+\alpha-1}}{\Gamma(b_1-a_1)\Gamma(b_2-a_2)\Gamma(a_3)\Gamma(b_3-2a_3+\alpha)},$$

$$E=\frac{(-x)^{a_1-b_1}(-y)^{a_2-b_2}(z)^{-a_3}(1-x-y)^{b_1-2a_1+b_2-2a_2+\alpha-1}}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_3-a_3)\Gamma(b_1-2a_1+b_2-2a_2+\alpha)},\quad F=\frac{(x)^{-a_1}(-y)^{a_2-b_2}(-z)^{a_3-b_3}(1-y-z)^{b_2-2a_2+b_3-2a_3+\alpha-1}}{\Gamma(b_1-a_1)\Gamma(a_2)\Gamma(a_3)\Gamma(b_2-2a_2+b_3-2a_3+\alpha)},$$

$$G=\frac{(-x)^{a_1-b_1}(y)^{-a_2}(-z)^{a_3-b_3}(1-z-x)^{b_1-2a_1+b_3-2a_3+\alpha-1}}{\Gamma(a_1)\Gamma(b_2-a_2)\Gamma(a_3)\Gamma(b_1-2a_1+b_3-2a_3+\alpha)},\quad H=\frac{(-x)^{a_1-b_1}(-y)^{a_2-b_2}(-z)^{a_3-b_3}(1-x-y-z)^{b_1-2a_1+b_2-2a_2+b_3-2a_3+\alpha-1}}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)\Gamma(b_1-2a_1+b_2-2a_2+b_3-2a_3+\alpha)}.$$

V. ANALYTIC CONTINUATION OF THE F_B FUNCTION

In this section we will obtain analytic continuations of the F_B series which are useful when its variables are as follows:

(a) $x\approx 1$, $y<1$, and $z<1$ (b) $x\approx 1$, $y>1$, and $z<1$ (c) $x<1$, $1<y\leq 2$, and $z>2$.

The Barnes integral representation for the F_B type of Lauricella function is as given in Eq. (10). This can be expressed as a single integral representation by identifying the terms for the Appell's hypergeometric function F_3 and is given as,

$$=\frac{\Gamma(c)}{\Gamma(a_3)\Gamma(b_3)}\frac{1}{2\pi i}\int_{k-i\infty}^{k+i\infty}du\,\frac{\Gamma(a_3+u)\Gamma(b_3+u)\Gamma(-u)(-z)^u}{\Gamma(c+u)}\,F_3(a_1,a_2,b_1,b_2;c+u;x,y).\tag{14}$$

The contour in the u-plane parallels the imaginary axis, except that where necessary it is indented so that poles of $\Gamma(a_3+u)$, $\Gamma(b_3+u)$ lie to the left of the contour, and the poles of $\Gamma(-u)$ lie to the right of the contour. The real parameter k is chosen such that $k=\mathrm{Re}(a_1+b_1-c)+\epsilon$, where ϵ is a small positive number.

Appell's hypergeometric function has a number of analytic continuations. We make use of the following one which is valid for $|y|<1$ and $|1-x^{-1}|<1$[6]:

$$F_3(a_1,a_2,b_1,b_2;c;x,y)=Q_1+Q_2.\tag{15}$$

Q_1 and Q_2 are explicitly given as

$$Q_1=x^{-a_1}\frac{\Gamma(c)\Gamma(c-a_1-b_1)}{\Gamma(c-a_1)\Gamma(c-b_1)}\sum_{n,n}\frac{(a_1)_m(b_2)_n(a_2)_n(a_1+1-c)_{m-n}(1-x^{-1})^m y^n}{(c-b_1)_n(a_1+b_1+1-c)_{m-n}m!\,n!}$$

$$Q_2=x^{a_1-c}(1-x)^{c-a_1-b_1}\frac{\Gamma(c)\Gamma(a_1+b_1-c)}{\Gamma(a_1)\Gamma(b_1)}\sum_{m,n}\frac{(a_2)_n(b_2)_n(1-a_1)_m(c-a_1)_{m+n}(1-x^{-1})^m[y(1-x^{-1})]^n}{(c-a_1)_n(1+c-a_1-b_1)_{m+n}m!\,n!}.\tag{16}$$

Substituting this continuation relation into Eq. (14), we obtain two integrals in the u plane. We will write these as $F_B(a_1,a_2,a_3,b_1,b_2,b_3;c;x,y,z)=I_1+I_2$, where I_1 and I_2 are given explicitly by the following:

$$I_1=\frac{\Gamma(c)}{\Gamma(a_3)\Gamma(b_3)2\pi i}\int_{k-i\infty}^{k+i\infty}du\,\Gamma(a_3+u)\Gamma(b_3+u)\Gamma(-u)(-z)^u(x)^{-a_1}\frac{\Gamma(c+u-a_1-b_1)}{\Gamma(c+u-a_1)\Gamma(c+u-b_1)}$$

$$\times\sum_{m,n}\frac{(a_1)_m(b_2)_n(a_2)_n(a_1+1-c-u)_{m-n}(1-x^{-1})^m y^n}{(c+u-b_1)_n(a_1+b_1+1-c-u)_{m-n}m!\,n!},$$

$$I_2=\frac{\Gamma(c)x^{a_1-c}(1-x)^{c-a_1-b_1}}{\Gamma(a_3)\Gamma(b_3)\Gamma(a_1)\Gamma(b_1)}\frac{1}{2\pi i}\int_{k-i\infty}^{k+i\infty}du\,\Gamma(a_3+u)\Gamma(b_3+u)\Gamma(-u)(-z)^u(x^{-1}-1)^u\,\Gamma(a_1+b_1-c-u)$$

$$\times\sum_{m,n}\frac{(a_2)_n(b_2)_n(1-a_1)_m(c+u-a_1)_{m+n}(1-x^{-1})^m[y(1-x^{-1})]^n}{(u+c-a_1)_n(1+c+u-a_1-b_1)_{m+n}m!n!}. \tag{17}$$

Two different analytic continuations of the F_B functions can be obtained by either closing the contour in the u plane on the right in both terms, or by closing the contour on the left for I_1 and on the right for I_2. By using the asymptotic behavior of the gamma function, we find the conditions for absolute convergence of I_1 and I_2 when the contour is closed on the right in u plane to be $\mathrm{Re}(a_3+b_3-c)<1$, $|z|<1$, and $\mathrm{Re}(a_3+b_3+a_1+b_1-c)<2$, $|z(1-x^{-1})|<1$, respectively. The conditions for absolute convergence for I_1 when the contour in the u plane is closed on the left is $\mathrm{Re}(a_3+b_3-c)<1$, $|1/z|<1$.

The integrand of I_1 has ascending sequences of poles at $u=n$ and $u=a_1+b_1-c+1+n$ lying in the right-hand contour, and decreasing sequences of poles at $u=-a_3-n$, $u=-b_3-n$ and $u=a_1+b_1-c-n$ lying on the left-hand contour where $n=0,1,2,\cdots$. The integrand of I_2 has ascending sequences of poles lying in the right-hand contour at $u=n$ and $u=a_1+b_1-c+1+n$ for $n=0,1,\cdots$. Note that the particular separation between the left and right contours depends on the choice of k given following equation (14), but since the original integrand contains no singularities at a_1+b_1-c+n, the final result is independent of the particular choice of k. When closing both contours on the right, the sequences beginning at a_1+b_1-c+1 cancel and we can write $F_B(a_1,a_2,a_3,b_1,b_2,b_3;c;x,y,z)=A_1+A_2$, where A_1 and A_2, obtained by explicit integration in the u plane and use of the residue theorem, are given by

$$A_1=x^{-a_1}\frac{\Gamma(c)\Gamma(c-a_1-b_1)}{\Gamma(c-a_1)\Gamma(c-b_1)}\sum_{m,n,l}\frac{(a_1)_m(a_2)_n(b_2)_n(a_3)_l(b_3)_l(a_1+1-c)_{m-n-l}(1-x^{-1})^m y^n z^l}{(c-b_1)_{n+l}(a_1+b_1+1-c)_{m-n-l}m!n!l!},$$

$$A_2=x^{a_1-c}(1-x)^{c-a_1-b_1}\frac{\Gamma(c)\Gamma(a_1+b_1-c)}{\Gamma(a_1)\Gamma(b_1)}\sum_{m,n,l}\frac{(a_2)_n(b_2)_n(a_3)_l(b_3)_l(1-a_1)_m(c-a_1)_{m+n+l}(1-x^{-1})^m[y(1-x^{-1})]^n[z(1-x^{-1})]^l}{(c-a_1)_{n+l}(1+c-a_1-b_1)_{m+n+l}m!n!l!}. \tag{18}$$

For $|z|>1$, we need to close the contour in the u plane for I_1 on the left and for I_2 on the right. Doing so we can write

$$F_B(a_1,a_2,a_3,b_1,b_2,b_3;c;x,y,z)=c_1+c_2+c_3+c_4+c_5 \tag{19}$$

where these are explicitly given as

$$c_1=\frac{\Gamma(c)\Gamma(a_1+b_1-c)x^{a_1-c}(1-x)^{c-a_1-b_1}}{\Gamma(a_1)\Gamma(b_1)}\sum_{m,n,l}\frac{(1-a_1)_m(a_2)_n(a_3)_l(b_2)_n(b_3)_l(c-a_1)_{l+m+n}(1-x^{-1})^m[y(1-x^{-1})]^n[z(1-x^{-1})]^l}{(c-a_1)_{l+n}(1+c-a_1-b_1)_{l+m+n}m!n!l!},$$

$$c_2=\frac{\Gamma(c)\Gamma(a_1+b_1+a_3-c+1)\Gamma(a_1+b_1+b_3-c+1)\Gamma(c-1-a_1-b_1)}{\Gamma(a_1)\Gamma(b_1)\Gamma(a_3)\Gamma(b_3)}x^{-b_1}z(1-x^{-1})(-z)^{a_1+b_1-c}$$

$$\times\sum_{m,n,l}\frac{(1-a_1)_m(a_2)_n(b_2)_n(1+a_1+b_1+a_3-c)_l(1+a_1+b_1+b_3-c)_l}{(1+b_1)_{n+l}(2)_{m+n+l}(2+a_1+b_1-c)_l m!n!l!}(1+b_1)_{m+n+l}(2)_l(1-x^{-1})^m[y(1-x^{-1})]^n[z(1-x^{-1})]^l,$$

$$c_3=\frac{\Gamma(c)\Gamma(b_3-a_3)\Gamma(c-a_1-b_1-a_3)x^{-a_1}(-z)^{-a_3}}{\Gamma(b_3)\Gamma(c-a_1-a_3)\Gamma(c-b_1-a_3)}\sum_{m,n,l}\frac{(a_1)_m(b_2)_n(a_2)_n(a_3)_l(1+a_1+a_3-c)_{m-n+l}(1-x^{-1})^m y^n(-z)^{-l}}{(1+a_3-b_3)_l(1+a_1+b_1+a_3-c)_{m-n+l}(c-b_1-a_3)_{n-l}m!n!l!},$$

$$c_4=\frac{\Gamma(c)\Gamma(a_3-b_3)\Gamma(c-a_1-b_1-b_3)x^{-a_1}(-z)^{-b_3}}{\Gamma(a_3)\Gamma(c-a_1-b_3)\Gamma(c-b_1-b_3)}\sum_{m,n,l}\frac{(a_1)_m(b_2)_n(a_2)_n(b_3)_l(1+a_1+b_3-c)_{m-n+l}(1-x^{-1})^m y^n(-z)^{-l}}{(1+b_3-a_3)_l(c-b_1-b_3)_{n-l}(1+a_1+b_1+b_3-c)_{m-n+l}m!n!l!},$$

$$c_5=\frac{\Gamma(c)\Gamma(a_1+b_1+a_3-c)\Gamma(a_1+b_1+b_3-c)\Gamma(c-a_1-b_1)x^{-a_1}(-z)^{a_1+b_1-c}}{\Gamma(a_1)\Gamma(b_1)\Gamma(a_3)\Gamma(b_3)}$$

$$\times\sum_{m,n,l}\frac{(a_1)_m(b_2)_n(a_2)_n(1-b_1)_{m-n+l}(c-a_1-b_1)_l(1-x^{-1})^m y^n(-z)^{-l}}{(a_1)_{n-l}(1)_{m-n+l}(1+c-a_1-b_1-a_3)_l(1+c-a_1-b_1-b_3)_l m!n!}.$$

VI. CONCLUSIONS

The results given in Eq. (9) provide one-term transformation relations for the F_A function. To demonstrate this more explicitly, consider the case of electron scattering in the presence of a point nucleus of charge z. The incident and final electron energies (momenta) are $E_1(P_1)$ and $E_2(P_2)$, where $P=(E^2-m^2)^{1/2}$ and the energy lost by the electron is $w=E_1-E_2$. The radial integrals describing this process in the distorted-wave

Born approximation can be expressed in terms of Lauricella's F_A function with variables.

$$x=\frac{2P_1}{P_1+P_2+w},\quad y=\frac{2P_2}{P_1+P_2+w},\quad \text{and}\quad z=\frac{2w}{P_1+P_2+w}.$$

Moreover, $x+y+z=2$, and, therefore, the Lauricella function F_A needs to be analytically continued. The use of Eq. (9) leads us to F_A functions having the following new sets of variables:

(I)

$$x=\frac{2P_1}{P_1-P_2-w},\quad y=\frac{2P_2}{P_2+w-P_1},\quad \text{and}\quad z=\frac{2w}{P_2+w-P_1},$$

(II)

$$x=\frac{2P_1}{P_1+w-P_2},\quad y=\frac{2P_2}{P_2-P_1-w},\quad \text{and}\quad z=\frac{2w}{P_1+w-P_2},$$

(III)

$$x=\frac{2P_1}{P_1+P_2-w},\quad y=\frac{2P_2}{P_1+P_2-w},\quad \text{and}\quad z=\frac{2w}{w-P_1-P_2}.$$

This in itself does not lead to convergent series for the F_A function, but the different combination of variables provided by one term transformation relations opens avenues for seeking new continuation relations for the F_A functions.

The use of Eq. (13) transforms the F_A functions in terms of eight F_B functions thus providing a new analytic continuation of the F_A function. In the problem of scattering that we are considering here, this leads to F_B series of four different sets of variables (two series for each set) which are,

(I)

$$\frac{P_1+P_2+w}{2P_1},\quad \frac{P_1+P_2+w}{2P_2},\quad \text{and}\quad \frac{P_1+P_2+w}{2w},$$

(II)

$$\frac{P_1-P_2-w}{2P_1},\quad \frac{P_2+w-P_1}{2P_2},\quad \text{and}\quad \frac{P_2+w-P_1}{2w},$$

(III)

$$\frac{P_1+w-P_2}{2P_1},\quad \frac{P_2-P_1-w}{2P_2},\quad \text{and}\quad \frac{P_1+w-P_2}{2w},$$

(IV)

$$\frac{P_1+P_2-w}{2P_1},\quad \frac{P_1+P_2-w}{2P_2},\quad \text{and}\quad \frac{w-P_1-P_2}{2w}.$$

In set I we have one variable $x<1$ whereas the other variables are for $w<\frac{1}{2}E_1$, $1<y<2$, $z>2$ and for $w>\frac{1}{2}E_1$, $y>2$ and $1<z<2$. The use of the analytic continuation relation given in Eq. (19) will result in absolutely convergent series for both regions. The variable set II is very small for all w except at the end point $P_2\approx 0$ and hence the F_B function with set II variable is absolutely convergent except very near the end point which we do not consider. One of the variables in set III is always very near unity ($z_{III}\approx 1$) and $x_{III}<1$. The remaining variable y_{III} depends upon the energy transfer, for $w<\frac{1}{2}E_1$, $y_{III}<1$ and for $w>\frac{1}{2}E_1$, $y_{II}>1$. The use of continuations relation given in Eq. (18), for $w<\frac{1}{2}E_1$, and Eq. (19) (for $w>\frac{1}{2}E_1$) will result in absolutely convergent series. The variable set IV needs the same continuation relations as used for the variable set III. In set IV we have $x_{IV}<1$, $y_{IV}\approx 1$ whereas the third variable is $z_{IV}>1$ (for $w<\frac{1}{2}E_1$) and $z_{IV}<1$(for $w>\frac{1}{2}E_1$).

To summarize, we have found a new analytic continuation of the Lauricella F_A function when $|x|+|y|+|z|=2$. This condition occurs in the analysis of the electron scattering from the nucleus and may be of use in calculating the radial matrix elements.

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Yang–Mills equations in Maxwell form[a)]

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The Yang–Mills field equations are written in a form analogous to Maxwell's equations. The inherent nonlinearities are to be thought of as arising from a medium: The gauge fields then look like waves propagating in a medium. Some well-known solutions are considered in this approach.

1. INTRODUCTION

It is a nontrivial step to go from an Abelian to a non-Abelian gauge field theory. It is therefore natural to ask how much a non-Abelian theory differs from an Abelian one. The crucial difference is, of course, that the non-Abelian fields themselves carry the gauge quantum numbers or that they couple back to themselves; instead of

$$F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu \tag{1}$$

one has

$$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\nu A^a_\mu+gc_{abd}A^b_\mu A^d_\nu. \tag{2}$$

From the mathematical point of view, the essential difference is that $F^a_{\mu\nu}$ is not an exact form anymore! Unusual magnetic properties are therefore expected. 't Hooft's monoploe[1] is just a manifestation of that state of affairs. The $gc_{abd}A^b_\mu A^d_\nu$ term is at the same time interesting and cumbersome. Kogut and Susskind[2] prefer to consider an Abelian model with Higgs scalars, proposing the idea that the latter can mimic the $gc_{abd}A^b_\mu A^d_\nu$ term. The role of those Higgs scalars is to provide a medium with negative dielectric susceptibility such that electric flux tubes will be created, leading to confinement. We want to pursue the idea somewhat but we wish to keep a non-Abelian theory. We shall identify the nonlinearities in the Yang–Mills equations with the presence of a "medium."

The point is that the complete Yang–Mills field equations (for any gauge group) can be thrown in the form of the Maxwell's equations.[3] Some partial results were obtained using the idea of the holonomy group.[4] General symmetry conditions of homogeneity and isotropy were found which lead to Maxwell's equations for *microscopic* media. Here, we obtain Maxwell's equations for *macroscopic* media. The main difference is that the Maxwell fields $\mathbf{E},\mathbf{B},\mathbf{H},\mathbf{D}$, the polarization $\mathbf{P}$, the magnetization $\mathbf{M}$, the charge density ρ and the current $\mathbf{j}$ beome matrices because those objects are elements of the gauge group algebra. The non-Abelian character of the gauge field tensor is contained in the polarization $\mathbf{P}$ and in the magnetization $\mathbf{M}$.

2. THE YANG-MILLS FIELD EQUATIONS

The gauge field equations are

$$D_\mu\Phi^{\mu\nu}=\partial_\mu\Phi^{\mu\nu}+\eta[\Gamma_\mu,\Phi^{\mu\nu}]=J^\nu, \tag{3}$$

where

$$D_\mu X=\partial_\mu X+\eta[\Gamma_\mu,X] \tag{4}$$

and J^ν is the current due to external fields and may, if one wishes, contain a term linear in Γ^ν. We want to write Eq. (3) in the Maxwell form. Split $\Phi^{\mu\nu}$ as follows:

$$\Phi_{\mu\nu}=f_{\mu\nu}+M_{\mu\nu}, \tag{5}$$

with

$$f_{\mu\nu}=\partial_\mu\Gamma_\nu-\partial_\nu\Gamma_\mu, \tag{6}$$

$$M_{\mu\nu}=\eta[\Gamma_\mu,\Gamma_\nu]. \tag{7}$$

This splitting is not gauge covariant. The question of gauge transformation is studied in the Appendix. Introduce the effect of a macroscopic medium with a polarization $\mathbf{P}$ and a magnetization $\mathbf{M}$

$$\mathbf{P}=\eta[\Gamma_0,\boldsymbol{\Gamma}], \tag{8}$$

$$\mathbf{M}=\eta\boldsymbol{\Gamma}\times\boldsymbol{\Gamma}=\eta\epsilon_{kim}\Gamma^a_i\Gamma^b_m L_a L_b\neq 0 \tag{9}$$

where $\epsilon_{123}=1$ and vanishes if two indices are equal. It is odd under permutation of two indices. The three-vector $\boldsymbol{\Gamma}=\{\Gamma_k\}$ satisfies

$$\Gamma_k=-\Gamma^k=-A_k, \tag{10}$$

$$\Gamma_0=\Gamma^0=\varphi. \tag{11}$$

Then we have, as in the usual Maxwell theory:

$$\mathbf{B}=\nabla\times\mathbf{A}, \tag{12}$$

$$\mathbf{E}=-\nabla\varphi-\partial_0\mathbf{A}, \tag{13}$$

$$\mathbf{D}=\mathbf{E}+\mathbf{P}, \tag{14}$$

$$\mathbf{H}=\mathbf{B}-\mathbf{M}. \tag{15}$$

Remember that the above quantities do not commute in general! The equations of motion (3) become

$$\nabla\cdot\mathbf{D}=\rho+\eta[\mathbf{A},\mathbf{D}], \tag{16}$$

$$\nabla\times\mathbf{H}-\partial_0\mathbf{D}=-\mathbf{j}+\eta[\varphi,\mathbf{D}]+\eta(\mathbf{A}\times\mathbf{H}+\mathbf{H}\times\mathbf{A}). \tag{17}$$

One can show that $\partial^*_\mu f^{\mu\nu}=0$ which boils down to

$$\nabla\cdot\mathbf{B}=0, \tag{18}$$

$$\partial_0\mathbf{B}+\nabla\times\mathbf{E}=0. \tag{19}$$

Let us define

$$\Lambda=D_\mu\Gamma^\mu=\partial_\mu\Gamma^\mu=\partial_0\varphi+\nabla\cdot\mathbf{A}. \tag{20}$$

The equations of motion (16) and (17) become

$$(\partial_0^2-\nabla^2)\varphi=\rho+\partial_0\Lambda-\nabla\cdot\mathbf{P}+\eta[\mathbf{A},\mathbf{D}] \tag{21}$$

$$(\partial_0^2-\nabla^2)A=-\mathbf{j}+\nabla\times\mathbf{M}+\eta(\mathbf{A}\times\mathbf{H}+\mathbf{H}\times\mathbf{A})-\nabla\Lambda+\partial_0\mathbf{P}+\eta[\varphi,\mathbf{D}]. \tag{22}$$

or in Lorentz-covariant form as

$$\Box\Gamma_\mu=J_\mu+\partial_\mu(\partial^\lambda\Gamma_\lambda)-\partial^\lambda M_{\lambda\mu}-\eta[\Gamma^\lambda,\Phi_{\lambda\mu}] \tag{23}$$

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where $\Box = \partial^\lambda \partial_\lambda$ is the D'Alambertian. We would like to get some insight from classical electrodynamics of media. We are still allowed to choose a gauge and a gauge group. Consider Eq. (23) and rewrite it as

$$\Box \Gamma_\mu = J_\mu + \partial_\mu \Lambda - \eta \nabla^\lambda M_{\lambda\mu} - \eta[\Gamma^\lambda, f_{\lambda\mu}]. \tag{24}$$

In our point of view, $M_{\lambda\mu}$ should represent the medium due to the nonlinearities of the field. If we assume that those nonlinearities are everywhere uniform, the "polarization" and the "magnetization" behave as covariant constants in all directions:

$$\nabla_\rho M_{\lambda\mu} = 0. \tag{25}$$

Let us choose a less stringent condition of the form

$$\nabla^\lambda M_{\lambda\mu} = 0, \tag{26}$$

i.e., we assume that there are no sources for $M_{\lambda\mu}$. Furthermore, choose the Lorentz gauge

$$\nabla^\lambda \Gamma_\lambda = \partial^\lambda \Gamma_\lambda = 0. \tag{27}$$

Using Eq. (26) and (27), Eq. (24) becomes

$$\Box \Gamma_\mu - \eta[\Gamma^\lambda, [\Gamma_\lambda, \Gamma_\mu]] - \eta[\Gamma^\lambda, \partial_\mu \Gamma_\lambda] = 0. \tag{28}$$

If we assume an ansatz where the space–time and internal degrees of freedom are related as follows,

$$\Gamma_\mu = j(x) L_\mu \tag{29}$$

where L_μ are constant matrices, we obtain

$$\Box \Gamma_\mu - \eta[\Gamma^\lambda, [\Gamma_\lambda, \Gamma_\mu]] = 0. \tag{30}$$

Such an equation was first obtained by Treat,[5] where he used some ad hoc assumptions. We obtain it as a consequence of a physical condition. This brings some support to our approach. Now, specify the system further: assume that

$$\Gamma_0 = \Gamma_z = 0, \quad \Gamma_x = \varphi(z,t) X, \quad \Gamma_y = \varphi(z,t) Y \tag{31}$$

so that X, Y, Z are related by an SO(3) algebra:

$$[X,Y] = Z, \quad [Z,X] = Y, \quad [Y,Z] = X. \tag{32}$$

One then gets a well known 1-space, 1-time dimensional problem:

$$\Box \varphi - \varphi^3 = 0. \tag{33}$$

The relevance of the φ-cubed equation as a limit of the Yang–Mills equation was stressed by many,[6] especially in relation to conformal invariance and the instanton.

For a source-free Yang–Mills field, the uniformity condition (25) or the ansatz (29) is not so general. We would like to evaluate our approach and see whether the quantities we defined previously characterize the known solutions or not. We see it is so indeed in the case of two well-known solutions.

3. TWO EXAMPLES

It is interesting to compare the different ansätzes people used to look for solutions of the Yang–Mills field equations. Let us first consider the Wu–Yang ansatz[7]:

$$\Gamma = \mathbf{r} \times \mathbf{L} (e r^2)^{-1}, \quad \Gamma \Gamma_0 = 0 \tag{34}$$

where $\mathbf{L} = (L_1, L_2, L_3)$ are the generators of the SU(2) algebra. In our framework, we can describe it as follows.

(1) It is a static solution: no time dependence.

(2) The scalar current density and all electric components vanish

$$\mathbf{E} = \mathbf{P} = \mathbf{D} = 0, \quad \rho = 0. \tag{35}$$

(3) The vector current density is essentially given by the vector potential

$$\mathbf{j} = -r^{-2} \Gamma. \tag{36}$$

(4) All the magnetic quantities are proportional and point in the same direction of isospace, $R = r_a L_a$

$$\mathbf{M} = \mathbf{H} = \tfrac{1}{2} \mathbf{B} = (e r^3)^{-1} \mathbf{r} R. \tag{37}$$

(5) The field equations reduce to:

$$\nabla \cdot \mathbf{B} = 0, \quad \partial_0 \mathbf{B} = 0, \quad \nabla \times \mathbf{H} = \mathbf{j}. \tag{38}$$

The next step is the version of Prasad and Sommerfield[8]:

$$\Gamma = (e r^2)^{-1} (1 - K(r)) \mathbf{r} \times \mathbf{L}, \quad \Gamma_0 = 0, \tag{39}$$

where

$$K(r) = Cr \operatorname{csch} Cr,$$

$$H(r) = Cr \coth Cr - 1.$$

Here also exact solutions have been found. We can summarize it as follows:

(1) It is a static solution: No time dependence.

(2) The scalar current density and all electric components vanish,

$$\mathbf{E} = \mathbf{P} = \mathbf{D} = 0, \quad \rho = 0. \tag{40}$$

(3) The magnetic components have more structure. The magnetization has the nice Wu–Yang behavior,

$$\mathbf{M} = (e r^3)^{-1} (K(r) - 1)^2 \hat{\mathbf{r}} R. \tag{41}$$

On the other hand, B and H need a superposition of two canonical directions in isospace:

$$\begin{aligned} \mathbf{B} &= (e r^3)^{-1} (2 - 2K - KH) \hat{\mathbf{r}} R + (e r^2)^{-1} KH \mathbf{L}, \\ \mathbf{H} &= -(e r^3)^{-1} (KH + K^2 - 1) \hat{\mathbf{r}} R + (e r^2)^{-1} KH \mathbf{L}. \end{aligned} \tag{42}$$

The conclusion to be drawn from those examples is that given a simple ansatz for Γ, the magnetization remains simple. On the other hand, the magnetic field is complicated due to the presence of the derivative $\nabla \times \Gamma$, although it has an Abelian look: $(\partial_k \Gamma_l - \partial_l \Gamma_k)$. The new approach is to look for a simple ansatz for $\mathbf{B} = \nabla \times \Gamma$ instead! Work is in progress and will be reported separately.

4. CONCLUSION

At the present time, the full Yang–Mills equations are untractable except for very special cases. It is thus welcome to gain as much physical insight as possible. The present note is an attempt to stress this point: nonlinearities should be thought of as a medium. We brought the Yang–Mills equations in a form which re-

sembles that of a wave propagating in some sort of medium; this is to be contrasted with all the static solutions discovered so far!

We have shown that a covariant divergence-free medium supplemented by some elementary assumption leads to a well known case related to the instanton. Using the Wu–Yang and the Prasad–Sommerfield solutions, we discover that the magnetic part contains all the information.

APPENDIX

Consider a general gauge transformation,

$$\Gamma'_\mu = \Lambda(\theta)\Gamma_\mu\Lambda^{-1}(\theta) - \eta^{-1}(\partial_\mu\Lambda(\theta))\Lambda^{-1}(\theta)$$

with the following infinitesemial properties

$$\delta\Gamma_\mu = i\eta^{-1}\partial_\mu\theta + i[\Gamma_\mu, \theta],$$

$$\delta\Phi_{\mu\nu} = i[\Phi_{\mu\nu}, \theta].$$

It is straightforward to show that D and H transform covariantly:

$$\delta\mathbf{D} = i[\mathbf{D}, \theta], \quad \delta\mathbf{H} = i[\mathbf{H}, \theta]$$

On the other hand, all the other fields transform with a noncovariant piece:

$$\delta\mathbf{E} = i[\mathbf{E}, \theta] + i\Delta\mathbf{E}, \quad \delta\mathbf{P} = i[\mathbf{P}, \theta] + i\Delta\mathbf{P},$$

where

$$\Delta\mathbf{E} = -\Delta\mathbf{P} = [\mathbf{\Gamma}, \partial_0\theta] - [\mathbf{\Gamma}_0, \nabla\theta],$$

$$\delta\mathbf{B} = i[\mathbf{B}, \theta] + i\Delta\mathbf{B},$$

$$\delta\mathbf{M} = i[\mathbf{M}, \theta] + i\Delta\mathbf{M},$$

where

$$\Delta\mathbf{B} = \Delta\mathbf{M} = \mathbf{\Gamma}\times\nabla\theta + \nabla\theta\times\mathbf{\Gamma}.$$

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Note on the entropy production in a discrete Markov system

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The Prigogine inequalities on the rate of entropy production are derived by information theoretic methods for a discrete open Markov system. A new inequality is proposed. A comparison is made with similar results due to Levine and co-workers.

1. INTRODUCTION

The information theory has been used with success by several authors[1–4] to determine the time-dependent orientational distribution function of molecules in liquids and gases from the experimentally measured dipolar and quadrupolar autocorrelation functions. A similar method has been applied by Bernstein, Levine, and co-workers[5–8] to predict the time evolution law of averaged values of observables, with practical applications for vibrational relaxation of a gas and chemical reactions.

These methods are based on the extremal properties of the information entropy or of the entropy deficiency, which have been studied extensively by Levine and co-workers[6–8] for systems obeying a linear discrete Markov equation.

The purpose of this article is to show that the existence of a master equation is not indispensable in these considerations. In particular, the Prigogine principle on the rate of entropy production[9–11] will be derived easily by using the characteristic evolution equation of a Markov system, which even provides additional informations on the entropy production.

In the first place we shall briefly review the definition and the properties of the entropy deficiency.

2. ENTROPY DEFICIENCY AND EVOLUTION OF A DISCRETE OPEN SYSTEM

2.1. Evolution equation

Following the model of Refs. 7, 12, or 13, we consider a discrete Markov system, satisfying the characteristic evolution equation

$$p_i(t+\tau)=\sum_{i'} p_{i'}(t)\,Y_{i'i}(\tau) \quad (\tau>0). \tag{1}$$

Here $p_i(t)$ is the probability of finding the system in state i at time t, and $Y_{i'i}(\tau)$ is the transition probability from i' to i during the time interval $[t, t+\tau]$; thus

$$\sum_{i} Y_{i'i}(\tau)=1. \tag{2}$$

The Markov process is supposed to be homogeneous, so that $Y_{i'i}(\tau)$ does not depend on the origin t of the time interval.

If the system is in contact with thermodynamic reservoirs, it usually tends to thermodynamic equilibrium with the reservoirs if they are in equilibrium between themselves, or more generally to a stationary state. Thus we admit the existence of a stationary solution $\{p_i^\circ\}$ of (1), satisfying the relation

$$\sum_{i'} p_{i'}^\circ Y_{i'i}(\tau)=p_i^\circ=\sum_{i'} p_i^\circ Y_{ii'}(\tau) \tag{3}$$

or in terms of the transition rates $W_{ii'}=\lim_{\tau\to 0}\tau^{-1}\cdot Y_{ii'}(\tau)$ $(i\neq i')$,

$$\sum_{i'} p_{i'}^\circ W_{i'i}=\sum_{i'} p_i^\circ W_{ii'}, \tag{3'}$$

a relation which replaces the bilateral normalization of the transition rates for an isolated system.[13–15]

However we shall use relation (2) rather than (3), since for our purpose it is not necessary to introduce the master equation corresponding to (1).

2.2. Entropy deficiency

In order to study the evolution of the system, it is convenient to define the function

$$F(t)=\sum_i p_i(t)\log\frac{p_i(t)}{p_i^\circ}. \tag{4}$$

With different notations, this function has been introduced by Tolman[16]; it was used by Levine, Bernstein, and co-workers[6,7] under the name of entropy deficiency: indeed when the system tends to equilibrium with a thermodynamic reservoir, $F(t)$ is the entropy produced in the system during its evolution from time t to equilibrium, excluding the entropy transferred from or to the reservoir.[7]

In this case the system interacts with the reservoir by exchanging n extensive quantities $X^1, \cdots, X^n$; the equilibrium distribution has the classical form

$$p_i^\circ=\frac{1}{Z_0}\exp\left(-\sum_{r=1}^{n}\lambda_r^\circ X_i^r\right), \tag{5}$$

X_i^r being the value of the quantity X^r corresponding to state i of the system.

Thus one may write

$$F(t)=A(t)-A^\circ=-\Delta A \tag{6}$$

using the thermodynamic potential

$$A^\circ=-\log Z^\circ \tag{7}$$

and its nonequilibrium value

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$$A(t)=\sum_r \lambda_r^\circ \sum_i p_i X_i^r + \sum_i p_i \log p_i$$

$$=\sum_r \lambda_r^\circ \langle X^r\rangle(t) - S(t) \tag{8}$$

with the usual definition of the time-dependent averages $\langle X^r\rangle\ (t)$ and of the entropy $S(t)$.

Noting that during the evolution of the system from time t the change in the entropy of the reservoir is

$$\Delta S_R = -\sum_r \lambda_r^\circ \Delta\langle X^r\rangle = \sum_r \lambda_r^\circ (\langle X^r\rangle(t) - \langle X^r\rangle^\circ),$$

Eq. (6) may be written

$$F(t)=\Delta S_R + \Delta S = \Delta(S_R + S)$$

which indeed shows that $F(t)$ is the entropy produced by the inversible process.

However the definition of the function $F(t)$ is not restricted to this case, since the distribution $\{p_i^\circ\}$ need only be stationary in order to established its main properties.

2.3. Properties of the entropy deficiency $F(t)$

The physical interpretation of $F(t)$ and its formal definition involves two well-known properties: $F(t)$ is positive and decreases to 0 as t tends to infinity.[7] It is worth noting that these properties may be proved easily with the aid of Eqs. (1), (2) and (3) only. Indeed, since the function $\varphi(x)=x\log x$ is concave ($d^2\varphi/dx^2>0$) and since by (2)

$$\sum_{i'} \frac{p_{i'}^\circ}{p_i^\circ} Y_{i'i}(\tau) = 1 \tag{9}$$

we have

$$\sum_{i'} \frac{p_{i'}^\circ}{p_i^\circ} Y_{i'i}(\tau)\varphi\left(\frac{p_{i'}(t)}{p_{i'}^\circ}\right) \geqslant \varphi\left(\sum_{i'} \frac{p_{i'}^\circ}{p_i^\circ} Y_{i'i}(\tau)\frac{p_{i'}(t)}{p_{i'}^\circ}\right)$$

$$=\varphi\left(\frac{p_i(t+\tau)}{p_i^\circ}\right). \tag{10}$$

Multiplying (10) by p_i° and summing on i give the classical result

$$F(t+\tau)\leqslant F(t). \tag{11}$$

The equality holding only if $p_i(t)=p_i^\circ$ for all i, in which case $F=0$. The positivity of F also follows from the concavity of φ since

$$F=\sum_i p_i^\circ \varphi\left(\frac{p_i}{p_i^\circ}\right) \geqslant \varphi\left(\sum_i p_i^\circ \frac{p_i}{p_i^\circ}\right) = 0. \tag{12}$$

As it has been pointed out by Levine[7] the same properties would hold if φ were any concave function such that $\varphi(1)=0$. Levine has shown that the present choice, leading to the entropy deficiency F, is more significant physically, but we shall see that the quadratic approximation of F near the stationary state may be mathematically simpler.

3. EXTREMAL PROPERTIES OF ENTROPY PRODUCTION

3.1. Rate of entropy production

It follows from Sec. 2.1 that $F(t)-F(t+\tau)$ may be identified[7] with the entropy produced between t and $t+\tau$ and that the rate of entropy production is

$$\sigma = -\frac{dF}{dt}. \tag{13}$$

With the aid of classical irreversible thermodynamics, Prigogine[9] has proved that $d\sigma/dt<0$ near equilibrium, when the linear relation between fluxes and forces hold, and that $d_X\sigma/dt<0$ in the general case, $d_X\sigma/dt$ being the time derivative of σ for constant fluxes.

By considering the discrete equilivalent of d^2F/dt^2,

$$\Delta^2 F = F(t-\tau)+F(t+\tau)-2F(t), \tag{14}$$

it will be shown that the method of Sec. 2.3, based on the direct application of the evolution equation (1), permits us to derive similar results in the framework of information theory.

This approach will partly follow the method of Levine,[7] with appreciable simplifications and additional results.

3.2. System near equilibrium

Let us suppose that the system is at the end of its irreversible evolution, so that the distribution $p_i(t)$ is not very different from the stationary distribution p_i°. Then writing

$$p_i(t)=p_i^\circ + x_i(t)$$

one may expand $F(t)$ in powers of $x_i(t)$, the quadratic approximation of F being

$$F_a(t)=\sum_i \frac{1}{2p_i^\circ}(x_i(t))^2. \tag{15}$$

Like $F(t)$, $F_a(t)$ is positive and decreases to 0 as t goes to infinity. Furthermore, we shall see that F_a is a concave function of time:

$$\frac{d^2F_a}{dt^2}>0 \tag{16}$$

if the detailed balance relation is satisfied by the distribution $\{p_i^\circ\}$. This relation is realized if $\{p_i^\circ\}$ corresponds to equilibrium with a thermodynamic reservoir[17,18] and may be written with the aid of the transition probabilities

$$p_{i'}^\circ Y_{i'i}(\tau)=p_i^\circ Y_{ii'}(\tau) \tag{17}$$

or, more conventionally, with the transition rates

$$p_{i'}^\circ W_{i'i}=p_i^\circ W_{ii'}. \tag{17'}$$

Then we have

$$F_a(t)=\sum_{i,i'} \frac{1}{2p_i^\circ} x_i(t)x_{i'}(t-\tau)Y_{i'i}(\tau)$$

$$=\sum_{i,i'} \frac{1}{2p_{i'}^\circ} x_{i'}(t-\tau)x_i(t)Y_{ii'}(\tau) \tag{18}$$

$$=\sum_i \frac{1}{2p_i^\circ} x_i(t-\tau)x_i(t+\tau),$$

so that

$$\Delta^2 F_a = F_a(t-\tau)+F_a(t+\tau)-2F_a(t)$$

$$=\sum_i \frac{1}{2p_i^\circ}(x_i(t-\tau)-x_i(t+\tau))^2 \geqslant 0, \tag{19}$$

the equality being only satisifed if $x_i(t-\tau)=x_i(t+\tau)$ for all i, which implies $F_a(t-\tau)=F_a(t)=F_a(t+\tau)$ and $\{p_i(t)\}=\{p_i^\circ\}$.

The inequality (19) is equivalent to (16) and may be considered as a microscopic version of the inequality of Prigogine. It should be noted that (19) applies if $\{p_i^\circ\}$ is not thermodynamic equilibrium but any stationary distribution satisfying the detailed balance (17).

3.3. General case

Far from equilibrium, (19) still holds, but $F_a(t)$ is no longer an approximation of $F(t)$.

In order to find an equivalent to the generalized inequality of Prigogine, one has to define forces and fluxes, which may be done according to the method of Levine and co-workers.[6,7]

Let us consider a number of physical quantities X^r associated with the system, and their average values at time t: $\langle X^r\rangle(t)$, which may be measured by real experiences. In principle, the nonequilibrium probability distribution $\{p_i(t)\}$ could be completely specified by giving the values $\langle X^1\rangle(t),\cdots,\langle X^N\rangle(t)$ of N such average quantities,[13] but Procaccia, Shimoni, and Levine[6] have shown that practically the evolution of the system is determined by the knowledge of a small number of $\langle X^r\rangle(t)$ only, say $\langle X^1\rangle(t),\cdots,\langle X^n\rangle(t)$, with $n\ll N$; the remaining quantities change in such a way that the entropy deficiency $F(t)$ has always the smallest value consistent with formula (4) and the constraints on $\{p_i\}$:

$$\sum_i p_i=1,\qquad \sum_i p_i X_i^r=\langle X^r\rangle(t)\quad (r=1,2,\ldots,n). \tag{20}$$

Then with the notations of formula (5), the desequilibrium distribution $\{p_i(t)\}$ is given by the semiequilibrium form

$$p_i(t)\cong\bar p_i(t)=\frac{1}{Z(t)}\exp\left(-\sum_r\lambda_r(t)X_i^r\right). \tag{21}$$

The time-dependent parameters $Z(t)$, $\lambda_1(t),\ldots,\lambda_n(t)$ are determined by the constraints (20), and tend to the equilibrium values Z°, $\lambda_1^\circ,\ldots,\lambda_n^\circ$ as $t\to\infty$.

$\lambda_r(t)$ is naturally identified with a force, corresponding to the flux $(d/dt)\langle X^r\rangle(t)$. [$(d/dt)\langle X^r\rangle(t)$ is a flux in the conventional sense only if X^r is an extensive quantity, as assumed in Sec. 2.1; this is generally true.]

We are now in a position to derive the generalized Prigogine inequality immediately. Indeed we may write

$$\Delta^{\bar 2}F=F(t-\tau)+F(t+\tau)-2F(t)=A+B, \tag{22}$$

with

$$A=\sum_i p_i(t-\tau)\log\frac{p_i(t-\tau)}{p_i(t)}+p_i(t+\tau)\log\frac{p_i(t+\tau)}{p_i(t)} \tag{23}$$

and

$$B=\sum_i\{p_i(t-\tau)+p_i(t+\tau)-2p_i(t)\}\log\frac{p_i(t)}{p_i^\circ} \tag{24}$$

The concavity of $x\log x$, which involves the positivity of F by (12), also involves the positivity of A; it may even be asserted that A decreases with time (see Sec. 4.2).

As for B, it may be written, by (21),

$$B=-\sum_{r=1}^n\mu_r(t)\{\langle X^r\rangle(t-\tau)+\langle X^r\rangle(t+\tau)-2\langle X^r\rangle(t)\}, \tag{25}$$

with

$$\mu_r(t)=\lambda_r(t)-\lambda^\circ \tag{26}$$

Thus B vanishes if the fluxes $(d/dt)\langle X^r\rangle(t)$ remain constant, and we may conclude, with obvious notation,

$$\Delta_X^{\bar 2}F=A\geq 0 \tag{27}$$

$$\Delta_X^{\bar 3}F=\Delta_X A\leq 0. \tag{28}$$

The inequalities (26) and (27) are equivalent to the generalized inequality of Prigogine,

$$\frac{d_X}{dt}\sigma\leq 0 \tag{29}$$

and to

$$\frac{d_X^2}{dt^2}\sigma\geq 0. \tag{30}$$

Another, still easier way to recover inequality (29) is to note that

$$\frac{dF}{dt}=\sum_i\left\{\log\frac{p_i(t)}{p_i^\circ}\right\}\cdot\frac{dp_i}{dt}=-\sum_r\mu_r(t)\cdot\frac{d}{dt}\langle X^r\rangle(t) \tag{31}$$

by (5), (21), and (26), and that

$$\frac{d^2F}{dt^2}=\sum_i\frac{1}{p_i(t)}\left(\frac{dp_i}{dt}\right)^2+\sum_i\left\{\log\frac{p_i(t)}{p_i^\circ}\quad\frac{d^2p_i}{dt^2}\right\}. \tag{32}$$

The first term on the right-hand side of (32) is positive; the second term may be expressed as

$$-\sum_r\mu_r(t)\cdot\frac{d^2}{dt^2}\langle X^r\rangle(t)$$

and it vanishes at constant fluxes. Inequality (29) follows, but (30) is not obtained so easily in this way.

4. DISCUSSION

We shall conclude with some remarks on the preceding results.

4.1. At first, it should be remembered that formula (21) for the probability $p_i(t)$, although convenient for practical purposes, is only an approximation: such a probability distribution need not satisfy the microscopic evolution equation (1) exactly.

Thus the positivity of the entropy production $\sigma=-dF/dt$, is given by (4) and (21), does not result from a rigorous derivation, but from a physical approximation. Contrarily, the generalized Prigogine inequality: $d_X\sigma/dt<0$ is exact when $p_i(t)$ takes the semiequilibrium form (21).

On the other hand, if the entropy production is computed with the exact probability distribution, its positivity is mathematically established, but the Prigogine principle follows from the approximation of F near equilibrium. However, from a macroscopic point of view, this principle does not simply express the micro-

scopic inequality (16), which only holds very near equilibrium: The domain of validity of the principle is probably much wider macroscopically than it is in its microscopic form. This is due to the fact that the Prigogine inequality follows from the generalized form (29) in the region where the fluxes depend on the forces linearly; but it is known[19,20] that linear macroscopic laws does not imply microscopic linearity.

These considerations are made more precise in Appendix A.

4.2. Finally, we shall note that definition (4) of $F(t)$ may be extended by replacing the stationary distribution $\{p_i^\circ\}$ by any distribution $\{q_i(t)\}$ solution of the evolution equation (1). It is easily verified the new function $F_{\{q_i\}}(t)$ obtained in this way is a positive and decreasing function of t, since the derivations of Sec. 2.3 apply word for word if (9) is replaced by

$$\sum_{i'} \frac{q_{i'}(t)}{q_i(t+\tau)} Y_{i'i}(\tau) = 1. \tag{33}$$

This remark has already be employed to derive (28), but it may have other applications. Let us suppose for instance that the external constraints due to the reservoirs are changed slowly, so that the "stationary" distribution $\{p_i^\circ\}$ follows these changes, that is to say, it varies slowly with time, but the relaxation proper to the system is much faster. Then it is natural to define the F function with the aid of the quasistationary distribution $\{p_i^\circ\}$: This function is positive and decreases to 0 as does the entropy deficiency defined with a time-independent distribution $\{p_i^\circ\}$.

This problem is similar to the evolution of a probability distribution $\{p_i(t)\}$, solution of Eq. (1), towards the semiequilibrium form $\bar{p}_i(t)$ given by (21). It is shown in Appendix B, with the aid of the previous discussion that the entropy deficiency $F(t)$, calculated with $\{p_i(t)\}$ is always greater than the entropy deficiency $\bar{F}(t)$ calculated with $\{\bar{p}_i(t)\}$ (which is obvious from the definition of $\bar{p}_i$) and that

$$\frac{dF}{dt} < \frac{d\bar{F}}{dt} < 0 \tag{34}$$

conformly to a result of Levine.[7]

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APPENDIX A: PRIGOGINE PRINCIPLE AND LINEAR LAWS NEAR EQUILIBRIUM

The flux of quantity $\langle X^r \rangle$ may be expressed with the aid of the master equation corresponding to (1), as[6,13]

$$\frac{d}{dt}\langle X^r \rangle = \sum_{i,i'} p_i(t)\, W_{ii'}(X_{i'}^r - X_i^r)$$

$$= \sum_{i,i'} p_i(t)\, L_{ii'} X_{i'}^r, \tag{A1}$$

with

$$L_{ii'} = W_{ii'} - \delta_{ii'}\left(\sum_{i''} W_{ii''}\right). \tag{A2}$$

If $p_i(t)$ has the semiequilibrium form (21), we may write

$$\frac{p_i(t)}{p_i^\circ} = \exp\left(-\sum_{r=0}^{n} \mu_r(t) X_i^r\right), \tag{A3}$$

with

$$\mu_0(t) = \log(Z(t)/Z^\circ),$$

$$\mu_r(t) = \lambda_r(t) - \lambda^\circ \quad (r = 1, \ldots, n).$$

As $t \to \infty$, $\mu_r(t) \to 0$, and near equilibrium

$$p_i(t) \cong p_i^\circ \left(1 - \sum_{r=0}^{n} \mu_r(t) X_i^r\right). \tag{A4}$$

Then, since $\sum_i p_i^\circ L_{ii'} = 0$, (A1) is transformed into the linear relation

$$\frac{d}{dt}\langle X^r \rangle = \sum_s M^{rs} \mu_s(t), \tag{A5}$$

with

$$M^{rs} = \sum_{i,i'} p_i^\circ L_{ii'} X_i^s X_{i'}^r. \tag{A6}$$

The Onsager symmetry relation

$$M^{rs} = M^{sr} \tag{A7}$$

corresponds to the relation of detailed balance,

$$p_i^\circ L_{ii'} = p_{i'}^\circ L_{i'i}.$$

Now, following the method of irreversible thermodynamics, one sees that by (A5) and (A6)

$$\sum_{r=0}^{n} \mu_r \cdot \frac{d^2}{dt^2}\langle X^r \rangle = \sum_{r=1}^{n} \frac{d}{dt}\mu_r \cdot \frac{d}{dt}\langle X^r \rangle. \tag{A8}$$

Thus the two terms on the right-hand side of (32) are equal and positive, and $d^2F/dt^2 > 0$, or $d^2\sigma/dt^2 < 0$.

APPENDIX B: COMPARISON OF $F(t)$ AND $\bar{F}(t)$

Let $p_i(t)$ be any probability distribution satisfying the evolution equation (1), and $\bar{p}_i(t)$ the semiequilibrium distribution (21), corresponding to the same average values $\langle X^r \rangle(t)$ as $p_i(t)$. $\bar{p}_i(t)$ is supposed to be also a solution of the evolution equation. Then the entropy deficiencies $F(t)$ and $\bar{F}(t)$, corresponding to $p_i(t)$ and $\bar{p}_i(t)$, are compared by noting that

$$F(t) - \bar{F}(t) = \sum_i \left\{ p_i(t) \log \frac{p_i(t)}{p_i^\circ} - \bar{p}_i(t) \log \frac{\bar{p}_i(t)}{p_i^\circ} \right\}$$

$$= \sum_i p_i(t) \log \frac{p_i(t)}{\bar{p}_i(t)} + \sum_i \{p_i(t) - \bar{p}_i(t)\} \log \frac{\bar{p}_i(t)}{p_i^\circ}. \tag{B1}$$

Now by (21), the second term in the right side of (B1) is

$$\sum_i \{p_i(t) - \bar{p}_i(t)\} \cdot \left\{ -\sum_{r=0}^{n} \mu_r(t) X_i^r \right\} = 0$$

since

$$\sum_i p_i(t) X_i^r = \sum_i \bar{p}_i(t) X_i^r.$$

Thus

$$F(t) - \bar{F}(t) = \sum_i p_i(t) \log \frac{p_i(t)}{\bar{p}_i(t)}. \tag{B2}$$

According to Sec. 4.2, this expression is positive and decreases with time, so that

$$\sigma = -\frac{dF}{dt} > \bar{\sigma} = -\frac{d\bar{F}}{dt} > 0, \tag{B3}$$

conformly to the result obtained by Levine[7] by a more general but rather complicated method.

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Criticality of neutron transport in a slab with finite reflectors

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The purpose of this paper is to investigate the subcriticality and the supercriticality for the neutron transport in a slab which is surrounded by two finite reflectors. The mathematical problem is to determine when the coupled boundary-value problem has or has no positive solution. It is shown under some explicit conditions on the material properties of the transport mediums and the size of the slab length that the coupled problem has a unique solution which insures the subcriticality of the system. It is also shown under some different conditions on the same physical quantities that the system cannot have a nonnegative solution when there is an external source, and it only has the trivial solution when there is no source in the system. This conclusion leads to the supercriticality of the system. Both upper and lower bounds for the critical length of the slab are explicitly given.

I. INTRODUCTION

A physically important and mathematically interesting problem in neutron transport in slab geometry is to predict the critical length of the slab in terms of the materials property of the transport medium. This problem has been discussed by many investigators, and various methods are proposed.[1-7] However most of the discussions are devoted either to vacuum boundary condition or with given incident neutrons at the slab faces. When the slab is surrounded by reflectors, then incoming neutrons at the slab faces are no longer known and its intensity is intrinsically related to the neutron's density in the reflectors. Although the critical size of the slab is independent of prescribed incoming fluxes at the slab faces, it may be affected by the surrounding reflectors. In order to investigate this effect and other related problems, we consider a nonhomogeneous monoenergetic slab of length $2a$ which is surrounded by two finite reflectors with equal length b. Then according to the neutrons balance relation, the equations governing the neutron densities $N_1(x, \mu)$ in the slab and $N_2(x, \mu)$, $N_3(x, \mu)$ in the right and the left reflectors are given, respectively, by

$$\mu \frac{\delta N_i}{\delta x} + N_i = \tfrac{1}{2} c_i \int_{-1}^{1} \sigma_i(x, \mu, \mu') N_i(x, \mu') d\mu' + q_i(x, \mu),$$

$$x \in I_i, \ \mu \in [-1, 1], \ i = 1, 2, 3, \tag{1.1}$$

where we have taken, for simplicity, the total cross sections of the slab and the reflectors as one (so that the values of $2a$ and b should be considered as optical thickness). In Eq. (1,1), c_i is the average number of secondary neutrons per collision, q_i is the external source, σ_i is the scattering cross section satisfying the condition

$$\tfrac{1}{2} \int_{-1}^{1} \sigma_i(x, \mu, \mu') d\mu' \leq 1,$$

and the intervals I_i are given, respectively, by

$$I_1 = [-a, a], \quad I_2 = [a, a+b], \quad I_3 = [-a-b, -a].$$

Suppose no neutron enters the reflectors from outside. Then the equations in (1.1) are coupled through the following boundary conditions:

$$\begin{aligned} &N_1(a, \mu) = N_2(a, \mu) && (-1 \leq \mu \leq 1), \\ &N_2(a+b, \mu) = 0 && (-1 \leq \mu < 0), \\ &N_1(-a, \mu) = N_3(-a_1 \mu) && (-1 \leq \mu \leq 1), \\ &N_3(-a-b, \mu) = 0 && (0 < \mu \leq 1). \end{aligned} \tag{1.2}$$

The slab problem with finite reflectors has been investigated by Busoni, Frosali, and Mangiarotti[8] in relation to the spectral properties of the corresponding transport operator and by Burkart, Ishiguro, and Siewert[9] for the case of one reflector in a linear anisotropic medium. The same problem with two finite reflectors has recently been discussed by the author[10] concerning the existence of a solution for a nonhomogeneous anisotropic medium. It was shown in Ref. 10 that under certain conditions on the physical quantities c_i, σ_i, a, b, the boundary value problem (1.1), (1.2) has a "maximal" solution and a "minimal" solution which can be constructed by a straightforward iteration process. The existence of these solutions is based on the notion of an upper solution and the construction of such a function. A natural question to be answered is whether the maximal solution coincides with the minimal solution and whether the system has a unique nonnegative solution. Moreover, it is interesting to know under what conditions on the physical parameters the coupled system (1.1), (1.2) has no nonnegative solution. The first problem involves the question of subcriticality while the second one concerns with supercriticality. The purpose of this paper is to investigate these questions. Specifically, we show, under some conditions on c_i, σ_i, a, b, that the system (1.1), (1.2) has exactly one nonnegative solution for every nonnegative source q_i. We also show under some different conditions on these quantities that this system has no nonnegative solution when the sources q_1, q_2, q_3 are not all identically zero and it only has the trivial solution when $q_i \equiv 0$ for every i. Hence the existence of a unique solution in

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the first case implies the subcriticality of the system while the nonexistence result means that the system is supercritical. An important aspect of these results is that it leads to a characterization of the subcriticality and supercriticality of the system and thus yields upper and lower bounds for the critical value of c_i in terms of the physical quantities σ_i, a, b. These conditions also give some interesting interrelating effect between the slab and the reflectors, and demonstrate the fact that criticality of the system depends only on the various cross sections of the transport mediums and the size of the transport region but not on the external sources. It is to be pointed out that the conclusions of this paper include the case of a slab surrounded by vacuum. In fact, we shall deduce some results for the no re-entry slab problem as those obtained in Refs. 6, 7.

2. UNIQUENESS PROBLEM—SUBCRITICALITY

Throughout the paper we assume that the functions q_i and $\int_{-1}^{1}\sigma_i(x, \mu, \mu')d\mu'$ are continuous nonnegative functions on $I_i\times[-1, 1]$. The aim of this section is to establish some conditions on the physical quantities σ_i, c_i, a, b such that the problem (1.1), (1.2) has exactly one nonnegative solution for every nonnegative source q_i. Since the existence of a nonnegative solution has already been shown in Ref. 10, we only need to show the uniqueness problem. Our uniqueness proof is based on the intrinsic property of the maximal and the minimal solution which are obtained through the construction of two monotone sequences from a corresponding integral equation by a suitable choice of the initial iterations. Specifically, if we set

$$(f_i(N_i))(x, \mu)\equiv \tfrac{1}{2}c_i\int_{-1}^{1}\sigma_i(x, \mu, \mu')N_i(x, \mu')d\mu' + q_i(x, \mu), \quad i=1, 2, 3, \tag{2.1}$$

then the integral equation corresponding to the boundary-value problem (1.1), (1.2) is in the form (cf. Ref. 10):

$$N_i(x, \mu)=(F_i(\mathcal{N}))(x, \mu), \quad x\in I_i, \quad \mu\in[-1, 1], \quad i=1, 2, 3, \tag{2.2}$$

where $\mathcal{N}=(N_1, N_2, N_3)$ and

$$(F_1(\mathcal{N}))(x, \mu) \equiv \begin{cases} \exp[-(a+x)/\mu](g_3(N_3))(\mu)+\int_0^{(a+x)/\mu}\exp(-\tau)(f_1(N_1))\times(x-\tau\mu, \mu)d\tau & (0<\mu\le 1), \\ \exp[(a-x)/\mu](g_2(N_2))(\mu)+\int_0^{(a-x)/(-\mu)}\exp(-\tau)(f_1(N_1))\times(x-\tau\mu, \mu)d\tau & (-1\le\mu<0), \end{cases}$$

$$(F_2(\mathcal{N}))(x, \mu) \begin{cases} \exp[-(x-a)/\mu][\exp(-2a/\mu)(g_3(N_3))(\mu)+(g_1(N_1))(\mu)] \\ +\int_0^{(x-a)/\mu}\exp(-\tau)(f_2(N_2))(x-\tau\mu, \mu)d\tau \quad (0<\mu\le 1) \\ \int_0^{(a+b-x)/\mu}\exp(-\tau)(f_2(N_2))(x-\tau\mu, \mu)d\tau \quad (-1\le\mu<0) \end{cases}$$

$$(F_3(\mathcal{N}))(x, \mu) \equiv \begin{cases} \int_0^{(a+b+x)/\mu}\exp(-\tau)(f_3(N_3))(x-\tau\mu, \mu)d\tau \quad (0<\mu\le 1), \\ \exp[-(a+x)/\mu][\exp(2a/\mu)(g_2(N_2))(\mu)+(\tilde{g}_1(N_1))(\mu)] \\ +\int_0^{(a+x)/\mu}\exp(-\tau)(f_3(N_3))(x-\tau\mu, \mu)d\tau \quad (-1\le\mu<0). \end{cases} \tag{2.3}$$

In the above expressions the functions $\tilde{g}_1(N_1)$ and $g_i(N_i)$, $i=1, 2, 3$, are given, respectively by

$$(\tilde{g}_1(N_1))(\mu) \equiv \int_0^{2a/(-\mu)}\exp(-\tau)(f_1(N_1))(-a-\tau\mu, \mu)d\tau \quad (-1\le\mu<0),$$

$$(g_1(N_1))(\mu) \equiv \int_0^{2a/\mu}\exp(-\tau)(f_1(N_1))(a-\tau\mu, \mu)d\tau \quad (0<\mu\le 1), \tag{2.4}$$

$$(g_2(N_2))(\mu) \equiv \int_0^{b/(-\mu)}\exp(-\tau)(f_2(N_2))(a-\tau\mu, \mu)d\tau \quad (-1\le\mu<0),$$

$$(g_3(N_3))(\mu) \equiv \int_0^{b/\mu}\exp(-\tau)(f_3(N_3))(-a-\tau\mu, \mu)d\tau \quad (0<\mu\le 1).$$

From the integral equation (2.2), we can construct a sequence $\{\mathcal{N}^{(k)}\}\equiv\{N_1^{(k)}, N_2^{(k)}, N_3^{(k)}\}$ successively from the recursion formula

$$N_i^{(k)}(x, \mu)=(F_i(\mathcal{N}^{(k-1)}))(x, \mu), \quad x\in[-1, 1], \quad i=1, 2, 3, \tag{2.5}$$

by a suitable choice of the initial iteration $\mathcal{N}^{(0)}\equiv(N_1^{(0)}, N_2^{(0)}, N_3^{(0)})$. Assume there exists an upper solution $\tilde{\mathcal{N}}\equiv(\tilde{N}_1, \tilde{N}_2, \tilde{N}_3)$ which is defined to be a continuous nonnegative function satisfying the inequality

$$\tilde{N}_i(x, \mu)\ge(F_i(\tilde{\mathcal{N}}))(x, \mu), \quad x\in I_i, \quad \mu\in[-1, 1], \quad i=1, 2, 3. \tag{2.6}$$

Then starting from the initial iteration $\mathcal{N}^{(0)}=\tilde{\mathcal{N}}$ and $\mathcal{N}^{(0)}=0$, respectively, we obtain two sequences from (2.5) which are denoted by $\{\overline{\mathcal{N}}^{(k)}\}$ and $\{\underline{\mathcal{N}}^{(k)}\}$. It can easily be shown that the sequence $\{\overline{\mathcal{N}}^{(k)}\}$ is monotone non-increasing while $\{\underline{\mathcal{N}}^{(k)}\}$ is monotone non-decreasing and $\underline{\mathcal{N}}^{(k)}\le\overline{\mathcal{N}}^{(k)}$ for every $k=1, 2, \cdots$ (cf. Ref. 10). Here $\underline{\mathcal{N}}^{(k)}\le\overline{\mathcal{N}}^{(k)}$ means that $\underline{N}_i^{(k)}(x, \mu)\le\overline{N}_i^{(k)}(x, \mu)$ for every $x\in I_i$, $\mu\in[-1, 1]$, $i=1, 2, 3$. Thus, if an upper solution does exist, then $\{\overline{\mathcal{N}}^{(k)}\}$ converges to a "maximal" solution $\overline{\mathcal{N}}$ and $\{\underline{\mathcal{N}}^{(k)}\}$ converges to a "minimal" solution $\underline{\mathcal{N}}$ and $\overline{\mathcal{N}}\ge\underline{\mathcal{N}}\ge 0$. Since every nonnegative solution is also an upper solution, it is clear that upper solution may or may not exist depending on the physical quantities σ_i, c_i, a, b. In order to give some conditions on these quantities so that Eq. (2.2) has a unique or has no nonnegative solution, it is convenient to use the following notations:

$$\bar{\sigma}_i(\mu')\equiv\sup\{\sigma_i(x, \mu, \mu'); \ x\in I_i, \ \mu\in[-1, 1]\},$$

$$\underline{\sigma}_i(\mu')\equiv\inf\{\sigma_i(x, \mu, \mu'); \ x\in I_i, \ \mu\in[-1, 1]\},$$

$$\overline{\sum}_i(\mu') \equiv \max\{\bar{\sigma}_i(\mu'),\ \bar{\sigma}_i(-\mu')\},$$
$$\underline{\sum}_i(\mu') \equiv \min\{\underline{\sigma}_i(\mu'),\ \underline{\sigma}_i(-\mu')\}. \tag{2.7}$$

Before proving our uniqueness result, we state the following existence theorem from Ref. 10.

Theorem 2.1: Assume that

$$\begin{aligned} &c_1\int_0^1 \overline{\sum}_1(\mu)\{1-\exp[-(a+b)/\mu]\}d\mu < 1,\\ &c_i\int_0^1 \overline{\sum}_i(\mu)\{1-\tfrac{1}{2}(\exp[-(2a+b)/\mu]+\exp(-b/\mu))\}d\mu < 1,\\ &(i=2,3). \end{aligned} \tag{2.8}$$

Then for any nonnegative source q_i, Eq. (2.2) has a maximal solution $\overline{N}$ and a minimal solution $\underline{N}$. Furthermore,

$$\overline{N} \geq \underline{N} \geq 0.$$

The above theorem has recently been proven through the construction of an upper solution $\tilde{N}$. A novelty of this theorem is the nonnegative property of the function $(\overline{N}-\underline{N})$ which is crucial in the proof of our uniqueness theorem.

Theorem 2.2: Assume that (2.8) holds and that

$$\begin{aligned} &c_1\int_0^1\{\overline{\sum}_1(\mu)(1-\exp(-a/\mu))\\ &\quad+\tfrac{1}{2}[\overline{\sum}_2(\mu)+\overline{\sum}_3(\mu)](1-\exp(-2a/\mu))\}d\mu \equiv c_1L_1<1,\\ &c_2\int_0^1\{\overline{\sum}_2(\mu)(1-\exp(-b/2\mu)+\tfrac{1}{2}[\overline{\sum}_1(\mu)\\ &\quad+\overline{\sum}_3(\mu)\exp(-2a/\mu)](1-\exp(-b/\mu))\}d\mu\\ &\quad\equiv c_2L_2<1,\\ &c_3\int_0^1\{\overline{\sum}_3(\mu)(1-\exp(-b/2\mu))\\ &\quad+\tfrac{1}{2}[\overline{\sum}_1(\mu)+\overline{\sum}_2(\mu)\exp(-2a/\mu)](1-\exp(-b/\mu))\}d\mu\\ &\quad\equiv c_3L_3<1. \end{aligned} \tag{2.9}$$

Then the maximal solution $\overline{N}\equiv(\overline{N}_1,\overline{N}_2,\overline{N}_3)$ coincides with the minimal solution $\underline{N}\equiv(\underline{N}_1,\underline{N}_2,\underline{N}_3)$. Moreover, Eq. (2.2) has exactly one nonnegative solution for every nonnegative source q_i.

Proof: Let $N_i=\overline{N}_i-\underline{N}_i\geq 0$ and set

$$\phi_i(x)\equiv\int_{-1}^1\overline{\sum}_i(\mu)N_i(x,\mu)d\mu,\quad x\in I_i,\quad i=1,2,3. \tag{2.10}$$

Since N_i satisfies Eq. (2.2) with $q_i\equiv 0$, we have

$$\phi_i(x)=\int_{-1}^1\overline{\sum}_i(\mu)(F_i(\mathcal{N}))(x,\mu)d\mu,\quad i=1,2,3, \tag{2.11}$$

where $F_i(\mathcal{N})$ is given by (2.3) with $q_i\equiv 0$ and $\mathcal{N}=(N_1,N_2,N_3)$.

Let $x_i\in I_i$ such that

$$\phi_i(x_i)=\max\{\phi(x);\ x\in I_i\},\quad i=1,2,3.$$

Then by (2.11) and the definition of $F_i(\mathcal{N})$,

$$\begin{aligned} \phi_1(x_1)=&\int_0^1\exp[-(a+x_1)/\mu]\overline{\sum}_1(\mu)(g_3(N_3))(\mu)d\mu\\ &+\int_0^1\int_0^{(a+x_1)/\mu}\overline{\sum}_1(\mu)\exp(-\tau)(f_1(N_1))(x_1-\tau\mu,\mu)d\tau\,d\mu\\ &+\int_0^1\exp[-(a-x_1)/\mu]\overline{\sum}_1(-\mu)(g_2(N_2))(-\mu)d\mu\\ &+\int_0^1\int_0^{(a-x_1)/\mu}\overline{\sum}_1(-\mu)\exp(-\tau)(f_1(N_1))(x_1+\tau\mu,-\mu)d\tau\,d\mu\\ \equiv& s_1(x_1)+s_2(x_1)+s_3(x_1)+s_4(x_1), \end{aligned} \tag{2.12}$$

where $s_j(x_1)$, $j=1,\ldots,4$, denote the four integrals in (2.12). In obtaining the above expression we have replaced μ by $(-\mu)$ in the last two integrals. Similar expressions for $\phi_2(x_2)$, $\phi_3(x_3)$ can be obtained from (2.11), (2.3). Since $x_1\in I_1$ and

$$\begin{aligned} &-a\leq(x_1-\tau\mu)\leq x_1 \quad\text{when } 0\leq\tau\leq(a+x_1)/\mu,\\ &x_1\leq x_1+\tau\mu\leq a \quad\text{when } 0\leq\tau\leq(a-x_1)/\mu, \end{aligned} \tag{2.13}$$

we see from (2.1) (with $q_i\equiv 0$) and the nonnegative property of N_1 that

$$\begin{aligned} &(f_1(N_1))(x_1-\tau\mu,\mu)\leq\tfrac{1}{2}c_1\\ &\quad\times\int_{-1}^1\overline{\sum}_1(\mu')N_1(x_1-\tau\mu,\mu')d\mu'\leq\tfrac{1}{2}c_1\phi_1(x_1),\\ &(f_1(N_1))(x_1+\tau\mu,-\mu)\leq\tfrac{1}{2}c_1\\ &\quad\times\int_{-1}^1\overline{\sum}_1(\mu')N_1(x_1+\tau\mu,\mu')d\mu'\leq\tfrac{1}{2}c_1\phi_1(x_1) \end{aligned}$$

for all τ in the indicated intervals in (2.13). The above inequalities imply that

$$\begin{aligned} &s_2(x_1)\leq\tfrac{1}{2}c_1\phi_1(x_1)\int_0^1\overline{\sum}_1(\mu)\{1-\exp[-(a+x_1)/\mu]\}d\mu\\ &s_4(x_1)\leq\tfrac{1}{2}c_1\phi_1(x_1)\int_0^1\overline{\sum}_1(\mu)\{1-\exp[-(a-x_1)/\mu]\}d\mu, \end{aligned} \tag{2.14}$$

where we have used the fact that $\overline{\sum}_1(-\mu)=\overline{\sum}_1(\mu)$. Similarly, since $(a+\tau\mu)\in I_2$, $(-a-\tau\mu)\in I_3$ for $0\leq\tau\mu\leq b$, we have

$$\begin{aligned} &(f_2(N_2))(a+\tau\mu,-\mu)\\ &\quad\leq\tfrac{1}{2}c_2\int_0^1\overline{\sum}_2(\mu')N_2(a+\tau\mu,\mu')d\mu'\leq\tfrac{1}{2}c_2\phi_2(x_2),\\ &(f_3(N_3))(-a-\tau\mu,\mu)\\ &\quad\leq\tfrac{1}{2}c_3\int_0^1\overline{\sum}_3(\mu')N_3(-a-\tau\mu,\mu')d\mu'\leq\tfrac{1}{2}c_3\phi_3(x_3) \end{aligned}$$

for $0\leq\tau\mu\leq b$. Hence by the definition of $g_2(N_2)$, $g_3(N_3)$, we obtain

$$\begin{aligned} &(g_2(N_2))(-\mu)\leq\tfrac{1}{2}c_2\phi_2(x_2)[1-\exp(-b/\mu)]\\ &(g_3(N_3))(\mu)\leq\tfrac{1}{2}c_3\phi_3(x_3)[1-\exp(-b/\mu)] \end{aligned} \qquad (0<\mu\leq 1).$$

It follows from (2.12) that

$$s_1(x_1)\leq\tfrac{1}{2}c_3\phi_3(x_3)$$

$$\times \int_0^1 \overline{\Sigma}_1(\mu) \exp[-(a+x_1)/\mu][1-\exp(-b/\mu)]d\mu, \tag{2.15}$$

$$s_3(x_1) \leq \tfrac{1}{2} c_2\phi_2(x_2)$$

$$\times \int_0^1 \overline{\Sigma}_1(\mu) \exp[-(a-x_1)/\mu\,[1-\exp(-b/\mu)]d\mu.$$

Application of the estimates given by (2.14), (2.15), in (2.12) yields

$$\phi_1(x_1) \leq \tfrac{1}{2} c_1\phi_1(x_1) \int_0^1 \overline{\Sigma}_1(\mu)$$

$$\times \{2-\exp[-(a+x_1)/\mu]-\exp[-(a-x_1)/\mu]\}d\mu$$

$$+ \tfrac{1}{2} c_2\phi_2(x_2) \int_0^1 \overline{\Sigma}_1(\mu) \exp[-(a-x_1)/\mu][1-\exp(-b/\mu)]d\mu$$

$$+ \tfrac{1}{2} c_3\phi_3(x_3) \int_0^1 \overline{\Sigma}_1(\mu) \exp[-(a+x_1)/\mu][1-\exp(-b/\mu)]d\mu. \tag{2.16}$$

Since for each fixed $\mu \in (0, 1]$ the function

$$\rho_1(x_1) \equiv 2-\exp[-(a+x_1)/\mu]-\exp[-(a-x_1)/\mu] \tag{2.17}$$

is convex, its maximum value occurs at $x_1 = 0$ and thus $\rho_1(x_1) \leq 2[1-\exp(-a/\mu)]$.

Hence

$$\phi_1(x_1) \leq c_1\phi_1(x_1)$$

$$\times \int_0^1 \overline{\Sigma}_1(\mu)[1-\exp(-a/\mu)]d\mu$$

$$+ \tfrac{1}{2} c_2\phi_2(x_2) \int_0^1 \overline{\Sigma}_1(\mu)[1-\exp(-b/\mu)]d\mu$$

$$+ \tfrac{1}{2} c_3\phi_3(x_3) \int_0^1 \overline{\Sigma}_1(\mu)[1-\exp(-b/\mu)]d\mu. \tag{2.18}$$

By an analogous argument for $\phi_2(x_2)$, $\phi_3(x_3)$, we obtain

$$\phi_2(x_2) \leq c_2\phi_2(x_2)$$

$$\times \int_0^1 \overline{\Sigma}_2(\mu)[1-\exp(-b/2\mu)]d\mu$$

$$+ \tfrac{1}{2} c_3\phi_3(x_3) \int_0^1 \overline{\Sigma}_2(\mu) \exp(-2a/\mu)[1-\exp(-b/\mu)]d\mu$$

$$+ \tfrac{1}{2} c_1\phi_1(x_1) \int_0^1 \overline{\Sigma}_2(\mu)[1-\exp(-2a/\mu)]d\mu, \tag{2.19}$$

$$\phi_3(x_3) \leq c_3\phi_3(x_3) \int_0^1 \overline{\Sigma}_3(\mu)[1-\exp(-b/2\mu)]d\mu$$

$$+ \tfrac{1}{2} c_1\phi_1(x_1) \int_0^1 \overline{\Sigma}_3(\mu)[1-\exp(-2a/\mu)]d\mu$$

$$+ \tfrac{1}{2} c_2\phi_2(x_2) \int_0^1 \overline{\Sigma}_3(\mu)\exp(-2a/\mu)[1-\exp(-b/\mu)]d\mu. \tag{2.20}$$

Addition of the inequalities (2.18)—(2.20) leads to the relation

$$\phi_1(x_1)+\phi_2(x_2)+\phi_3(x_3) \leq c_1L_1\phi_1(x_1)$$

$$+ c_2L_2\phi_2(x_2) + c_3L_3\phi_3(x_3),$$

where L_1, L_2, L_3 are the integrals appeared in (2.9). It follows from the hypothesis that $\phi_1(x_1)+\phi_2(x_2)+\phi_3(x_3) = 0$. But $\phi_i(x_i) \geq 0$ we must have $\phi_1(x_1) = \phi_2(x_2) = \phi_3(x_3) = 0$, that is,

$$\int_{-1}^1 \overline{\Sigma}_i(\mu) N_i(x, \mu)d\mu = 0 \quad \text{for all } x \in I_i,\ i = 1, 2, 3.$$

In view of (2.1) with ($q_i \equiv 0$), we see that $(f_i(N_i))(x, \mu) = 0$ for $x \in I_i$, $\mu \in [-1, 1]$ and, in particular, $(\tilde{g}_1(N_1))(\mu) = 0$ and $(g_i(N_i))(\mu) = 0$, $i = 1, 2, 3$. It follows from (2.3) that $(F_i(\mathcal{N})) = 0$ and thus, by (2.2), $N_i(x, \mu) = 0$ on $I_i \times [-1, 1]$. This proves $\mathcal{N} = \underline{\mathcal{N}}$. Now if $\mathcal{N}^*$ is any nonnegative solution of (2.2). Then by definition it is also an upper solution. The above-established conclusion shows that $\mathcal{N}^* = \underline{\mathcal{N}}$. Therefore, Eq. (2.2) has only one nonnegative solution. This completes the proof of the theorem.

If the two reflectors on the sides of the slab are identical, then $c_2 = c_3$ and $\sigma_2 = \sigma_3$. In this case, condition (2.9) reduces to

$$c_1 \int_0^1 [\overline{\Sigma}_1(\mu)[1-\exp(-a/\mu)] + \overline{\Sigma}_2(\mu)[1-\exp(-2a/\mu)]d\mu < 1,$$

$$c_2 \int_0^1 \{\tfrac{1}{2}\overline{\Sigma}_1(\mu)[1-\exp(-b/\mu)]$$

$$+ \overline{\Sigma}_2(\mu)[(1-\exp(-b/2\mu)$$

$$+ \tfrac{1}{2}\exp(-2a/\mu)]\}d\mu < 1. \tag{2.21}$$

In particular, if the slab and the reflectors are homogenoeus isotropic, then we may take $\sigma_i = 1$ for each i. In this situation, (2.9) becomes

$$c_1 \int_0^1 [2-\exp(-a/\mu)-\exp(-2a/\mu)]d\mu < 1,$$

$$c_2 \int_0^1 [(1-\exp(-b/2\mu)$$

$$+ \tfrac{1}{2}[1-\exp(-b/\mu)(1+\exp(-2a/\mu)]d\mu < 1. \tag{2.22}$$

In conclusion we have the following:

Corollary: Let the two reflectors be identical and let (2.8) hold. Then the system (2.2) is subcritical if (2.21) is satisfied. In case the slab and the reflectors are homogeneous isotropic, then (2.2) is subcritical if (2.22) holds.

Remark 2.1: When there is no reflector at the slab faces, that is, when the slab is embedded in vacuum, we may set $c_2 = c_3 = \overline{\Sigma}_2 = \overline{\Sigma}_3 = 0$ in (2.9) to obtain the condition

$$c_1 \int_0^1 \overline{\Sigma}_1(\mu)[1-\exp(-a/\mu)]\,d\mu < 1. \tag{2.23}$$

Under this condition the requirement (2.8) is also fulfilled by letting $b = 0$. In this situation, condition (2.23) alone is sufficient to insure the subcriticality of the system. This result coincides with the one obtained in Ref. 6 for the slab problem without reflectors. Notice that in the general case with reflectors the second term in the first integral in (2.21) gives the effect of the reflectors on the subcriticality of the slab problem.

3. NONEXISTENCE PROBLEM—SUPERCRITICALITY

It is seen from Theorem 2.2 that if (2.8), (2.9) hold, then the system (1.1), (1.2) is subcritical. A natural question about this system is that under what condition on the same physical parameters the system has no nonnegative solution. The purpose of this section is to establish a sufficient condition for insuring the nonexistence of nonnegative solution. Specifically, we show under a suitable condition on σ_i, c_i, a, b that the integral equation (2.2) has no nonnegative solution when the sources q_i are not all identically zero, and it only has the trivial solution when q_i are all identically zero. To accomplish this, we first prepare the following lemma.

Lemma 3.1: Let $\mathcal{N} \equiv (N_1, N_2, N_3)$ be a nontrivial nonnegative solution of (2.2) and let $\underline{\sum}_i(\mu) > 0$, where $\underline{\sum}_i$ is defined by (2.7). Then the function

$$\psi_i(x) \equiv \int_{-1}^{1} \underline{\sum}_i(\mu) N_i(x, \mu) d\mu \quad (x \in I_i) \tag{3.1}$$

is strictly positive on I_i for each $i = 1, 2, 3$.

Proof: Let $x_i \in I_i$ such that $\psi_i(x_i) = \min\{\psi_i(x); x \in I_i\}$. Then by (2.2), (3.1)

$$\psi_i(x_i) = \int_{-1}^{1} \underline{\sum}_i(\mu)(F_i(\mathcal{N}))(x_i, \mu) d\mu, \quad i = 1, 2, 3. \tag{3.2}$$

In view of (2.3) the value of $\psi_1(x_1)$ is given by the right side of (2.12) except with $\overline{\sum}_1(\mu)$ replaced by $\underline{\sum}_1(\mu)$. We again denote the four integrals in (2.12) by $s_1(x_1), \cdots, s_4(x_1)$, that is, $\psi_1(x_1) = s_1(x_1) + \cdots + s_4(x_1)$. Similar expressions can be obtained for $\psi_2(x_2)$, $\psi_3(x_3)$. It is easily seen by a suitable change of the integration variable τ that,

$$\begin{aligned}
s_2(x_1) &= \int_0^1 \int_{-a}^{x_1} \mu^{-1} \underline{\sum}_1(\mu) \exp[-(x_1 - \xi)/\mu] \\
&\quad \times \tfrac{1}{2} c_1 \int_{-1}^{1} \sigma_1(\xi, \mu, \mu') N_1(\xi, \mu') d\mu' + q_1(\xi, \mu)] d\xi\, d\mu \\
s_4(x_1) &= \int_0^1 \int_{x_1}^{a} \mu^{-1} \underline{\sum}_1(-\mu) \exp[-(\xi - x_1)/\mu] \\
&\quad \times \tfrac{1}{2} c_1 \int_{-1}^{1} \sigma_1(\xi, -\mu, \mu') N_2(\xi, \mu') d\mu' + q_2(\xi, -\mu)] d\xi\, d\mu \\
(g_2(N_2))(-\mu) &= \int_a^{a+b} \mu^{-1} \exp[-(\xi - a)/\mu] \\
&\quad \times \tfrac{1}{2} c_2 \int_{-1}^{1} \sigma_2(\xi, -\mu, \mu') N_2(\xi, \mu') d\mu' \\
&\quad + q_2(\xi, -\mu)] d\xi \\
(g_3(N_3))(\mu) &= \int_{-a-b}^{-a} \mu^{-1} \exp[(\xi + a)/\mu] \\
&\quad \times \tfrac{1}{2} c_3 \int_{-1}^{1} \sigma_3(\xi, \mu, \mu') N_3(\xi, \mu') d\mu' \\
&\quad + q_3(\xi, \mu)] d\xi.
\end{aligned} \tag{3.3}$$

Now if $N_1(x, \mu) \not\equiv 0$ then since $\underline{\sum}_1(\mu) > 0$ the first two integrals in (3.3) imply that $s_2(x_1) + s_4(x_1) > 0$. Similarly, if $N_2(x, \mu) \not\equiv 0$ or $N_3(x, \mu) \not\equiv 0$, then by the third and the fourth integrals in (3.3), respectively, we have

$$(g_2(N_2))(-\mu) > 0 \text{ or } (g_3(N_3))(\mu) > 0 \quad (0 < \mu \leq 1)$$

and thence $s_3(x_1) > 0$ or $s_1(x_1) > 0$. In any case, we obtain $s_1(x_1) + \cdots + s_4(x_1) > 0$, which shows that $\psi_1(x_1) > 0$. Therefore, $\psi_1(x) > 0$ for all $x \in I_1$. The proofs for $\psi_2(x_2) > 0$ and $\psi_3(x_3) > 0$ are similar, and we omit the details.

It is interesting to note that the positivity of the function ψ_i holds for every $i = 1, 2, 3$ when at least one of the solution components in $\mathcal{N}$ is not identically zero. Moreover, this property remains valid even if $q_i \equiv 0$ for all i. This fact will be used in the proof of the following:

Theorem 3.1: Assume that $\underline{\sum}_i(\mu) > 0$ and that one of the following conditions hold:

$$\begin{aligned}
&\text{(i)} \quad \tfrac{1}{2} c_1 \int_0^1 \underline{\sum}_1(\mu)[1 - \exp(-2a/\mu)] d\mu \geq 1, \\
&\text{(ii)} \quad \tfrac{1}{2} c_2 \int_0^1 \underline{\sum}_2(\mu)[1 - \exp(-b/\mu)] d\mu \geq 1, \\
&\text{(iii)} \quad \tfrac{1}{2} c_3 \int_0^1 \underline{\sum}_3(\mu)[1 - \exp(-b/\mu) d\mu \geq 1.
\end{aligned} \tag{3.4}$$

Then the system (2.2) has no nonnegative solution when q_i is not identically zero for at least one i, and it only has the trivial solution when q_i is identically zero for all $i = 1, 2, 3$. Thus in this case the system is supercritical.

Proof: Assume by contradiction that $\mathcal{N} \equiv (N_1, N_2, N_3)$ is a nontrivial solution of (2.2). Then, by Lemma 3.1, $\psi_i(x) > 0$ on I_i and satisfies (3.2) with $\psi_i(x_i) = \min \psi_i(x) > 0$ for some $x_i \in I_i$. Consider the case for $\psi_1(x_1)$. Since for every $\xi \in I_i$, $-1 \leq \mu \leq 1$,

$$\begin{aligned}
&\int_{-1}^{1} \sigma_i(\xi, \mu, \mu') N_i(\xi, \mu') d\mu' \\
&\quad \geq \int_{-1}^{1} \underline{\sum}_i(\mu') N_i(\xi, \mu') d\mu' = \psi_i(\xi) \geq \psi_i(x_i).
\end{aligned} \tag{3.5}$$

We see from (3.3) and the nonnegative property of q_i that

$$\begin{aligned}
s_2(x_1) &\geq \tfrac{1}{2} c_1 \psi_1(x_1) \int_0^1 \underline{\sum}_1(\mu)\{1 - \exp[-(a + x_1)/\mu]\} d\mu, \\
s_4(x_1) &\geq \tfrac{1}{2} c_1 \psi_1(x_1) \int_0^1 \underline{\sum}_1(\mu)\{1 - \exp[-(a - x_1)/\mu]\} d\mu, \\
(g_2(N_2))(-\mu) &\geq \tfrac{1}{2} c_2 \psi_2(x_2)[1 - \exp(-b/\mu)], \\
(g_3(N_3))(\mu) &\geq \tfrac{1}{2} c_3 \psi_3(x_3)[1 - \exp(-b/\mu)].
\end{aligned} \tag{3.6}$$

Notice that the above inequalities hold for every source $q_i \geq 0$ including $q_i \equiv 0$. Now from $\psi_1(x_1) = s_1(x_1) + \cdots + s_4(x_1)$, where $s_i(x_1)$ are given in (2.12) (with $\overline{\sum}$ replaced by $\underline{\sum}$), we obtain

$$\begin{aligned}
\psi_1(x_1) &\geq \tfrac{1}{2} c_1 \psi_1(x_1) \int_0^1 \underline{\sum}_1(\mu)\{2 - \exp[-(a + x_1)/\mu] \\
&\quad - \exp[-(a - x_1)/\mu]\} d\mu \\
&\quad + \tfrac{1}{2} c_2 \psi_2(x_2) \int_0^1 \underline{\sum}_1(\mu)[1 - \exp(-b/\mu)] \exp[-(a - x_1)/\mu] d\mu \\
&\quad + \tfrac{1}{2} c_3 \psi_3(x_3) \int_0^1 \underline{\sum}_1(\mu)[1 - \exp(-b/\mu)] \exp[-(a + x_1)/\mu] d\mu.
\end{aligned} \tag{3.7}$$

Since, for each $\mu \in (0,1]$, the minimum value of the function $\rho_1(x_1)$ given by (2.17) occurs at $x_1 = \pm a$, we have

$$\psi_1(x_1) \geq c_1\psi_1(x_1)\int_0^1 \underline{\Sigma}_1(\mu)[1-\exp(-2a/\mu)]d\mu$$
$$+\tfrac{1}{2}c_2\psi_2(x_2)\int_0^1 \underline{\Sigma}_1(\mu)\exp(-2a/\mu)[1-\exp(-b/\mu)]d\mu$$
$$+\tfrac{1}{2}c_3\psi_3(x_3)\int_0^1 \underline{\Sigma}_1(\mu)\exp(-2a/\mu)[1-\exp(-b/\mu)]d\mu. \tag{3.8}$$

An analogous argument leads to

$$\psi_2(x_2) \geq \tfrac{1}{2}c_1\psi_1(x_1)\int_0^1 \underline{\Sigma}_2(\mu)\exp(-b/\mu)[1-\exp(-2a/\mu)]d\mu$$
$$+\tfrac{1}{2}c_2\psi_2(x_2)\int_0^1 \underline{\Sigma}_2(\mu)[1-\exp(-b/\mu)]d\mu$$
$$+\tfrac{1}{2}c_3\psi_3(x_3)\int_0^1 \underline{\Sigma}_2(\mu)\exp[-(2a+b)/\mu)][1-\exp(-b/\mu)]d\mu, \tag{3.9}$$

$$\psi_3(x_3) \geq \tfrac{1}{2}c_1\psi_1(x_1)\int_0^1 \underline{\Sigma}_3(\mu)\exp(-b/\mu)[1-\exp(-2a/\mu)]d\mu$$
$$+\tfrac{1}{2}c_2\psi_2(x_2)\int_0^1 \underline{\Sigma}_3(\mu)\exp[-(2a+b)/\mu]$$
$$\times[1-\exp(-b/\mu)]d\mu + \tfrac{1}{2}c_3\psi_3(x_3)\int_0^1 \underline{\Sigma}_3(\mu)$$
$$\times[1-\exp(-b/\mu)]d\mu. \tag{3.10}$$

It follows from $\psi_i(x_i) > 0$ that the inequality (3.8) is impossible if condition (i) in (3.4) holds. Similarly, (3.9) [respectively, (3.10)] cannot be fulfilled if condition (ii) [respectively, (iii)] holds. In each case we obtain a contradiction. Therefore, Eq. (2.2) has no nonnegative solution when the sources q_i are not all identically zero. When $q_i \equiv 0$ for every $i = 1,2,3$, the above argument shows that Eq. (2.2) cannot have nonnegative solution except the trivial solution $\mathcal{N} = 0$. This completes the proof of the theorem.

When the slab is embedded in vacuum without reflectors, the nonexistence problem is insured under the first condition (i) in (3.4). This result together with the conclusion in Remark 2.1 implies that the slab problem is subcritical if (2.23) holds and is supercritical if condition (i) in (3.4) holds. In particular, if σ_1 is a constant (say $\sigma_1 = 1$), these conditions become, respectively,

$$c_1 < [1-E_2(a)]^{-1} \quad \text{and} \quad c_1 > 2[1-E_2(2a)]^{-1},$$

where $E_n(z)$ is the nth-order exponential integral given by (cf. Ref. 11)

$$E_n(z) = \int_0^1 \mu^{n-2}\exp(-z/\mu)d\mu, \quad n = 1,2,\cdots. \tag{3.11}$$

The above observation leads to the following conclusions as those obtained in Ref. 6, 7.

Corollary: The slab problem without reflectors is subcritical if (2.23) holds and is supercritical if condition (i) in (3.4) holds. Thus, if the critical value of c_1 is denoted by c_1^*, then

$$\left[\int_0^1 \overline{\Sigma}_1(\mu)[1-\exp(-a/\mu)d\mu\right]^{-1} \leq c_1^*$$
$$\leq 2\left[\int_0^1 \overline{\Sigma}_1(\mu)[1-\exp(-2a/\mu)]d\mu\right]^{-1}. \tag{3.12}$$

In particular, if $\sigma_1 \equiv 1$, then c_1^* is bounded by

$$[1-E_2(a)]^{-1} \leq c^* \leq 2[1-E_2(2a)]^{-1}, \tag{3.13}$$

where $E_2(z)$ is the second order exponential integral.

Remark 3.1: Since the values of the exponential integrals $E_n(z)$ have been tabulized in standard handbooks (e.g., see Ref. 11), numerical results for the subcriticality can easily be obtained from the integrals in (3.12) when the functions $\overline{\Sigma}_1(\mu)$ and $\underline{\Sigma}_1(\mu)$ are polynomials in μ. The same remark holds for the general system (1.1), (1.2) when $\overline{\Sigma}_i(\mu)$ and $\underline{\Sigma}_i(\mu)$ are polynomials in μ. Some of the numerical results have been given for the special case $\sigma_1 \equiv 1$ (cf. Ref. 7). It is interesting to note that if the difference between $\overline{\Sigma}_1(\mu)$ and $\underline{\Sigma}_1(\mu)$ is small, then (3.12) yields good estimate for the critical value c_1^* for small values of optical thickness $2a$.

The argument given in the proof of Theorem 3.1 indicates that it is possible to obtain a different set of conditions for the nonexistence problem. Indeed, we have the following.

Theorem 3.2: Let $\underline{\Sigma}_i(\mu) > 0$. If all the inequalities

$$\tfrac{1}{2}c_1\int_0^1 [1-\exp(-2a/\mu)][\underline{\Sigma}_1(\mu)+\underline{\Sigma}_2(\mu)\exp(-b/\mu)$$
$$+\underline{\Sigma}_3(\mu)\exp(-b/\mu)]d\mu \equiv c_1L_1' \geq 1,$$
$$\tfrac{1}{2}c_2\int_0^1 [1-\exp(-b/\mu)][\underline{\Sigma}_1(\mu)\exp(-2a/\mu)+\underline{\Sigma}_2(\mu) \tag{3.14}$$
$$+\underline{\Sigma}_3(\mu)\exp[-(2a+b)/\mu]d$$
$$\equiv c_2L_2' \geq 1,$$
$$\tfrac{1}{2}c_3\int_0^1 [1-\exp(-b/\mu)]\{\underline{\Sigma}_1(\mu)\exp(-2a/\mu)+\underline{\Sigma}_2(\mu)$$
$$\times\exp[-(2a+b)/\mu]+\underline{\Sigma}_3(\mu)\}d\mu \equiv c_3L_3' \geq 1$$

hold and at least one strict inequality holds, then the system (2.2) is supercritical; that is, the conclusions in Theorem 3.1 remain true.

Proof: Let $\mathcal{N} \equiv (N_1, N_2, N_3)$ be a nontrivial nonnegative solution of (2.2). Then by adding the inequalities (3.8)–(3.10) established in the proof of Theorem 3.1, we obtain

$$\psi_1(x_1)+\psi_2(x_2)+\psi_3(x_3) \geq c_1L_1'\psi_1(x_1)$$
$$+c_2L_2'\psi_2(x_2)+c_3L_3'\psi_3(x_3). \tag{3.15}$$

But by the hypothesis (3.14) and the positivity of $\psi_i(x_i)$ the above inequality is impossible. This contradiction leads to the conclusion of the theorem.

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Exact solitary ion acoustic waves in a magnetoplasma

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It is shown that finite amplitude ion acoustic solitary waves propagating obliquely to an external magnetic field can occur in a plasma.

I. INTRODUCTION

Sagdeev[1,2] demonstrated that the equations governing the dynamics of nonlinear ion acoustic waves can be written in the form of the energy integral of a classical particle in a potential well. By analyzing the behavior of the potential one can show that finite amplitude localized density humps with a speed V, for $c_s < V < 1.6\, c_s$, where $c_s = (T_e/m_i)^{1/2}$ is the ion acoustic speed, can occur. When the wave amplitude is small, and the dispersion weak, the ion acoustic waves are described by a Korteweg—de Vries (KdV) equation,[3] whose localized solution is the well-known square hyperbolic secant. Zakharov and Kuznetsov[4] investigated the nonlinear development of small amplitude slow ion acoustic waves in a magnetized plasma. Here, the dispersion arising from charge separation as well as finite gyroradius effects can balance the nonlinearity. It is found that these nonlinear waves obey a modified KdV equation, which admits stationary three-dimensional localized solutions.

In this paper, we show that exact stationary solutions can be found for ion acoustic waves propagating obliquely to a magnetic field. In Sec. II, we present the basic equations and briefly review the linear wave propagation problem. For obliquely planar propagation, we solve the appropriate equations looking for stationary nonlinear solutions. An equation analogous to the energy integral of a classical particle is obtained. The potential is analyzed in Sec. III and the criteria for the existence of localized solutions are presented. Section IV contains a discussion of the small amplitude limit. Our results and their applications are discussed in Sec. V.

II. FORMULATION

Consider a two-component (electron—ion) low-β ($\beta = 8\pi n_0 T_e/B_0^2$) nonisothermal ($T_e \gg T_i$) plasma in the presence of a constant magnetic field $B_0\hat{z}$. The wave dynamics is governed by

$$\partial_t n + \nabla\cdot(n\mathbf{v}) = 0, \tag{1}$$

$$\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v} = -\frac{e}{m_i}\nabla\phi + \mathbf{v}\times\boldsymbol{\Omega}_i, \tag{2}$$

$$\nabla^2\phi = -4\pi e(n - n_e), \tag{3}$$

$$n_e = n_0 \exp(e\phi/T_e), \tag{4}$$

where n and $\mathbf{v}$ are the ion density and velocity, $\boldsymbol{\Omega}_i = eB_0\hat{z}/m_i c$ is the ion gyrofrequency, and ϕ is the ambipolar field. Since the perturbations are of low frequency ($\omega < \Omega_i$), electron inertia is neglected and the usual Boltzmann distribution (4) is assumed. The notations are standard.

Linearizing Eqs. (1)—(4), we find for $\omega \ll \Omega_i$ the following linear dispersion relation:

$$\omega = k_z c_s/(1 + k^2\lambda_D^2 + k_x^2 R_s^2)^{1/2}, \tag{5}$$

where $R_s = c_s/\Omega_i$, $\lambda_D = v_{Te}/\omega_{pe}$, and $k^2 = k_x^2 + k_z^2$. When the amplitude of the waves is sufficiently large, nonlinear effects cannot be neglected. Zakharov and Kuznetsov showed that when the nonlinearity and dispersion are weak, the wave propagation is governed by[4]

$$\partial_t v_z + c_s\partial_z[1 + \tfrac{1}{2}(R_s^2 + \lambda_D^2)\nabla_\perp^2 + \tfrac{1}{2}\lambda_D^2\partial_z^2 + v_z/2c_s]v_z = 0. \tag{6}$$

They found that three-dimensional stationary localized solutions of Eq. (6) exist. These solutions are stable against perturbations.

In the following, we investigate finite amplitude slow ion acoustic waves in a magnetized plasma, taking into account exact ion and electron nonlinearities. All variations are assumed to be in the x—z plane. We shall also assume charge neutrality, $n_i = n_e$, so that dispersion is solely due to gyroradius effects.

Nondimensionalizing n, t, x, z, v, and ϕ by n_0, L/c_s, R_s, L, c_s, and T/e, respectively, we obtain from Eqs. (1)—(4)

$$\partial_t n + (L/R_s)\partial_x(nv_x) + \partial_z(nv_z) = 0, \tag{7}$$

$$v_x = (R_s/L)\partial_x\partial_t\phi, \tag{8}$$

$$\partial_t v_z + (L/R_s)v_x\partial_x v_z + v_z\partial_z v_z = -\partial_z\phi, \tag{9}$$

$$n = n_e, \tag{10}$$

$$n_e = \exp\phi. \tag{11}$$

In obtaining (8) and (10), we have assumed R_s, $\lambda_D \ll L$, where L is the scale length of the solution.

Consider as solution a one-dimensional simple wave propagating obliquely with respect to the external magnetic field. The wave is assumed to be stationary in the moving frame defined by

$$\eta = k_x x + k_z z - Mt, \tag{12}$$

where k_x and $k_z = (1 - k_x^2)^{1/2}$ are the direction cosines. The Mach number $M = V/c_s$ gives the velocity of the wave along the η direction.

We are interested in the localized planar solutions of Eqs. (7)—(11). Thus, for $\eta \to \pm\infty$ we require

$$n = 1, \quad \mathbf{v} = 0, \quad \phi = 0,$$

and $\tag{13}$

$$\partial_\eta n = 0, \quad \partial_\eta\phi = 0.$$

From Eqs. (7) and (9), using (12) and (13), one obtains

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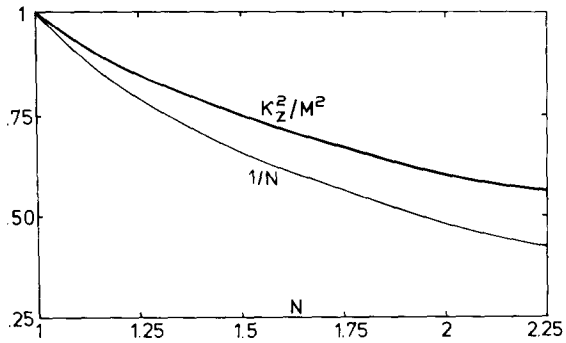

FIG. 1. K_z^2/M^2 vs N. This diagram shows the region of existence as well as the propagation characteristics of ion acoustic solitary waves in a magnetized plasma. See Eq. (21) and the paragraph following it.

$$M\partial_\eta v_z = k_z n \partial_\eta \phi. \tag{14}$$

This surprisingly simple result appears because the factor $(L/R_s)k_x v_x + k_z v_z$ occurs in both Eqs. (7) and (9), leading to a partial cancellation of the ion inertia terms in the latter equation.

Substituting the expression (11) for n into the above equation and integrating, we get

$$Mv_z = k_z(n-1). \tag{15}$$

Combining (7), (8), and (15), one obtains

$$\partial_\eta^2(\ln n) + b(n-1) + c(n^{-1}-1) = 0 \tag{16}$$

where $b = (k_z/Mk_x)^2$ and $c = k_x^{-2}$.

Multiplying throughout Eq. (16) by $\partial_\eta(\ln n)$ and integrating, we obtain

$$\tfrac{1}{2}(\partial_\eta n)^2 + \psi(n;\ M,\ k_x) = 0, \tag{17}$$

where

$$\psi(n;\ M,\ k_x) = bn^3 - (b-c)n^2 - cn - (b+c)n^2 \ln n. \tag{18}$$

Equation (17) is in the form of the energy integral of a classical particle in a potential well. In the next section, we shall analyse the Sagdeev potential $\psi(n)$ to determine the existence conditions and the behavior of possible localized solutions.

III. ANALYSIS

We now discuss the conditions under which localized solutions of Eq. (17) exist. From the analogy of the motion of a classical particle in a potential well, it follows that localized solutions are possible provided that $\psi(n)$ is negative between the point $n=1$ and a point, say at $n=N$, which we choose to be at $\eta = 0$ without loss of generality, corresponding to the maximum variation of n. In order that the "particle" is reflected at $n=N$ and not reflected at $n=1$ $(\eta = \pm\infty)$, we also require $\psi(N) = \psi(1) = \psi'(1) = 0$ as the conditions for the existence of solitary wave solutions. It is therefore necessary to study the behavior of $\psi(n)$ at $n=1$ and N.

Near the points $n \approx 1$ and $n \approx N$, Taylor expansion of Eq. (18) leads to

$$\psi(n) \approx -\tfrac{1}{2}(c-b)(n-1)^2 \quad \text{for } n \approx 1, \tag{19}$$

$$\psi(n) \approx -(N-n)(N-1)(bN-c) \quad \text{for } n \approx N, \tag{20}$$

In deriving Eq. (20), we have used a relation which emerges from applying the condition at the apex of the electric field profile, namely $\partial_\eta n = 0$ and $n = N$ at $n = 0$, to Eq. (17). That is,

$$\frac{b}{c} = \frac{k_z^2}{M^2} = \frac{1 - N + N\ln N}{N^2 - N - N\ln N}. \tag{21}$$

Equation (21) relates the Mach number M to N and k_z. That Eq. (21) does have solution also proves the existence of the maximum density N. Furthermore, Eqs. (19) and (20) show that in order for $\psi(n)$ to be negative, one should require $N^{-1} < (k_z/M)^2 < 1$. It is readily verified that these conditions are satisfied for $N > 1$. Figure 1 exhibits a plot of k_z^2/M^2 vs N. We note that the dependence of the parameter k_z/M on the soliton height N is strongest for small amplitude solitons.

IV. SMALL AMPLITUDE LIMIT

For $N \approx 1$, it is readily verified that

$$\psi(\delta n) = \tfrac{1}{2}(b-c)\delta n^2 + (\tfrac{2}{3}b + c)\delta n^3, \tag{22}$$

where $\delta n = n - 1 = O(\epsilon)$, $\epsilon \ll 1$. We have also assumed $b - c = O(\epsilon)$. The latter condition is equivalent to $k_z \approx M$, so that sonic solitons propagates almost parallel to the external magnetic field. For this case, one can write down an explicit analytical solution

$$\delta n = \delta N \operatorname{sech}^2\{[\delta N(2b+c)/6]^{1/2}\eta\}, \tag{23}$$

where $\delta N \equiv 3(c-b)/2b$, which can also be obtained from Eq. (21) by letting $N = 1 + \delta N$, is the maximum for the density. The projection of the solition width in the x direction is $L = k_x R_s/[\delta N(2b+c)/6]^{1/2}$, while that in the z direction is $k_z L^2/k_x R_s$.

Equation (23) can be recognized as the expression for the KdV soliton. Indeed, one can show that whithin the approximation $\delta n \approx b - c$, the set of equations (7)—(11) can be reduced by means of a suitable perturbation technique to a two-dimensional KdV equation, whose localized planar solution in the η-coordinate is given by Eq. (23). The corresponding linear dispersion is

$$\omega = k_z c_s(1 - \tfrac{1}{2}k_x^2 R_s^2), \tag{24}$$

which is simply the dispersion relation (5) in the limit of weak dispersion and charge neutrality.

V. DISCUSSION

We have considered the problem of nonlinear ion—acoustic waves in a magnetized plasma. It is found that the waves can propagate as a soliton whose motion is oblique to the external magnetic field. A relation is found between the angle of propagation, the speed, and the amplitude of the soliton. We have also presented an exact analytical formula for the electric field in the small amplitude limit.

We have assumed that the scale length L of the soliton should be larger than the Debye length λ_D as well as the gyroradius R_s. This assumption, which allows us to use charge neutrality and neglect some inertia terms in the perpendicular ion momentum equation, is valid as long as the soliton amplitude remains moderate, since the width of the soliton decreases as its amplitude increases.

As we have used the ion fluid equations, individual particle, as well as collective effects, such as ion Landau damping, trapping, acceleration, and reflection by the electric field potential are neglected. It is expected that such effects, which can lead to dissipation of wave energy, may cause the solitons to evolve into shock waves.[5] On the other hand, $\underset{\sim}{E}\times\underset{\sim}{B}_0$ drift effects can cause evolution of the soliton into the y direction. The latter effect is precluded in the plane wave solution presented here, and can be included only in a fully two-dimensional analysis.

Although we have considered only localized solutions here, our calculations can readily be extended to include nonlinear periodic solutions, such as conoidal waves. For this purpose, one needs only to change the boundary conditions.

Our results are applicable to any low β plasma in which $T_e \gg T_i$. The large amplitude ion acoustic waves may stem from an external source such as a grid within the plasma, a linear instability such as the two stream instability, as well as nonlinear instabilities such as the parametric decay instability.

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A generalized eigenvalue distribution

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The statistical properties of the eigenvalues of random unitary matrices may be determined from the joint probability density function of the matrix eigenvalues. Earlier theorems have derived the density function for the unitary and symplectic circular ensembles from that for the circular orthogonal ensemble. A method is presented here for successively eliminating variables from the probability density function for the orthogonal circular ensemble; the method generalizes an earlier result, and the resulting function appears to represent the behavior of eigenvalues from a new series of matrix ensembles.

The statistical properties of the eigenvalues of random unitary matrices, which have been studied by Dyson and Mehta,[1] may be determined from the joint probability density function of the matrix eigenvalues. Such functions typically take the form

$$P_{N,\beta}(\theta_1, \cdots, \theta_N) = C_{N,\beta} \prod_{j<k} |\exp(i\theta_j) - \exp(i\theta_k)|^\beta, \tag{1}$$

where $\beta = 1$, 2, or 4, corresponding to matrices of the orthogonal, unitary or symplectic circular ensembles.

The motivation for this discussion is the knowledge that there are simple ways to transform the orthogonal circular ensemble eigenvalue density into the circular unitary or symplectic densities. These methods involve eliminating eigenvalues, according to a particular procedure, from the orthogonal ensemble. Such procedures can in principle be generalized, and this suggests the possibility that there is some significance to be attached to the density functions their application would determine. In what follows, we generate a class of functions by generalizing one such procedure.

1. RELATIONS BETWEEN EIGENVALUE DENSITY FUNCTIONS

The transformations referred to are two physically meaningful and nontrivial methods of generating the unitary and symplectic circular ensembles from the orthogonal ensemble.

That is, one can perform operations D, G on the eigenvalues of the orthogonal circular ensemble such that

$$D: P_{2N,1}(\theta_1, \cdots, \theta_{2N}) \to P_{N,4}(\theta_2, \theta_4, \cdots, \theta_{2N}), \tag{2a}$$

$$G: \text{Two copies of } P_{N,1}(\theta_1, \cdots, \theta_N) \to P_{N,2}(\phi_1, \phi_2, \cdots, \phi_N). \tag{2b}$$

These two transformations are defined by two theorems, the former due to Mehta and Dyson,[2] the latter suggested by Dyson[3] and proved by Gunson.[4]

The meaning of (2a) is that, given a sequence of $2N$ eigenvalues belonging to the circular orthogonal ensemble, one may pick N alternate eigenvalues from that sequence; the N eigenvalues chosen will have the same statistical properties as those of a naturally occurring sequence of N eigenvalues belonging to the symplectic ensemble. That is, the eigenvalue density functions of the former sequence (made by choosing alternate eigenvalues) and of the latter sequence (belonging to the symplectic ensemble) are of the same form. The theorem is stated explicitly below [Eq. (7)].

The relationship (2b) means that if one takes two independent sequences of eigenvalues belonging to the orthogonal ensemble, superimposes them (randomly), and then picks from that mixed sequence N alternate eigenvalues, the chosen eigenvalues will have a density function which is the same as that for a unitary ensemble of order N.

There are thus explicit relations between $P_{2N,1}$ and $P_{N,4}$, and between $P_{N,1}$ and $P_{N,2}$. Two obvious questions may be asked: Can we find a similar relationship between $P_{N,2}$ and $P_{N,4}$, and can either of the two relationships in Eq. (2) be generalized, for β not restricted to the values 1, 2, 4.

Both questions are reasonable, the first because we would like to know whether the three ensembles are symmetrical in their relationships to each other, the second on the supposition that generalized eigenvalue densities may have some statistical significance. Since the functions $P_{N,\beta}$ as given by Dyson are well defined and properly normalized for all (complex) values of β—and intuitively appealing generalizations of the Mehta–Dyson or Gunson theorems should involve relationships between various $P_{N,\beta}$ with positive integral β—the proposed generalizations should have at least a mathematical interest.

In answer to the questions posed above, we may say the following.

First, we have been unable to find a relationship between $P_{N,2}$ and $P_{N,4}$ with either physical or mathematical interest. This is not to say that such a relationship does not exist, but we are inclined to be doubtful. In view of the ground fields underlying the various ensembles, we note that (2a) implies in a sense a mapping between the real field and the quaternion field; (2b) is, again in a sense, a mapping between the real field and the complex field. A relation of the sort desired would be a similar kind of mapping between the complex field and the field of real quaternions.

As regards a generalization of (2b), the proper result would be a theorem that could predict the properties of a sequence of eigenvalues formed by superimposing two

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or more independent sequences, and picking N eigenvalues, according to a prescribed formula, from the mixed sequence. If the probability density function for the eigenvalues of the resultant sequence were similar to $P_{N,\beta}$, for some integral β, that might be a result of physical interest. We have no reason to believe that some such formula might not exist, but there is not one available at the present time.

A generalization of the theorem indicated by Eq. (2a) has been proved, and is given by Eq. (8) below. It depends on the possibility of writing certain kinds of products as confluent alternant[5] determinants.

With the exception of the above argument based on the ground fields underlying the respective ensembles, there exists, to our knowledge, no explanation for the existence of the theorems implied by Eqs. (2a), (2b). However, Porter[6] has suggested the possibility of restating (2a), (2b) for the Gaussian ensembles; if such restatements are in fact possible, it would seem that these theorems must be connected in a very powerful way with the foundations of random matrix theory.

It is possible to state a number of theorems similar to (8). Such a theorem must eliminate a particular number $(\beta N - N)$ of arguments (eigenvalues) from $P_{\beta N,1}$, and must do so in a particular number of steps (integrations). An essential element of the procedure, however, is that the arguments—eigenvalues or dummy variables—be maintained in a certain fixed relationship to each other.

What (8) does is perform a series of integrations over the eigenvalues to be eliminated. The limits of integration may be other eigenvalues (in the last set of integrations), or dummy variables (in the preceding sets of integrations).

The limits of integration in the earlier integrations may, however, be other eigenvalues, provided that they are chosen in a symmetrical way from among only those eigenvalues over which the number of integrations to be performed is exactly the same as is that for the eigenvalues for which they will serve as limits; if any other eigenvalues were to be chosen as limits of integration, the essential fixed relationship between the arguments would be disrupted.

We have chosen the most general possible statement of the theorem, using dummy variables as limits of integration, rather than choosing one of the many possible equivalent statements without dummy variables.

2. GENERALIZATION OF THE MEHTA-DYSON THEOREM

The normalization constant $C_{N,\beta}$ appearing in Eq. (1), which is correct for all values of β, is given by[7]

$$C_{N,\beta} = \frac{1}{(2\pi)^N} \frac{[\Gamma(1+\frac{1}{2}\beta)]^N}{\Gamma(1+\frac{1}{2}N\beta)} \tag{3}$$

If we order the angles

$$0 \leq \theta_1 \leq \theta_2 \leq \cdots \leq \theta_N \leq 2\pi, \tag{4}$$

we can use the identity

$$\begin{aligned} &|\exp(i\theta_m) - \exp(i\theta_n)| = i^{-1} \exp[-\tfrac{1}{2}i(\theta_m + \theta_n)] \\ &\times (\exp[i\theta_m] - \exp[i\theta_n]), \quad \theta_n \leq \theta_m, \end{aligned} \tag{5}$$

to write

$$P_{N,1}(\theta_1, \cdots, \theta_N) = C_{N,1}(i)^{-N(N-1)/2} \det[\exp(ij\theta_s)], \tag{6}$$

$$j = \frac{-(N-1)}{2}, \frac{-(N-3)}{2}, \cdots, \frac{+(N-1)}{2},$$

$$s = 1, 2, \cdots, N.$$

Theorem (2a), relating the orthogonal and symplectic ensembles, is derived using the determinantal form (6) of the orthogonal ensemble eigenvalue density. It is given by

$$\begin{aligned} &\int_{\theta_{2N-1}}^{\theta_{2N}} d\theta_{2N-1} \cdots \int_{\theta_2}^{\theta_4} d\theta_3 \int_{\theta_{2N}-2\pi}^{\theta_2} d\theta_1 P_{2N,1}(\theta_1, \cdots, \theta_{2N}) \\ &= \frac{C_{2N,1}}{C_{N,4}} 2\left(\frac{2^{2N}N!}{(2N)!}\right)^2 P_{N,4}(\theta_2, \theta_4, \cdots, \theta_{2N}), \end{aligned} \tag{7}$$

where we have neglected constant factors on the right-hand side of (7) that result from the ordering (4) of the eigenvalues.

Note that in (7), integrals are performed over the odd numbered eigenvalues between the neighboring even numbered eigenvalues; the results would clearly be unchanged if instead we were to integrate over the even numbered eigenvalues between the neighboring odd numbered eigenvalues.

As has already been indicated, the meaning of the theorem is that N alternate eigenvalues, taken from a series of $2N$ belonging to the orthogonal ensemble, are distributed in the same way as N eigenvalues taken from the symplectic ensemble of order N. An obvious question to ask is, what will happen if instead of choosing alternate eigenvalues, we choose instead every third eigenvalue, or every fourth.

The confluent alternant determinant indicates how the choices of eigenvalues (the integrations) should be made: While the symplectic ensemble generated by (7) corresponds to the simplest sort of confluent alternant, generalizations of (7) (for $\beta > 2$) will generate ensembles corresponding to confluent alternants of higher degree.

We are of course concerned with (eigenvalue density) functions that are symmetric in all their arguments. In general, a confluent alternant determinant can describe (symmetric) functions of the form P_{N,A^2} (for A positive integral); these are the kinds of functions that are produced by the theorem below.

Theorem: For βN even, β, N positive integers, $N \geq 2$, $\beta \geq 2$,

$$\left[\int_{\theta_{N\beta}-2\pi}^{\theta_\beta} d\theta_{\beta-1}\left(\prod_{q=1}^{N-1} \int_{\theta_{q\beta}}^{\theta_{(q+1)\beta}} d\theta_{(q+1)\beta-1}\right)\right]$$

$$\times\left[\prod_{\alpha=1}^{\beta-2}\int_{\theta_{N\beta}-2\pi}^{\theta_\beta} d\phi_\alpha^{\beta-2}\left(\prod_{q=1}^{N-1}\int_{\theta_{q\beta}}^{\theta_{(q+1)\beta}} d\phi_{q\beta+\alpha}^{\beta-2}\right)\right]$$

$$\times\prod_{\gamma=1}^{\beta-2}\left\{\left[\prod_{q=0}^{N-2}\left(\prod_{r=\gamma}^{\beta-3}\int_{\phi_{q\beta+\gamma}^{r+1}}^{\phi_{(q+1)\beta+\gamma}^{r+1}} d\phi_{q\beta+\gamma}^{r}\right)\int_{\phi_{q\beta+\gamma}^{\gamma}}^{\phi_{(q+1)\beta+\gamma}^{\gamma}} d\theta_{q\beta+\gamma}\right]\right.$$

$$\left.\times\left[\left(\prod_{r=\gamma}^{\beta-3}\int_{\phi_{(N-1)\beta+\gamma}^{r+1}}^{\phi_\gamma^{r+1}+2\pi} d\phi_{(N-1)\beta+\gamma}^{r}\right)\int_{\phi_{(N-1)\beta+\gamma}^{\gamma}}^{\phi_\gamma^{\gamma}+2\pi} d\theta_{(N-1)\beta+\gamma}\right]\right\}$$

$$\times P_{\beta N',1}(\theta_1,\ldots,\theta_{N\beta})$$

$$=\frac{1}{K}(i)^{N\beta(\beta-1)/2}\frac{C_{\beta N',1}}{C_{N',\beta}^{\ 2}}(i)^{-N\beta(N\beta-1)/2}[\Gamma(1)\cdots\Gamma(\beta)]^N$$

$$\times(i)^{N\beta^2(N-1)/2}2^{(\beta-1)}(\pm 2)^{(\beta-1)(\beta-2)/2}\quad/2$$

$$\times P_{N',\beta}^{\ 2}(\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta}). \tag{8}$$

The constant K is given by

$$K=\left[\prod_{p=1}^{\beta N}(ij_p)\right]^{\beta-1}, \tag{9}$$

where

$$j_1=-\frac{(\beta N-1)}{2},\quad j_2=-\frac{(\beta N-3)}{2},\quad\ldots,\quad j_N=+\frac{(\beta N-1)}{2}, \tag{10}$$

so that

$$K=\left[(\beta N)!/(2)^{\beta N}\left(\frac{\beta N}{2}\right)!\right]^{2(\beta-1)}. \tag{11}$$

We can then write the right-hand side of (8) as

$$=\left[\frac{2^{\beta N}(\beta N/2)!}{(\beta N)!}\right]^{2(\beta-1)}\frac{C_{\beta N',1}}{C_{N',\beta}^{\ 2}}[\Gamma(1)\cdots\Gamma(\beta)]^N 2^{\beta-1}(\pm 2)^{(\beta-1)(\beta-2)/2}$$

$$\times P_{N',\beta}^{\ 2}(\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta}). \tag{12}$$

In (8) and (12) the + sign is for N even, and the − sign is for N odd.

Note that (8) reduces exactly to (7) in the case $\beta=2$: the products over α, γ, and r all vanish; the remaining integrals are over θ_p, p odd, and have the correct limits. The constant, as can be seen in (12), also reduces to the proper form.

Note also the introduction of the $(\beta-2)$ series of dummy variables, ϕ_p^γ, where γ labels each series $(1\leq\gamma\leq\beta-2)$; the subscript p of the dummy variables will obey $\gamma\leq p\leq q\beta+\gamma$ $(q=0,1,\ldots,N-1)$.

Proof of Theorem (8): We can write $P_{N',\beta}^{\ 2}(\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta})$ as a confluent alternant determinant

$$P_{N',\beta}^{\ 2}=\frac{C_{N',\beta}^{\ 2}}{(i)^{\beta^2N(N-1)/2}[\Gamma(1)\cdots\Gamma(\beta)]^N}$$

$$\times\det[\exp(ij\theta_p),\ j\exp(ij\theta_p),\ldots,j^{\beta-1}\exp(ij\theta_p)], \tag{13}$$

where the column index p takes the values $\beta,\ 2\beta,\ldots,N\beta$, and the row index j takes the values indicated in (10).

Similarly, we can order the eigenvalues, $0\leq\theta_1\leq\theta_2\leq\cdots\leq\theta_{N\beta}\leq 2\pi$, and use (5) and (6) to write as a determinant

$$P_{\beta N',1}(\theta_1,\ldots,\theta_{\beta N})=\frac{C_{\beta N',1}}{(i)^{\beta N(\beta N-1)/2}}\det[\exp(ij\theta_s)], \tag{14}$$

where j is given by (10), and $s=1,2,\ldots,\beta N$.

In the statement of the theorem we neglect constant factors on the right-hand side of (8) that result from the ordering of the eigenvalues leading to (14).

In order to transform the determinant in (14) into the determinant in (13), divide the βN variables into groups, with β variables in each group. Consider the first set of β variables: $\theta_1,\theta_2,\ldots,\theta_\beta$. The first variable—$\theta_1$—will be integrated a total of $\beta-1$ times; θ_2 will be integrated a total of $\beta-2$ times; the tth variable $(t=1,2,\ldots,\beta)$ will be integrated $\beta-t$ times.

Consider again the tth variable. The first $\beta-t-1$ integrations will transform θ_t into a succession of dummy variables—$\phi^1,\phi^2,\ldots,\phi^{\beta-t-1}$. The final, $\beta-t$, integration will transform $\phi^{\beta-t-1}$ into θ_β. In general, the first β variables of (14)—$\theta_1,\theta_2,\ldots,\theta_\beta$—are transformed finally into θ_β. The next set of β variables—$\theta_{\beta+1},\theta_{\beta+2},\ldots,\theta_{2\beta}$—is transformed finally into $\theta_{2\beta}$. The final set of β variables—$\theta_{(N-1)\beta+1},\ldots,\theta_{N\beta}$—is transformed finally into $\theta_{N\beta}$.

The integrations in (8), inside the product over γ, encompass all the integrations that are necessary to transform any of the θ's into the dummy variables ϕ^1, and to transform any set of the dummy variables ϕ^a into the succeeding set of dummy variables ϕ^{a+1}.

The other factors in (8) (those outside the product over γ) do the final integrations, by transforming the final sets of dummy variables into $\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta}$. Of course, since there is only one integration to be performed on each of $\theta_{\beta-1},\theta_{2\beta-1},\ldots,\theta_{N\beta-1}$, these variables are transformed directly into $\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta}$, respectively.

The integrals in (8) are performed from right to left. Begin by considering the integrations inside the product over γ, which act on variables initially labeled $\theta_{q\beta+\gamma'}$, where γ' is a given, fixed value of γ, and $q=0,1,\ldots,N-2$. That is, consider

$$\left[\prod_{q=0}^{N-2}\left(\prod_{r=\gamma'}^{\beta-3}\int_{\phi_{q\beta+\gamma'}^{r+1}}^{\phi_{(q+1)\beta+\gamma'}^{r+1}} d\phi_{q\beta+\gamma'}^{r}\right)\int_{\phi_{q\beta+\gamma'}^{\gamma'}}^{\phi_{(q+1)\beta+\gamma'}^{\gamma'}} d\theta_{q\beta+\gamma'}\right]$$

$$\times\left[\left(\prod_{r=\gamma'}^{\beta-3}\int_{\phi_{(N-1)\beta+\gamma'}^{r+1}}^{\phi_{\gamma'}^{r+1}+2\pi} d\phi_{(N-1)\beta+\gamma'}^{r}\right)\int_{\phi_{(N-1)\beta+\gamma'}^{\gamma'}}^{\phi_{\gamma'}^{\gamma'}+2\pi} d\theta_{(N-1)\beta+\gamma'}\right], \tag{15}$$

acting on $\det[\exp(ij\theta_s)]$.

These integrals do the first $\beta-t-1$ integrations on the tth variable of each set of β variables. The integrals in the second line of (15) do these integrations on the last set of β variables—$\theta_{(N-1)\beta+1},\theta_{(N-1)\beta+2},\ldots,\theta_{N\beta}$—while the integrals in the first line of (15) do these integrations on all other sets of β variables. Of course, as mentioned, the variables $\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta}$ are not integrated over at all, while the variables $\theta_{\beta-1},\theta_{2\beta-1},\ldots,\theta_{N\beta-1}$ are transformed directly into $\theta_\beta,\theta_{2\beta},\ldots,\theta_{N\beta}$ by integrals not included in (15) [by integrals in the first line of (8)].

Now, write out (15) explicitly for the fixed value $\gamma=\gamma'$. These integrals do not vanish for $\beta-3\geq 1$, and are given by

$$\int_{\phi^{\gamma'+1}_{\gamma'}}^{\phi^{\gamma'+1}_{\beta+\gamma'}} d\phi^{\gamma'}_{\gamma'} \int_{\phi^{\gamma'+1}_{\beta+\gamma'}}^{\phi^{\gamma'+1}_{2\beta+\gamma'}} d\phi^{\gamma'}_{\beta+\gamma'} \cdots \int_{\phi^{\gamma'+1}_{(N-2)\beta+\gamma'}}^{\phi^{\gamma'+1}_{(N-1)\beta+\gamma'}} d\theta^{\gamma'}_{(N-2)\beta+\gamma'} \int_{\phi^{\gamma'}_{\gamma'}}^{\phi^{\gamma'}_{\beta+\gamma'}} d\theta_{\gamma'}$$

$$\times \int_{\phi^{\gamma'}_{\beta+\gamma'}}^{\phi^{\gamma'}_{2\beta+\gamma'}} d\theta_{\beta+\gamma'} \cdots \int_{\phi^{\gamma'}_{(N-2)\beta+\gamma'}}^{\phi^{\gamma'}_{(N-1)\beta+\gamma'}} d\theta_{(N-2)\beta+\gamma'}$$

$$\times \int_{\phi^{\gamma'+1}_{(N-1)\beta+\gamma'}}^{\phi^{\gamma'+1+2\pi}_{\gamma'}} d\phi^{\gamma'}_{(N-1)\beta+\gamma'} \int_{\phi^{\gamma'}_{(N-1)\beta+\gamma'}}^{\phi^{\gamma'+2\pi}_{\gamma'}} d\theta_{(N-1)\beta+\gamma'} (\det[\exp(ij\theta_s)]). \tag{16}$$

The integrations in (16) are performed only on the γ', $\beta+\gamma', 2\beta+\gamma', \cdots, (N-1)\beta+\gamma'$ columns of the matrix. The integrations over the θ's transform these columns as shown: The columns

$$\{\exp(ij\theta_{\gamma'}), \exp(ij\theta_{\beta+\gamma'}), \ldots, \exp[ij\theta_{(N-1)\beta+\gamma'}]\} \tag{17}$$

become

$$\left\{\frac{\exp(ij\phi^{\gamma'}_{\beta+\gamma'})-\exp(ij\phi^{\gamma'}_{\gamma'})}{ij}, \frac{\exp(ij\phi^{\gamma'}_{2\beta+\gamma'})-\exp(ij\phi^{\gamma'}_{\beta+\gamma'})}{ij}, \right.$$

$$\left. \cdots, \frac{\exp[ij(\phi^{\gamma'}_{\gamma'}+2\pi)]-\exp[ij\phi^{\gamma'}_{(N-1)\beta+\gamma'}]}{ij}\right\}. \tag{18}$$

Since j is half-integral for βN even, $\exp[ij(\phi+2\pi)] = -\exp(ij\phi)$, and we can add columns in (18) so as to obtain

$$\pm\left\{\frac{\exp(ij\phi^{\gamma'}_{\gamma'})}{ij}, \frac{\exp(ij\phi^{\gamma'}_{\beta+\gamma'})}{ij}, \ldots, \frac{\exp[ij\phi^{\gamma'}_{(N-1)\beta+\gamma'}]}{ij}\right\}, \tag{19}$$

where the + sign holds for N even, and the − sign for N odd.

We can now perform the integrations over the $\phi^{\gamma'}$'s, as indicated in (16), and the integrations over the $\phi^{\gamma'+1}$, $\phi^{\gamma'+2}$, $\cdots$, until all of the $\beta-\gamma'+1$ (with $t=\gamma'$) integrations, over the t, $\beta+t$, $2\beta+t$, $\cdots$, columns have been performed. All the integrations proceed in essentially the same way as (17)–(19); when the integrations in (15) have all been performed, the γ', $\beta+\gamma'$, $\cdots$, $(N-1)\beta+\gamma'$ columns will have been transformed into

$$(\pm 2)^{\beta-\gamma'-1}\left\{\frac{\exp(ij\phi^{\beta-2}_{\gamma'})}{(ij)^{\beta-\gamma'-1}}, \frac{\exp(ij\phi^{\beta-2}_{\beta+\gamma'})}{(ij)^{\beta-\gamma'-1}}, \ldots, \frac{\exp[ij\phi^{\beta-2}_{(N-1)\beta+\gamma'}]}{(ij)^{\beta-\gamma'-1}}\right\}. \tag{20}$$

Since the integrals in (15) commute for different values of γ', it is clear that once they have been performed, in whatever order, we can perform all the integrals in (8) inside the product over γ, for $\gamma=1, \cdots, \beta-2$. These integrals transform

$$\det[\exp(ij\theta_s)] \to (\pm 2)^{(\beta-1)(\beta-2)/2} \det\left\{\frac{\exp(ij\phi^{\beta-2}_{p\beta+1})}{(ij)^{\beta-2}}, \right.$$

$$\left. \frac{\exp(ij\phi^{\beta-2}_{p\beta+2})}{(ij)^{\beta-3}}, \cdots, \frac{\exp(ij\phi^{\beta-2}_{p\beta+\beta-2})}{(ij)}, \exp(ij\theta_{p\beta+\beta-1}), \right.$$

$$\left. \exp[ij\theta_{(p+1)\beta}]\right\}, \quad p=0, 1, \cdots, N-1. \tag{21}$$

Now consider the remaining integrals in (8); they are outside the product over γ [the first two brackets (counting from the left)] and can be written

$$\int_{\theta_{N\beta-2\pi}}^{\theta_\beta} d\theta_{\beta-1} \int_{\theta_\beta}^{\theta_{2\beta}} d\theta_{2\beta-1} \int_{\theta_{2\beta}}^{\theta_{3\beta}} d\theta_{3\beta-1} \cdots \int_{\theta_{(N-1)\beta}}^{\theta_{N\beta}} d\theta_{N\beta-1}$$

$$\times \prod_{\alpha=1}^{\beta-2} \left(\int_{\theta_{N\beta-2\pi}}^{\theta_\beta} d\phi^{\beta-2}_{\alpha} \int_{\theta_\beta}^{\theta_{2\beta}} d\phi^{\beta-2}_{\beta+\alpha} \int_{\theta_{2\beta}}^{\theta_{3\beta}} d\phi^{\beta-2}_{2\beta+\alpha} \right. \tag{22}$$

$$\left. \times \cdots \int_{(N-1)\beta}^{\theta_{N\beta}} d\phi^{\beta-2}_{(N-1)\beta+\alpha} \right).$$

They operate on the determinant on the right-hand side of (21); the result is evident, and (21) is transformed into

$$(\pm 2)^{(\beta-1)(\beta-2)/2} \det\left\{\frac{\exp(ij\theta_\beta)-\exp[ij(\theta_{N\beta}-2\pi)]}{(ij)^{\beta-1}}, \right.$$

$$\times \frac{\exp(ij\theta_\beta)-\exp[ij(\theta_{N\beta}-2\pi)]}{(ij)^{\beta-2}}$$

$$\times \cdots, \frac{\exp(ij\theta_\beta)-\exp[ij(\theta_{N\beta}-2\pi)]}{(ij)}, \tag{23}$$

$$\left. \times \exp(ij\theta_\beta), \cdots \right\}.$$

Here we have written only the first β columns of the determinant. The effect on the other (groups of β) columns is exactly the same, except that θ_β is replaced by $\theta_{2\beta}$ (columns $\beta+1$ through 2β), by $\theta_{3\beta}$ (columns $2\beta+1$ through 3β), $\cdots$, $\theta_{N\beta}$ [columns $(N-1)\beta+1$ through $N\beta$]. If we let $p=\beta, 2\beta, \cdots, N\beta$, we can add columns, and rewrite (23) so as to obtain

$$\det[\exp(ij\theta_s] \to (\pm 2)^{(\beta-1)(\beta-2)/2} 2^{\beta-1} \det\left[\frac{\exp(ij\theta_p)}{(ij)^{\beta-1}}, \right.$$

$$\left. \frac{\exp(ij\theta_p)}{(ij)^{\beta-2}}, \cdots, \frac{\exp(ij\theta_p)}{(ij)}, \exp(ij\theta_p)\right]. \tag{24}$$

Now multiply (24) by K as defined in (9). This in effect multiplies the first row on the right-hand side of (24) by $(ij_1)^{\beta-1}$, the second row by $(ij_2)^{\beta-1}, \ldots$, the βNth row by $(ij_{\beta N})^{\beta-1}$. That is,

$$K\det[\exp(ij\theta_s)] \to (\pm 2)^{(\beta-1)(\beta-2)/2} 2^{\beta-1} \det[\exp(ij\theta_p)$$

$$\times (ij)\exp(ij\theta_p), \cdots, (ij)^{\beta-2}\exp(ij\theta_p), (ij)^{\beta-1}\exp(ij\theta_p)]$$

$$= (\pm 2)^{(\beta-1)(\beta-2)/2} 2^{\beta-1} (i)^{N\beta(\beta-1)/2} \det[\exp(ij\theta_p), \tag{25}$$

$$\times j\exp(ij\theta_p), \cdots, j^{\beta-2}\exp(ij\theta_p), j^{\beta-1}\exp(ij\theta_p)].$$

This concludes the proof. The integrals on the left-hand side of (8), operating on $\det[\exp(ij\theta_s)]$, produce the confluent alternant in (25), which is identical to the form (18) for $P_{N,\beta}{}^2$. The remaining constant factors in (8) come from the definitions (13) and (14) of $P_{\beta N,1}$ and of P_{N,β^2} as determinants.

Alternative forms of the theorem, with different limits of integration, can easily be stated, but as indicated above, the form in (8) seems most natural. The first set of integrals in (8) [in the first square brackets in

the first line of (8)], in their present form, reduce exactly to (7) in the case $\beta=2$. The other integrals largely involve dummy variables as limits of integration, and changes in these may be rather arbitrary.

Finally, we note that P_{N,β^2} might be interpreted as the eigenvalue density for an ensemble of unitary matrices with β^2 independent components in each off-diagonal matrix element.

The application of (8) can be seen most easily in a simple example. Let $\beta N=6$, $\beta=3$, $N=2$. Then (8) becomes

$$\int_{\theta_6-2\pi}^{\theta_3} d\theta_2 \int_{\theta_3}^{\theta_6} d\theta_5 \int_{\theta_6-2\pi}^{\theta_3} d\phi_1^1 \int_{\theta_3}^{\theta_6} d\phi_4^1 \int_{\phi_1^1}^{\phi_4^1} d\theta_1 \int_{\phi_4^1}^{\phi_1^1+2\pi} d\theta_4 P_{6',1}(\theta_1,\cdots,\theta_6) \tag{26}$$
$$=\left(\frac{2^6 3!}{6!}\right)^4 \frac{C_{6',1}}{C_{2',9}} 2^5 P_{2',9}(\theta_3, \theta_6).$$

The integrals in (26) can easily be performed in succession from right to left.

The statistical meaning of (26) can be seen in Fig. 1. Two eigenvalues, θ_1 and θ_4, are chosen by the first two integrations, and allowed to move within the indicated interval; this destroys their ordering with respect to the other eigenvalues, but preserves it with respect to each other.

The third and fourth integrations fix ϕ_4^1 and ϕ_1^1 in the intervals $[\theta_6, \theta_3]$ and $[\theta_3, \theta_6]$, respectively, but without saying anything about the relation of ϕ_4^1 to θ_4 or θ_5, or about the relation of ϕ_1^1 to θ_1 or θ_2.

The last two integrations destroy the orderings of θ_2 with respect to θ_1 and θ_3, and of θ_5 with respect to θ_4 and θ_6: θ_2 and θ_5 are integrated out, just as the odd variables are in Theorem (7).

Note that allowing $N=2, 4, 6, \cdots$ (βN even) would make no significant change in (26). This is clear from Fig. 1, which for $N>2$ would simply be repeated horizontally.

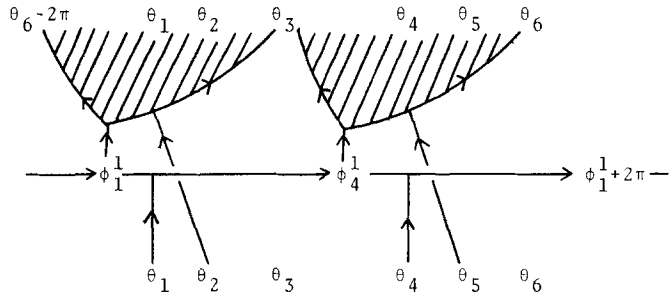

FIG. 1.

From (26), the first integrations are performed over θ_1 and θ_4, in the intervals $[\phi_1^1, \phi_4^1]$ and $[\phi_4^1, \phi_1^1+2\pi]$, respectively; the second set of integrations is over ϕ_1^1 and ϕ_4^1, in the intervals $[\theta_6-2\pi, \theta_3]$ and $[\theta_3, \theta_6]$, respectively. The final set of integrations, which may in fact be performed at any time, is over θ_2 and θ_5, in the respective intervals $[\theta_6-2\pi, \theta_3]$ and $[\theta_3, \theta_6]$. With the final integrations, the variables θ_1, θ_2, θ_4 and θ_5 have been eliminated.

If we were to allow $N=4, 6, 8, \cdots$, the diagram in Fig. 1 would appear 2, 3, 4, $\cdots$, times.

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Explicit decomposition of tensor products of certain analytic representations of symplectic groups[a),b)]

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For any integer $k>1$ let $E=\mathbb{C}^{2k\times 1}$, $E'=\mathbb{C}^{1\times 2k}$, and $G=\mathrm{Sp}(k,\mathbb{C})$. If $P_m(E)$ denotes the linear space of all homogeneous polynomial functions of degree m on E, then the representation L_m of G, obtained by left translation on $P_m(E)$, is irreducible with signature $(m,0,\cdots,0)$. Similarly, $P_n(E')$ and R_n are defined by replacing E by E', m by n, and left translation by right translation. In this article, an explicit decomposition of the tensor product representation $R_n\otimes L_m$ on $P_n(E')\otimes P_m(E)$ is given in terms of the solid symplectic Stiefel harmonics.

I. INTRODUCTION

Let k be an integer $\geqslant 1$, and let I_k denote the identity matrix of order k. In general, the transpose of a matrix m will be denoted by m'. Set

$$s_k=\begin{bmatrix}0 & -I_k\\ I_k & 0\end{bmatrix},$$

and define the complex symplectic group G by the equation

$$G=\{g\in\mathrm{GL}(2k,\mathbb{C}):\ gs_kg'=s_k\}.$$

Set $E=\mathbb{C}^{2k\times 1}$, $E'=\mathbb{C}^{1\times 2k}$, $\mathbb{C}^*=\mathbb{C}-\{0\}$; let $P(E)$ and $P(E')$ denote the algebras of all complex valued polynomial functions on E and E', respectively. For non-negative integers m and n define

$$P_m(E)=\{q\in P(E):q(xc)=c^m q(x),\ \forall\ (x,c)\in E\times\mathbb{C}^*\}$$

and

$$P_n(E')=\{p\in P(E'):p(c\xi)=c^n p(\xi),\ \forall\ (c,\xi)\in\mathbb{C}^*\times E'\}$$

If D_n denotes the representation of $\mathrm{GL}(2k,\mathbb{C})$ obtained by right translation on $P_n(E')$, then it is well known that D_n is irreducible with signature $(n,0,\ldots,0)$ (cf., e.g., Ref. 1). Similarly, the left representation T_m of $\mathrm{GL}(2k,\mathbb{C})$ in $P_m(E)$ is irreducible with signature $(0,\ldots,-m)$. If R_n (resp. L_m) denotes the restriction of D_n (resp. T_m) to G, then R_n (resp. L_m remains irreducible with signature

$$\underbrace{(n,0,\ldots,0)}_{k\text{ factors}}\ [\text{resp. } (m,0,\ldots,0)].$$

(In a more general context, the study of restrictions of analytic representations of $\mathrm{GL}(2k,\mathbb{C})$ to G was investigated in Ref. 2. The above assertion is a special case of Theorem 2.1 in Ref. 2, but the proof is much simpler by observing that G acts transitively on the dense subset $\{\xi\in E':\xi\neq 0\}$ of E'.)

Now, define an action of $\mathrm{GL}(2k,\mathbb{C})$ on $E'\times E$ by

$$((\xi,x),y)\to(\xi,x)\cdot y=(\xi y,y^{-1}x),$$

$$\forall\ (\xi,x)\in E'\times E,\ \forall\ y\in\mathrm{GL}(2k,\mathbb{C});$$

and consider the tensor product representation $D_m\otimes T_m$ of $\mathrm{GL}(2k,\mathbb{C})$ given by

$$[(D_n\otimes T_m)(y)](p\otimes q)(\xi,x)=[p\otimes q]((\xi,x)\cdot y)$$

for all $p\otimes q\in P_n(E')\otimes P_m(E)$, and $y\in\mathrm{GL}(2k,\mathbb{C})$. Then, it was shown in Ref. 3 (see also Ref. 4) that one has the following decomposition.

$$P_n(E')\otimes P_m(E)=\sum_{j=0,\ldots,r}\oplus p_0^j H_{m-j}^{n-j},\quad\text{where}$$

$r=\min(m,n)$; p_0 is defined by $p_0(\xi,x)=\Sigma_{i=0,\ldots,2k}\Sigma_i\xi_{ii}x_i$, and each subspace H_{m-j}^{n-j} consists of elements f in $P_{n-j}(E')\otimes P_{m-j}(E)$ which also satisfy the Hermite–Laplace equation

$$\Delta f=0,\ \text{with}\ \Delta f(\xi,x)=\sum_{j=0,\ldots,2k}\frac{\partial^2 f}{\partial\xi_j\partial x_j}(\xi,x).$$

In addition, each subrepresentation of $D_n\otimes T_m$ on $p^jH_{m-j}^{n-j}$ $(0\leqslant j\leqslant r)$ is irreducible with signature $[n-j,0,\ldots,-(m-j)]$.

With the exception of the case $k=1$ for which $G=\mathrm{SL}(2,\mathbb{C})$, the restriction of $D_n\otimes T_m$ to G does not decompose as simply as in Eq. (1.1) (the case $k=1$ was completely solved by H. Weyl in Ref. 5(a), p. 128). We shall give an explicit decompositon of the tensor product representation $R_n\otimes L_m$ of G on $P_n(E')\otimes P_m(E)$. The simple submodules that occur in this decomposition consist of symplectic Stiefel harmonics which are equipped with an inner product invariant under the unitary symplectic group (cf. Ref. 2 for details). This is a natural setting to study the Clebsch–Gordan coefficients problem of these tensor product representations which we shall discuss in another article.

In connection with this decomposition, we shall also give an explicit description of the restriction of two classes of irreducible analytic representations of $\mathrm{GL}(2k,\mathbb{C})$ to its subgroup G (Theorem 2.2 and Theorem 3.2). To obtain these results we must further our study on the ξ-covariant and ρ-covariant polynomial functions that we first investigated in Refs. 1 and 2.

There is an extensive literature on Clebsch–Gordan series. (A detailed and comprehensive bibliography on this subject can be found in Louck's article.[6]) Starting with the

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[b)]The author wishes to thank the referee for several helpful comments, especially on the connection between the authors's work and the boson calculus [cf. C. Quesne, J. Math. Phys. **14**, 366 (1973)] and on the discussion of the last equality in Eq. (3.2).

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work of Brauer,[7] Weyl,[5(b)] Kostant,[8] and Steinberg[9] on the relationship between the inner and outer multiplicity structure of complex simple Lie groups (or equivalently, their compact real forms), Biedenharn established in Ref. 10 an important lemma which, in turn, generated a very effective method to compute Clebsch–Gordan series (see also Klimyk[11]). The explicit conditions for the validity of Biedenharn's lemma for simple classical groups were derived by MacFarlane, O'Raifeartaigh, and Rao[12] and Beck.[13] (Incidentally, these conditions are not fulfilled in our problem with the exception for the simple cases where $k=1$ or $m=n=0$.) The relationship between inner and branching (or restriction) multiplicities were also investigated by Delaney and Gruber in Ref. 14 and by Stone in Ref. 15.

II. THE ξ- AND ρ-COVARIANT SYMPLECTIC STIEFEL HARMONICS

Let l denote an arbitrary integer satisfying $2\leqslant l\leqslant k$, set $V=\mathbb{C}^{l\times 2k}$, and let m_i $(1\leqslant i\leqslant l)$ be integers satisfying $m_1\geqslant m_2\geqslant\cdots\geqslant m_l\geqslant 0$. Let B denote the subgroup of lower triangular matrices of $GL(l,\mathbb{C})$ and define a holomorphic character $\xi=\xi(m_1,\cdots,m_l)$ on B by setting

$$\xi(b)=b_{11}^{m_1}\cdots b_{ll}^{m_l},\ \forall\ b\in B.$$

A polynomial function f on V will be called ξ-covariant if $f(bX)=\xi(b)f(X)$ for all $(b,X)\in B\times V$; furthermore, f will be called *symplectic Stiefel harmonic* if $p_{ij}(D)f=0$, $1\leqslant i<j\leqslant l$ [see Ref. 2, for the definition of the $p_{ij}(D)$'s]. If $H_\xi(V)$ denotes the linear space of all ξ-covariant symplectic Stiefel harmonics then it was shown in Ref. 2 (Theorem 2.1) that the representation R_ξ of G obtained by right translation on $H_\xi(V)$ is irreducible and its signature is $(m_1,m_2,\ldots,m_l,0,\ldots,0)$.

Now, set

$$W_\rho=\{f:\mathbb{C}^{l\times l}\to\mathbb{C}: f \text{ polynomial}; f(ba)=\xi(b)f(a),$$
$$\forall\ (b,a)\in B\times\mathbb{C}^{l\times l}\}$$

and let ρ denote the representation of $GL(l,\mathbb{C})$ obtained by right translation on W_ρ. Then, according to Theorem 1.5 in Ref. 1, ρ is irreducible with signature $(m_1,\ldots m_l)$.

Set

$$P_\rho(V)=\{F: V\to W_\rho : F \text{ polynomial}; F(aX)$$
$$=\rho(a)F(X),\forall\ (a,X)\in GL(l,\mathbb{C})\times V\}$$

and call an element $F\in P_\rho(V)$ symplectic Stiefel harmonic if $p_{ij}(D)(\lambda\circ F)=0$ for all linear functionals λ on W_ρ and for all i,j, $1\leqslant i<j\leqslant l$. Let $H_\rho(V)$ denote the subspace of $P_\rho(V)$ consisting of all symplectic Stiefel harmonics, and let R_ρ denote the right shift representation of G on $H_\rho(V)$. Then we have the following:

Theorem 2.1: The representation R_ρ is equivalent to the representation R_ξ.

The proof of this theorem is similar to that of Corollary 3.2 in Ref. 1. Thus, in our context we must show only that if $a\in\mathbb{C}^{l\times l}$ and θ_a denotes the mapping $X\to aX$ $(X\in V)$, then $[p_{ij}(D)(f\circ\theta_a)](X)=0$ for all $f\in H_\xi(V)$ and all i,j $(i\leqslant i<j\leqslant l)$. But an easy computation shows that

$$[p_{ij}(D)(f\circ\theta_a)](X)$$
$$=\sum_{1\leqslant u<v\leqslant l}(a_{vj}a_{ui}-a_{uj}a_{vi})[p_{uv}(D)f](aX),$$

which must vanish for every $(a,X)\in\mathbb{C}^{l\times l}\times V$ since $f\in H_\xi(V)$.

Henceforth, we shall assume that $V=\mathbb{C}^{2\times 2k}$ with $k\geqslant 2$. Under this additional condition, our study of the symplectic Stiefel harmonics in Ref. 2 can now be symplified and completed. In particular, to prove that the ideal J^*S is prime it suffices to observe that it is generated by a single irreducible polynomial p_{12} defined by

$$p_{12}(X)=\sum_{t=1}^{k}X_{1,t+k}X_{2t}-X_{1t}X_{2,t+k},$$
$$X\in V.$$

Moreover, we have the following:

Theorem 2.2: The space $P_{\xi(m_1,m_2,0,\ldots0)}(V)$ can be expressed as direct sum

$$P_{\xi(m_1,m_2,0,\ldots0)}(V)=\sum_{i=0}^{m_2}\oplus p_{12}^{i}H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V),$$

where each $p_{12}^{i}H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V)$, is a simple G-module with signature $(m_1-i,m_2-i,0,\ldots,0)$.

Proof: From Ref. 2 (Theorem 2.1) we know that each $H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V)$ is a simple G-module with signature $(m_1-i,m_2-i,0,\ldots,0)$. Define a mapping from $H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V)$ into $P_{\xi(m_1,m_2,0,\ldots,0)}(V)$ by

$$f\to p_{12}^{i}f;\ \forall f\in H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V).$$

Obviously this map is well defined since

$$(p_{12}f)(bX)=b_{11}^{m_1}b_{22}^{m_2}p_{12}(X)f(X),\ \forall(b,X)\in B\times V.$$

The fact that it is injective follows from Theorem 1.10 in Ref. 2. Now since p_{12} is G-invariant

$$[D_{\xi(m_1,m_2,\ldots,0)}(g)(p_{12}^{i}f)](X)$$
$$=p_{12}^{i}(X)f(Xg)$$
$$=p_{12}^{i}(X)\{R_{\xi(m_1-i,m_2-i,0,\ldots,0)}(g)f\},\quad\forall\ g\in G$$

(see Refs. 1 and 2 for notations). Thus the mapping $f\to p_{12}^{i}f$ is also a G-module homomorphism. Since $P_{\xi(m_1,m_2,0,\ldots,0)}(V)$ is a semisimple G-module, and $p_{12}^{i}H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V)$, $p_{12}^{j}H_{\xi(m_1-j,m_2-j,0,\ldots,0)}(V)$ are nonisomorphic simple G-modules for $i\neq j$ $(0\leqslant i,j\leqslant m_2)$, it follows from a well known fact (cf., e.g., *Theory of Lie Groups* by C. Chevalley, Propositions 1 and 3, pp. 174–175) that the sum of the simple G-modules $p_{12}^{i}H_{\xi(m_1-i,m_2-i,0,\ldots,0)}(V)$ $(0\leqslant i\leqslant m_2)$ is direct. Thus, to achieve the proof of the theorem, we only need to show that

$$d^0(m_1,m_2,0,\ldots,0)=\sum_{i=0}^{m_2}d_G^0(m_1-i,m_2-i,0,\ldots,0) \tag{2.1}$$

if $d^0(m_1,m_2,0,\ldots,0)$ [resp. $d_G^0(m_1-i,m_2-i,0,\ldots,0)$] represents the degree of the representation of $GL(2k,\mathbb{C})$ (resp. of G) with signature $(m_1,m_2,0,\ldots,0)$ [resp. $(m_1-i,m_2-i,0,\ldots,0)$].

According to Ref. 5(b) (Theorem 7.5.B, p. 201 and Theorem 7.8.C, p. 218), Formula (2.1) becomes

$$\frac{(m_1-m_2+1)\{(m_1+2k-1)!(m_2+2k-2)!\}}{(m_1+1)!m_2!(2k-1)!(2k-2)!}$$

$$=\sum_{i=0}^{m_2}(m_1-m_2+1)(m_1+m_2+2k-2i-1)$$

$$\times\{(m_1+2k-i-2)!)(m_2+2k-i-3)!\}$$

$$\times[(m_1+1-i)!(m_2-i)!(2k-1)!(2k-3)!\ ]^{-1}. \tag{2.2}$$

which can be easily verified by induction on m_2, or may be deduced from a well-poised ${}_3F_2$ series (cf. Ref. 16, p. 57). □

III. THE MAIN THEOREM

We shall now return to the main problem of this article. Assume $k\geqslant 2$ and preserve the notations introduced in Sec. I.

Theorem 3.1: The semisimple G-module $P_n(E')\otimes P_m(E)$ can be represented as a direct sum

$$P_n(E')\otimes P_m(E)=\sum_{j=0}^{r}\sum_{i=0}^{r-j}\oplus p_0^j\mathscr{H}(n+m-2j-i,i), \tag{3.1}$$

where in (3.1)

$$H_{m-j}^{n-j}=\sum_{i=0}^{r-j}\oplus\mathscr{H}(n+m-2j-i,i).$$

Morevoer, each subrepresentation of $R_n\otimes L_m$ on $p_0^j\mathscr{H}(n+m-2j-i,i)$ is equivalent to an irreducible analytic representation of G with signature $(n+m-2j-i,i,0,\ldots,0)$.

From Eq. (1.1) we know that each subrepresentation of $D_n\otimes T_m$ on $p_0^jH_{m-j}^{n-j}$ is irreducible, and since each H_{m-j}^{n-j} is obviously a G-module, to obtain Theorem 3.1 it suffices to prove the following:

Theorem 3.2: Under the restriction $\mathrm{GL}(2k,\mathbb{C})\mid G$ each simple $\mathrm{GL}(2k,\mathbb{C})$-module $H_{m-j}^{n-j}(0\leqslant j\leqslant r)$ is decomposed into simple G-modules as

$$H_{m-j}^{n-j}=\sum_{i=0}^{r-j}\oplus\mathscr{H}(n+m-2j-i,i).$$

Without loss of generality we may assume that $n\geqslant m$; thus $r=m$. The proof of this theorem will be achieved via several lemmas.

Fix i, and in Sec. II let $l=2$, $\xi=\xi(n+m-2j-i,i)$. This character ξ corresponds to the representation ρ of $\mathrm{GL}(2,\mathbb{C})$ on the linear space W_ρ. Equip W_ρ with the inner product

$$\langle f_1f_2\rangle=[f_1(D)\tilde{f}_2](0)$$

(cf. Ref. 1, p. 31 for justification) for all f_1f_2 in W_ρ.

Lemma 3.3: Let α,β be nonnegative integers such that $\alpha+\beta=n+m-2j-2i$ and set

$$C_{\alpha\beta}=\left\{\sum_{u=0,\ldots,i}\binom{i}{u}^2(\alpha+i-u)!(\beta+u)!u!(i-u)!\right\}^{-1/2}$$

$$=\left[\frac{i!\alpha!\beta!(\alpha+\beta+i+1)!}{(\alpha+\beta+1)!}\right]^{-1/2}. \tag{3.2}$$

For $y\in\mathbb{C}^{2\times 2}$ let $|y|$ denote the determinant of y and define

$$\varphi_{\alpha\beta}(y)=C_{\alpha\beta}y_{11}^{\alpha}y_{12}^{\beta}|y|^i.$$

Then the system $\{\varphi_{\alpha\beta}\}_{(\alpha\beta)}$ is an orthonormal basis for W_ρ.

Proof: We have

$$\varphi_{\alpha\beta}(y)$$

$$=C_{\alpha\beta}\left(\sum_{u=0,\ldots,i}(-1)^u\binom{i}{u}y_{11}^{\alpha+i-u}y_{12}^{\beta+u}y_{21}^{u}y_{22}^{i-u}\right);$$

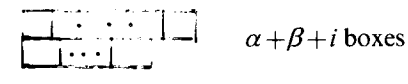
it follows immediately from relation (2.2) in Ref. 1 that $\{\varphi_{\alpha\beta}\}_{(\alpha\beta)}$ is an orthonormal system. Now, for

$$b=\begin{bmatrix}b_{11}&0\\b_{21}&b_{22}\end{bmatrix}$$

in B, we verify easily that

$$\varphi_{\alpha\beta}(by)=b_{11}^{m+n-2j-i}b_{22}^{i}\varphi_{\alpha\beta}(y)\ \text{ for all } y\in\mathbb{C}^{2\times 2}.$$

The last equality in Eq. (3.2) is obtained by observing that the normalization factor $C_{\alpha\beta}$ is the square root of the measure factor M of the Young tableaux



filled in with $\alpha+i$ 1's followed by β 2's in row 1 and i 2's in row 2. It can also be derived from the formula defining the basis of boson polynomials in the article by Baird and Biedenharn, J. Math. Phys. **4**, 1459 (1963):

$$\left|\begin{pmatrix}m_{12}&m_{22}\\m_{11}\end{pmatrix}\right\rangle=M^{-1/2}(a_1^1)^{m_{12}-m_{22}}$$

$$\times(a_1^2)^{m_{12}-m_{11}}(a_1^1a_2^2-a_2^1a_1^2)^{m_{22}}|0\rangle.$$

The relations between notations are

$$m_{12}=\alpha+\beta+i,\ m_{22}=i,\ m_{11}=\alpha+i,$$

$$a_j^i=y_{ij},\ 1\leqslant i,j\leqslant 2.$$

But from Ref. 5(b) (Theorem 7.5.B, p. 201), we known that W_ρ has dimension $m+n-2j-2i+1$; so that $\{\varphi_{\alpha\beta}\}_{(\alpha\beta)}$ is indeed an orthonormal basis for W_ρ. □

To this Hilbert space W_ρ we associate as in Sec. II the representation R_ρ on the linear space $H_\rho(V)$. Let G_0 denote the unitary symplectic group corresponding to G. Set $U=U(2)$, and let ρ_0 and R_ρ^0 denote the restrictions of ρ and R_ρ to U and G_0 respectively. It follows from the "unitarian trick" that ρ_0 and R_ρ^0 remain irreducible. If W_ρ^* denotes the dual of W_ρ we define the linear space K by

$$K=\{\lambda\circ F:\lambda\in W_\rho^*,\ F\in H_\rho(V)\}.$$

Define a representation of G_0 on K by the equation

$$[\pi^0(g)(\lambda\circ F)](X)=(\lambda\circ F)(Xg)=[\lambda\circ R^0_\rho(g)F](X)$$

for all $\lambda\circ F\in K$, $g\in G_0$, and $X\in V$.

If $\{\lambda^{\alpha\beta}\}_{(\alpha\beta)}$ denotes the dual basis for $\{\varphi_{\alpha\beta}\}_{(\alpha\beta)}$ we set $K_{\alpha\beta}=\{\lambda^{\alpha\beta}\circ F: F\in H_\rho(V)\}$. As in Ref. 1 (p. 31) we equip $H_\rho(V)$ and $K_{\alpha\beta}$ with appropriate inner products which render R^0_ρ and π^0 unitary. Invoking Theorem 3.8 in Ref. 1 we obtain the following:

Lemma 3.4: The Hilbert space K is decomposed into primary irreducible components under the representation π^0 as

$$K=\sum_{(\alpha\beta)}\oplus K_{\alpha\beta},$$

where the summation is taken over all nonnegative integers α,β satisfying $\alpha+\beta=m+n-2j-2i$. Moreover, each subrepresentation $\pi^0_{\alpha\beta}$ of π^0 on $K_{\alpha\beta}$ is equivalent to the representation R^0_ρ.

Lemma 3.5: For fixed i,j $(0\leqslant j\leqslant m, 0\leqslant i\leqslant m-j)$ if we let $\alpha=n-j-i$ and $\beta=m-j-i$, then the space $K_{(n-j-i,m-j-i)}$ consists of symplectic Stiefel harmonics f which also satisfy the condition

$$f(aX)=a_1^{n-j}a_2^{m-j}f(X) \tag{3.3}$$

for all

$$a=\begin{pmatrix}a_1 & 0\\ 0 & a_2\end{pmatrix}$$

in U, and all X in V.

Proof: For F in $H_\rho(V)$ write $F(X)=\Sigma_{(\alpha\beta)}F^{\alpha\beta}(X)\varphi_{\alpha\beta}$, where $F^{\alpha\beta}=\lambda^{\alpha\beta}\circ F\in K_{\alpha\beta}$, and $X\in V$. Thus, for all $a\in U$ and all $y\in\mathbb{C}^{2\times 2}$ we have

$$F(aX)(y)=\sum_{(\alpha\beta)}F^{\alpha\beta}(aX)\varphi_{\alpha\beta}(y).$$

Since F is ρ-covariant, we must also have

$$F(aX)(y)=(\rho(a)F(X))(y)=[F(X)](ya)$$

$$=\sum_{(\alpha\beta)}F^{\alpha\beta}(X)\varphi_{\alpha\beta}(ya).$$

Now, $\varphi_{\alpha\beta}(ya)=a_1^{\alpha+i}a_2^{\beta+i}\varphi_{\alpha\beta}(y)$. In conclusion,

$$\sum_{(\alpha\beta)}F^{\alpha\beta}(aX)\varphi_{\alpha\beta}(y)=\sum_{(\alpha\beta)}a_1^{\alpha+i}a_2^{\beta+i}F^{\alpha\beta}(X)\varphi_{\alpha\beta}(y)$$

for all $y\in\mathbb{C}^{2\times 2}$. It follows that

$$F^{\alpha\beta}(aX)=a_1^{\alpha+i}a_2^{\beta+i}F^{\alpha\beta}(X)$$

for all $(a,X)\in U(2)\times V$. In particular, when $\alpha=n-j-i$, $\beta=m-j-i$ we obtain

$$F^{(n-j-i,m-j-i)}(aX)=a_1^{n-j}a_2^{m-j}F^{(n-j-i,m-j-i)}(X).$$

□

By an easy argument involving analytic continuation, one can strengthen Relation (3.3) to

$$f\left(\begin{pmatrix}b_1 & 0\\ 0 & b_2\end{pmatrix}X\right)=b_1^{n-j}b_2^{m-j}f(X) \tag{3.4}$$

for all $b_1,b_2\in\mathbb{C}^*$. Also, it follows from the "unitarian trick" that if we denote by $\pi^{(n-j-i)}_{(m-j-i)}$ the representation of G which is obtained by right translation on $K_{n-j-i,m-j-i)}$ then it is irreducible with signature $(m+n-2j-i,i,0,\ldots,0)$.

Let Ω^{n-j}_{m-j} denote the representation of G on H^{n-j}_{m-j}. Fix i and j, and consider the linear space $K_{(n-j-i,m-j-i)}$ as given in Lemma 3.5.

Let Φ denote the linear map defined by

$$[\Phi f](\xi,x)=f\left(\begin{bmatrix}\xi\\ x\text{'s}\end{bmatrix}\right)$$

for all f in $K_{(n-j-i,m-j-i)}$ and all $\begin{bmatrix}\xi\\ x\text{'s}\end{bmatrix}$ in V. For all $b_1,b_2\in\mathbb{C}^*$ Eq. (3.4) implies

$$[\Phi f](b_1\xi,xb_2)=f\left(\begin{bmatrix}b_1 & 0\\ 0 & b_2\end{bmatrix}\begin{bmatrix}\xi\\ x\text{'s}\end{bmatrix}\right)$$

$$=b_1^{n-j}b_2^{m-j}[\Phi f](\xi,x).$$

Also, by a simple computation we see that

$$[\Delta(\Phi F)](\xi,x)=[p_{12}(D)f]\left(\begin{bmatrix}\xi\\ x\text{'s}\end{bmatrix}\right);$$

since $f\in K_{(n-j-i,m-j-i)}$ it follows that $\Delta(\Phi f)=0$. Hence Φf belongs to H^{n-j}_{m-j}.

By definition, $g\in G$ implies $(g^{-1})'s=sg$; it follows that

$$[\Omega^{n-j}_{m-j}(g)\Phi f](\xi,x)$$

$$=\Phi f(\xi g,g^{-1}x)$$

$$=f\left(\begin{bmatrix}\xi g\\ (g^{-1}x)\text{'s}\end{bmatrix}\right)=f\left(\begin{bmatrix}\xi g\\ x\text{'s}g\end{bmatrix}\right)=f\left(\begin{bmatrix}\xi\\ x\text{'s}\end{bmatrix}g\right)$$

$$=[\pi^{n-j-i}_{m-j-i}(g)f]\left(\begin{bmatrix}\xi\\ x\text{'s}\end{bmatrix}\right)=\{\Phi(\pi^{n-j-i}_{m-j-i}(g)f)\}(\xi,x).$$

Thus, Φ is an intertwining operator. Since Φ is obviously injecive, if we denote by $\mathscr{H}(n+m-2j-i,i)$ the image of $K_{(n-j-i,m-j-i)}$ under Φ, then $\mathscr{H}(n+m-2j-i,i)]$ is a simple G-submodule of H^{n-j}_{m-j}. Since for different i $(0\leqslant i\leqslant m-j)$ the $\mathscr{H}(n+m-2j-i,i)]$ are nonisomorphic simple G-modules, by the same argument used at the end of the proof of Theorem 2.2, we see that it suffices to verify that the dimension of H^{n-j}_{m-j} is equal to the sum of the dimensions of the $\mathscr{H}(n+m-2j-i,i)$'s to achieve the proof of Theorem 3.2. According to Ref. 5(b),

$$\dim(H^{n-j}_{m-j}) = \frac{(2k+(n-j)+(m-j)-1)\ [(2k+(n-j)-2)!(2k+(m-j)-2)!\ ]}{(2k-1)!(2k-2)!(n-j)!(m-j)!}$$

and

$$\dim(\mathscr{H}(n+m-2j-i,i)) = \frac{(n+m-2j-2i+1)(n+m-2j+2k-1)\ [(n+m-2j-i+2k-2)!(i+2k-3)!\ ]}{(2k-1)!(2k-3)!(n+m-2j-i+1)!i!}$$

Thus, if we set $u=n-j$, $v=m-j$, then $u\geqslant v\geqslant i\geqslant 0$, and we must establish the following relation:

$$\frac{(2k+u+v-1)\ [(2k+u-2)!(2k+v-2)!\ ]}{(2k-1)!(2k-2)!u!v!} = \sum_{i=0}^{v} \frac{(u+v-2i+1)(u+v+2k-1)\ [(u+v-i+2k-2)!(i+2k-3)!\ ]}{(2k-1)!(2k-3)!(u+v-i+1)!i!} \tag{3.5}$$

Remark 3.6: Explicit decompositions of the restriction of representations of several classical groups to their various subgroups, similar to our result in Theorems 2.2 and 3.2, were investigated in Refs. 14, 15, 5(b), and 17. In Ref. 5(b), Weyl gave a general formula which, in principle, would allow us to compute the multiplicity of each equivalence class of irreducible analytic representations of G that occurs in the restriction to G of an analytic representation of $\mathrm{GL}(2k,\mathbb{C})$. In the appendix we perform such a computation for a simple case ($k=2$); however, this technique doesn't seem tractable for more complex cases.

APPENDIX

In this appendix we will utilize the notations and results in Ref. 5(b) Sec. 8 (pp. 216–222), especially Theorem 7.8.G. Let $\pi(e_1,\ldots,e_{2k})$ [resp. $\pi_G(m_1,\ldots,m_k)$] denote the representation of $\mathrm{GL}(2k,\mathbb{C})$ (resp. of G) of signature $(e_1,\ldots,e_{2k})$ [resp. $(m_1,\ldots,m_k)$]. Our objective is to investigate the decomposition of the representation $\pi(n,0,\ldots,0,-m)$ when restricted to G. Since G is a subgroup of $\mathrm{SL}(2k,\mathbb{C})$, this is equivalent to studying the restriction of $\pi(n+m,m,\ldots,m,0)$ to G.

If $z_1,\ldots,z_{2k}$ are $2k$ complex variables, let $|z^{\alpha_1},\ldots,z^{\alpha_{2k}}|$ denote the determinant of the matrix of order $2k$ having $[z_j^{\alpha_1},\ldots,z_j^{\alpha_{2k}}]$, $(1\leqslant j\leqslant 2k)$, as the jth row. Set

$$L_{n+m-i,i,0,\ldots,0}(z_1,\ldots,z_k) = |z^{n+m-1+2k-1}, z^{i+2k-2}, z^{2k-3},\ldots, \times z^{k-1}, z^{k-2}+z^{k}, z^{k-3}+z^{k+1},\ldots,1+z^{2k-2}|,$$

then by virtue of Theorem 7.8.G in Ref. 5 one has the following formula:

$$L_{n+m-i,i,0,\ldots,0}(z_1,\ldots,z_{2k}) \Big/ \prod_{1\leqslant j<l\leqslant 2k}(1-z_jz_l) = \sum_{(l_1\geqslant\cdots\geqslant l_k\geqslant 0} \mu\begin{pmatrix} l_1,\ldots,l_{2k} \\ n+m-i,i,0,\ldots,0\end{pmatrix} \times |z_1^{l_1+(2k-1)},\ldots,z^{l_{2k}}|, \tag{A1}$$

where

$$\mu\begin{pmatrix} l_1\cdots l_{2k} \\ n+m-i,i,0,\ldots,0\end{pmatrix}$$

represents the multiplicity with which the irreducible representation $\pi_G(n+m-i,i,0,\ldots,0)$ occurs in $\pi(l_1,\ldots,l_{2k})$.

Clearly, we have

$$L_{n+m-i,i,0,\ldots,0}(z_1,\ldots,z_{2k}) = (|z^{n+m+2k-i-1}, z^{i+2k-2}, z^{2k-3},\ldots,z,1| + |z^{n+m+2k-i-1}, z^{i+2k-2}, z^{2k-3}\ldots,z,z^{2k-2}|)\,(\Pi_{1\leqslant j<l\leqslant 2k}(1-z_jz_l)$$

Suppose $n\geqslant m$ and $k=2$. A moment's consideration will show that, for this particular case,

$$\mu\begin{pmatrix} n+m,m,\ldots,m,0 \\ n+m-i,i,0,\ldots,0,0\end{pmatrix}$$

represents precisely the coefficient of the polynomial $z_1^{n+m+3}z_2^{m+2}z_3^{m+1}$ in the expression of the left side of Formula (A1). A simple argument shows that this coefficient represents the number of solutions of the equation

$$z_1^{n+m+3}z_2^{m+2}z_1^{m+1} = z_1^{n+m+3-i}(z_2^{i+2}z_3)\,[(z_1z_2)^u(z_1z_3)^v(z_2z_3)^w]$$

for all nonnegative integers u,v,w. This leads to the unique solution $u=0$, $v=i$, and $w=m-i$. Further systematic use of Formula (A1) for more complex cases leads to unmanageable calculations.

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The point form of quantum dynamics and a 4-vector coordinate operator for a spinless particle

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We construct the analog in the quantum mechanics of a free spinless particle, of Dirac's formula for the generators of space–time translations in his point form of classical dynamics, where one takes as fundamental variables the generators of homogeneous Lorentz transformations and the coordinate 4-vector of the point where the world line of the particle meets one sheet of a two-sheeted hyperboloid in space–time. A 4-vector coordinate operator is determined for such a particle, with commuting Hermitian components. The corresponding observable is the analog of the coordinate 4-vector of the point on the hyperboloid. This operator bears the same relation to such a surface as the Newton–Wigner operator does to an instant.

1. INTRODUCTION

Dirac[1] has shown that in classical mechanics there are many ways to set up a dynamical discription of a free point particle with nonzero rest mass, consistent with the requirements of the special theory of relativity. An observer in any inertial frame of reference need make use only of variables specifying the condition of the particle at the point in space—time where its world line crosses an arbitrarily chosen spacelike surface. (Even a surface on which every two points are separated by either a spacelike or a null interval may be chosen.) These dynamical variables will include the energy—momentum 4-vector for the particle, P_λ; the relativistic angular—momentum tensor $J_{\lambda\mu}(=-J_{\mu\lambda})$; and three coordinates specifying the location of the particle on the surface.

A Poisson bracket (A,B) must be introduced for every pair of dynamical variables A, B in such a way that

$$(P_\lambda, P_\mu)=0, \quad (P_\lambda, J_{\mu\nu})=g_{\lambda\mu}P_\nu - g_{\lambda\nu}P_\mu,$$
$$(J_{\lambda\mu}, J_{\nu\rho})=g_{\mu\nu}J_{\lambda\rho}+g_{\lambda\rho}J_{\mu\nu}-g_{\mu\rho}J_{\lambda\nu}-g_{\lambda\nu}J_{\mu\rho}, \tag{1}$$

in order that the ten variables P_λ and $J_{\lambda\mu}$ will generate a group of transformations isomorphic to $\mathcal{P}$, the inhomogeneous Lorentz group.

If the observer adopts a system of space—time coordinates x_λ, an obvious choice for the spacelike surface is an instant, say $x_0=0$. The three coordinates q_r for the particle may then be taken to form a 3-vector. Following Dirac, one may choose to regard this as the 3-vector part of a 4-vector q_λ associated with the particle, and subject to the constraint $q_0=0$; and one may further suppose the existence of a 4-vector p_λ conjugate to q_λ, so that one has the Poisson bracket relations

$$(q_\lambda, q_\mu)=0=(p_\lambda, p_\mu), \quad (p_\lambda, q_\mu)=g_{\lambda\mu}. \tag{2}$$

However, the constraint $q_0=0$ is required to be invariant under canonical transformations generated by all dynamical variables of physical importance—called *physical variables* by Dirac—and it follows that these can be functions only of the q_r and p_r. In particular, Dirac argued that P_λ and $J_{\lambda\mu}$ are given by

$$P_r=p_r, \quad J_{rs}=q_rp_s-q_sp_r, \tag{3a}$$
$$P_0=(p_rp_r+m^2c^2)^{1/2} \tag{3b}$$
$$J_{r0}=(p_sp_s+m^2c^2)^{1/2}q_r, \tag{3c}$$

where m is the rest mass of the particle, and c the speed of light. It is well known that these definitions lead, in consequence of (2), to the required relations (1), as well as to the relations

$$P_\lambda P^\lambda=m^2c^2, \tag{4a}$$
$$P_0\gtrless mc, \tag{4b}$$
$$\epsilon_{\lambda\mu\nu\rho}J^{\mu\nu}P^\rho=0, \tag{4c}$$

which characterize a system with rest mass m, positive energy, and no internal angular momentum. As Dirac pointed out, the choice of the surface $x_0=0$ singles out the Euclidean subgroup of $\mathcal{P}$, because coordinate transformations in that subgroup leave this surface invariant. Some consequences of this are the relatively simple expressions for the associated generators P_r and J_{rs} in (3) as compared with those for P_0 and J_{r0}, and a complicated transformation law for q_r with respect to Lorentz boosts.[2]

Dirac called this the "instant" form of dynamics, and presented corresponding results for two other forms of classical dynamics:

(I) The "point" form, in which the selected surface is taken to be one sheet of a two-sheeted hyperboloid or cone, such as $x_\lambda x^\lambda=k^2$, $x_0\gtrless k\gtrless 0$.

(II) The "front" form, in which the selected surface is a plane light wave front, such as $x_0=x_3$.

We are concerned with the point form of relativistic quantum dynamics (in the case $k>0$) for a free, spinless particle with nonzero rest mass and positive energy, in particular as it bears upon the much-discussed question of the definition of position operators for such a particle. We do not consider the special limiting case $k=0$, which has been discussed from a slightly different viewpoint by Peres,[3] and when we speak of the point form below, we shall generally be referring to the case $k>0$.

In order to establish the line of our argument, we describe briefly in Sec. 2 the familiar instant form of quantum dynamics for such a particle. The operator analog of the classical coordinate 3-vector q_r is easily seen to be the Newton—Wigner operator[4], which therefore corresponds to the measurement of the position of

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the particle on an instant. The complicated transformation properties of this operator in respect of Lorentz boosts are from this point of view not to be regarded as a defect when this operator is used to define the concept of localization of the particle (on an instant). On the contrary, they are a necessary consequence of the fact that an instant is not a Lorentz-invariant surface, and they are quite analogous to the transformation properties of the classical 3-vector q_r. (See however the relevant discussion in Ref. 2.) When the papers of Dirac[1] and Newton and Wigner[4] are studied side by side, one's initial reaction may be that the question of localization of an elementary particle (or system) on an instant has been resolved, at least in the spinless case, in a perfectly satisfactory way with due regard for the correspondence principle. One may feel less sure when one remembers that "manifestly covariant" descriptions of particles apparently need to be used if a (field) theory of local interactions is to be developed. Associated with such descriptions one has conserved current densities, which seem to point the way to other concepts of localization. (See for example Barut and Malin[5].)

In Sec. 3 we review Dirac's formula for the generators of space—time translation in the point form of classical mechanics and formulate the problem of finding the analog of this formula in quantum mechanics. We find that a mathematically equivalent problem can also be formulated—that of finding in terms of the group generators an expression for a 4-vector operator which is the analog in quantum mechanics of the coordinate 4-vector of the point where the world line of the classical particle meets the hyperboloid sheet described in (I) above.

Some of the properties of this 4-vector coordinate operator have been summarized by us elsewhere[6] without proof. It has commuting, Hermitian components, and bears the same relation to the surface described in (I) as does the Newton—Wigner operator to the instant; and just as the latter transforms simply under the Euclidean group, but not under Lorentz boosts, so the former transforms simply under the homogeneous Lorentz group (as a 4-vector) but not simply under translations in space or time. No doubt this explains why it does not seem to have been mentioned in the extensive literature on the localization of elementary particles. (See for example Refs. 4, 5, 7-11 and references therein.)

In Sec. 4, we solve the problem formulated in Sec. 3, relegating some proofs to two Appendices. Our conclusions are summarized in Sec. 5.

Notation: In what follows, we use the same symbol to denote a classical variable and its operator counterpart in quantum mechanics, relying on context to distinguish the two. Greek indices run over 0, 1, 2, 3 and Latin over 1, 2, 3. The metric tensor is diagonal with $g_{00} = -g_{11} = -g_{22} = -g_{33} = 1$, and the alternating tensor is defined with $\epsilon_{0123} = 1$.

2. THE INSTANT FORM OF RELATIVISTIC QUANTUM DYNAMICS

We proceed by analogy with the development of the classical case in Eqs. (2)—(4) now taking p_λ and q_λ to be operators in a suitable vector space, and replacing the Poisson bracket relations (2) by commutation relations

$$[q_\lambda, q_\mu] = 0 = [p_\lambda, p_\mu], \quad [p_\lambda, q_\mu] = i\hbar g_{\lambda\mu} \tag{5}$$

The constraints $q_0 = 0$ must now be interpreted as an operator equation valid in the physically relevant portion of the vector space, and it again restricts the physical variables to be functions only of the p_r and q_r. In quantum mechanics one also requires that physical variables be Hermitian operators in Hilbert space. Thus q_r should be taken to be Hermitian, and the assumption that p_r also is Hermitian guarantees the hermiticity of P_r and J_{rs} if we take over the classical formulas (3a) to define these variables. Moreover, P_0 as defined in (3b) will then also be Hermitian provided the operator square root is suitably interpreted. However, the formula (3c) for J_{r0} is then not consistent with the hermiticity requirement, and in order to obtain Hermitian J_{r0} without violating the correspondence principle, we are naturally led to adopt instead the symmetrized expression

$$J_{r0} = \tfrac{1}{2} q_r (p_s p_s + m^2 c^2)^{1/2} + \tfrac{1}{2} (p_s p_s + m^2 c^2)^{1/2} q_r. \tag{6}$$

It is then readily checked that with these definitions, P_λ and $J_{\lambda\mu}$ satisfy the required relations

$$\begin{aligned} &[P_\lambda, P_\mu] = 0, \quad [P_\lambda, J_{\mu\nu}] = i\hbar (g_{\lambda\mu} P_\nu - g_{\lambda\nu} P_\mu), \\ &[J_{\lambda\mu}, J_{\nu\rho}] = i\hbar (g_{\mu\nu} J_{\lambda\rho} + g_{\lambda\rho} J_{\mu\nu} - g_{\mu\rho} J_{\lambda\nu} - g_{\lambda\nu} J_{\mu\rho}), \end{aligned} \tag{7}$$

as well as the "representation relations" (4), now interpreted as operator equations.

As q_r and p_r are by assumption Hermitian operators satisfying the canonical commutation relations, one may take the Hilbert space to be that of square-integrable functions $\Phi(p_1, p_2, p_3)$ with scalar product

$$(\Phi, \Psi) = \int\int\int_{-\infty}^{\infty} \Phi^*(p_1, p_2, p_3)\, \Psi(p_1, p_2, p_3)\, d^3p, \tag{8}$$

and take $q_r = i\hbar\, \partial/\partial p_r$. It is well-known (see, for example, Foldy[12]) that in this space the operators P_λ and $J_{\lambda\mu}$ defined above generate the unitary representation $(m^2c^2, 0, +)$ of $\mathcal{P}$, apprpriate to the description in the Heisenberg picture of a positive-energy spinless particle with rest mass m. The operators q_r are seen to form the Newton—Wigner 3-vector position operator (at $x_0 = 0$), which is thus revealed as the analogue in quantum mechanics of the position vector of the classical particle where its world line meets an instant.

Since the operators P_λ and $J_{\lambda\mu}$ do generate an irreducible representation of $\mathcal{P}$ one may hope that any given operator on the Hilbert space can be expressed in terms of those generators. This is true for the operator q_r: It can be seen from (3a), (3b), and (6) that

$$q_r = J_{r0} (P_0)^{-1} + \tfrac{1}{2} i\hbar P_r (P_0)^{-2}. \tag{9}$$

Moreover it is not hard to see that if one takes (9) as a definition of q_r, *assuming* the commutation relations (7) *and* representation relations (4), then one can *deduce* the relations

$$[q_r, q_s] = 0, \quad [q_r, P_s] = i\hbar\, \delta_{rs}, \quad J_{rs} = q_r P_s - q_s P_r,$$

and

$$J_{r0} = \tfrac{1}{2} q_r (P_s P_s + m^2 c^2)^{1/2} + \tfrac{1}{2} (P_s P_s + m^2 c^2)^{1/2} q_r \tag{10}$$

From this point of view, it is the group generators which play the more fundamental role, the variables q_r

being derived quantities. In such a formulation one does not need to introduce the unphysical variables p_0 and q_0.

3. THE POINT FORM OF RELATIVISTIC DYNAMICS

The preceding discussion should have its counterpart for each of the other forms of classical dynamics described by Dirac— and in principle, for the form corresponding to an arbitrary choice of spacelike surface. Fleming[11] has found the counterpart for the case of a general spacelike hyperplane, in which case the constraint $q_0 = 0$ is replaced by

$$q_\mu \eta^\mu = \tau,$$

where τ and η^μ are real constants, with $\eta_\mu \eta^\mu = 1$. In the case of a nonplanar surface, such as that defining the point form, the counterpart is more difficult to discover.

In the point form, the three coordinates specifying the point at which the world line of the classical particle meets the surface $x_\lambda x^\lambda = k^2$, $x_0 \geqq k \geqq 0$, may be written as a 4-vector q_λ subject to the constraints

$$q_\lambda q^\lambda = k^2, \quad q_0 \geqq k. \tag{11}$$

Again introducing variables p_λ conjugate to q_λ as in (2), and noting these constraints, we expect that in this case physical variables can be functions only of q_λ and $l_{\lambda\mu}$, where

$$l_{\lambda\mu} = q_\lambda p_\mu - q_\mu p_\lambda.$$

Dirac argued that P_λ and $J_{\lambda\mu}$ in particular have the forms

$$\begin{aligned} J_{\lambda\mu} &= l_{\lambda\mu} \\ k^2 P_\lambda &= k^2 p_\lambda + q_\lambda \{[(p_\mu q^\mu)^2 - k^2(p_\mu p^\mu - m^2c^2)]^{1/2} - p_\mu q^\mu\} \\ &= -\, l_{\lambda\mu} q^\mu + q_\lambda (m^2c^2k^2 - \tfrac{1}{2} l_{\mu\nu} l^{\mu\nu})^{1/2}, \end{aligned} \tag{12}$$

which one readily checks imply the required relations (1) and (4).

One then sees that

$$q_\lambda P_\mu - q_\mu P_\lambda = J_{\lambda\mu} \tag{13}$$

and that the Poisson bracket (q_λ, P_μ) $[= -\partial P_\mu / \partial p^\lambda]$ has the form

$$(q_\lambda, P_\mu) = -g_{\lambda\mu} + q_\lambda P_\mu (q_\nu P^\nu)^{-1}, \tag{14}$$

so that

$$(q_\lambda, P^\lambda) = -3. \tag{15}$$

There is a remarkable symmetry between the roles of the timelike 4-vectors P_λ and q_λ in this form of dynamics. Apart from Eqs. (13— 15), ones sees that as a result of Eqs. (4a), (11), (12), and (13)

$$k^2 P_\lambda = -J_{\lambda\mu} q^\mu + q_\lambda (m^2c^2k^2 - \tfrac{1}{2} J_{\mu\nu} J^{\mu\nu})^{1/2} \tag{16}$$

$$m^2c^2 q_\lambda = J_{\lambda\mu} P^\mu + P_\lambda (m^2c^2k^2 - \tfrac{1}{2} J_{\mu\nu} J^{\mu\nu})^{1/2} \tag{17}$$

All equations in the point form of dynamics, such as (13)— (17) above, can be expressed in a manifestly covariant way using four-dimensional tensor notation. As Dirac stressed, this reflects the special role chosen for the homogeneous Lorentz subgroup of $\mathcal{P}$ by the observer's choice of a special surface which is invariant under Lorentz transformations of his coordinate system. It is this feature of the point form, and the associated fact that this subgroup is simple in the mathematical sense, which makes it attractive and will be responsible for any advantages it may have over the other forms.

Turning now to the point form of *quantum* dynamics for a spinless particle, we proceed initially as in the case of the instant form (Sec. 2), introduce a set of operators q_λ, p_λ satisfying the commutation relations (5), and impose the operator constraints

$$q_\lambda q^\lambda = k^2, \quad q_0 \geqq k > 0, \tag{18}$$

now to be satisfied by Hermitean operators q_λ on a Hilbert space $\mathcal{H}$.

We also take $l_{\lambda\mu} (= q_\lambda p_\mu - q_\mu p_\lambda)$ to be Hermitian operators in $\mathcal{H}$, and identify $J_{\lambda\mu} = l_{\lambda\mu}$. Then we wish to find the analog in the quantum theory of the formula (16), defining Hermitean P_λ in terms of q_λ and $J_{\lambda\mu}$ in such a way that the P_λ and $J_{\lambda\mu}$ satisfy the relations (4) and (7).

A suitable realization of the space $\mathcal{H}$ is that of functions $\Phi(q_0, q_1, q_2, q_3)$ defined on the sheet $q_0 \geqq k > 0$ of the hyperboloid $q_\lambda q^\lambda = k^2$, with scalar product

$$(\Phi, \Psi) = \int \Phi^*(q_0, q_1, q_2, q_3)\, \Psi(q_0, q_1, q_2, q_3) d\Omega,$$

where the integral is over the whole sheet, and $d\Omega (= dq_1\, dq_2 dq_3 / q_0)$ is the Lorentz-invariant volume element on the sheet. Then q_λ and also $l_{\lambda\mu}$, which is now given by

$$l_{\lambda\mu} = i\hbar (q_\lambda \partial/\partial q^\mu - q_\mu \partial/\partial q^\lambda), \tag{19}$$

are Hermitian as required. In these terms, the problem is to exhibit the unitary representation $(m^2c^2, 0, +)$ of $\mathcal{P}$ in this function space, with generators

$$J_{\lambda\mu} = i\hbar (q_\lambda \partial/\partial q^\mu - q_\mu \partial/\partial q^\lambda) \tag{20}$$

and P_λ, defined in such a way that the classical formula (13), and consequently (16), can be recovered in the classical limit.

Peres[3] has solved the corresponding problem in the limiting case $k = 0$ (for particles with spin 0 or $\frac{1}{2}$.) However, his solution is not expressed in a manifestly covariant way, so that the peculiar advantage of the point form is to some extent lost in his treatment. While Fubini, Hanson, and Jackiw,[13] Sommerfield,[14] and Gromes, Rothe, and Stech[15] have considered the initial-value problem for quantum or classical fields with the surface $x_\lambda x^\lambda = k^2$, $x_0 \geqq k > 0$ as Cauchy surface, no one to our knowledge has tackled the specific problem posed above, although Fubini *et al.* make passing reference to its difficulty.

Supposing that a solution P_λ exists, it is clear that $q_\lambda P_\mu - q_\mu P_\lambda$ and $P_\mu q_\lambda - P_\lambda q_\mu$ can differ from $J_{\lambda\mu}$ only by terms which in some sense vanish in the classical limit. We shall see that it is possible to find a solution P_λ with

$$J_{\lambda\mu} = \tfrac{1}{2}(q_\lambda P_\mu - q_\mu P_\lambda) + \tfrac{1}{2}(P_\mu q_\lambda - P_\lambda q_\mu),$$

but *not* with $J_{\lambda\mu}$ equal to either of the asymmetrical forms. The solution is uniquely determined if we require in addition the analogue of (15), viz.

$$[q_\lambda, P^\lambda] = -3i\hbar.$$

In the representation space $\mathcal{H}$ the P_λ and $J_{\lambda\mu}$ must satisfy the representation relations (4) as well as the commutation relations (7). We note that in $\mathcal{H}$ we shall have the relations (18), and also

$$\epsilon_{\lambda\mu\nu\rho}J^{\mu\nu}q^{\rho}=0 \tag{21}$$

by virtue of (2). Furthermore, it is clear that in $\mathcal{H}$

$$[q_\lambda,q_\mu]=0$$
$$[q_\lambda,J_{\mu\nu}]=i\hbar(g_{\lambda\mu}q_\nu-g_{\lambda\nu}q_\mu). \tag{22}$$

Comparing (18) and (21) with (4a)– (4c), and (22) with (7), we see that the Hermitian operators q_λ and $J_{\lambda\mu}$ may be regarded as generators in $\mathcal{H}$ of a unitary irreducible representation $(k^2,0,+)$ of a group isomorphic to $\mathcal{P}$.

Just as in the case of the instant form of dynamics, one can look at the problem posed above for the point form from a different point of view, supposing the generators $P_\lambda, J_{\lambda\mu}$ of the representation $(m^2c^2,0,+)$ to be given, and arguing that other operators in the Hilbert space, such as q_λ, might be expressible in terms of those generators. From this point of view, one has Hermitian operators P_λ, $J_{\lambda\mu}$ satisfying (4, 7), and wishes to express in terms of them, Hermitian operators q_λ via a formula reducing to (17) in the classical limit.

One sees that mathematically, this problem is essentially the same as the former one. In its most abstract form, *each* problem can be formulated as follows:

One has a set of Hermitian operators a_λ, $J_{\lambda\mu}$ which generate in a Hilbert space $\mathcal{H}$ a unitary irreducible representation $(1,0,+)$ of a group isomorphic to $\mathcal{P}$, and hence satisfy

$$[a_\lambda,a_\mu]=0,\quad [a_\lambda,J_{\mu\nu}]=i\hbar(g_{\lambda\mu}a_\nu-g_{\lambda\nu}a_\mu), \tag{23a,b}$$
$$[J_{\lambda\mu},J_{\nu\rho}]=i\hbar(g_{\mu\nu}J_{\lambda\rho}+g_{\lambda\rho}J_{\mu\nu}-g_{\lambda\nu}J_{\mu\rho}-g_{\mu\rho}J_{\lambda\nu}), \tag{23c}$$

as well as

$$a_\lambda a^\lambda=1,\quad a_0\gtrless 1,\quad \epsilon_{\lambda\mu\nu\rho}J^{\mu\nu}a^\rho=0; \tag{24a,b,c}$$

and one wishes to find, in terms of a_λ and $J_{\lambda\mu}$, Hermitian operators b_λ satisfying the same relations as a_λ in (23) and (24). In addition, one wants to obtain in the classical limit

$$a_\lambda b_\mu-a_\mu b_\lambda=\alpha J_{\lambda\mu} \tag{25}$$

and (consequently)

$$b_\lambda=-\alpha J_{\lambda\mu}a^\mu+a_\lambda(1-\tfrac{1}{2}\alpha^2J_{\mu\nu}J^{\mu\nu})^{1/2}, \tag{26}$$

where α is a nonzero constant with the dimensions of $\hbar^{-1}$. In the first problem posed, $\alpha=1/mck$, $a_\lambda=q_\lambda/k$, $b_\lambda=P_\lambda/mc$; in the second $\alpha=-1/mck$, $a_\lambda=P_\lambda/mc$, $b_\lambda=q_\lambda/k$.

As indicated above, in order to specify a solution uniquely, we shall find it necessary to require

$$[a_\lambda,b^\lambda]=-3i\hbar\alpha, \tag{27}$$

the analog of the classical relation $(a_\lambda,b^\lambda)=-3\alpha$.

4. SOLUTION OF THE PROBLEM

It is known[16] that the operator $\frac{1}{2}J_{\lambda\mu}J^{\lambda\mu}$ has in $\mathcal{H}$ a continuous spectrum of points $-(1+\beta^2)\hbar^2$, $0\leqq\beta<\infty$; we introduce an Hermitian Lorentz-scalar operator B satisfying

$$[B,J_{\lambda\mu}]=0,\quad \tfrac{1}{2}J_{\lambda\mu}J^{\lambda\mu}=-(1+B^2)\hbar^2 \tag{28a,b}$$

(Here and below, a numerical multiple of the identity operator on $\mathcal{H}$ is denoted by the corresponding complex number.) The specification of B is completed by the requirement that its spectrum be of points β, $0\leqq\beta<\infty$, corresponding to that of $\frac{1}{2}J_{\lambda\mu}J^{\lambda\mu}$ in the obvious way. Then $\hbar B$ is an analog in quantum theory of the positive square root of the positive classical quantity $(-\frac{1}{2}J_{\lambda\mu}J^{\lambda\mu})$.

The identity

$$J_{\lambda\mu}J^{\mu\nu}a_\nu-2i\hbar J_{\lambda\nu}a^\nu+(\tfrac{1}{2}J_{\rho\sigma}J^{\rho\sigma})a_\lambda=0 \tag{29}$$

holds as a consequence of (23c) and (24c), as can be checked by substitution of index values. This is a special case of a more general type of identity, discussed in detail elsewhere.[6,17]

Combining (28b) and (29) we have

$$(J_{\lambda\mu}-(i-B)\hbar g_{\lambda\mu})(J^{\mu\nu}-(i+B)\hbar g^{\mu\nu})a_\nu=0. \tag{30}$$

We define

$$v^{(\pm)}{}_\lambda=(2\hbar B)^{-1}(J_{\lambda\mu}-(i\mp B)\hbar g_{\lambda\mu})a^\mu \tag{31}$$

so that

$$a_\lambda=v^{(+)}{}_\lambda-v^{(-)}{}_\lambda. \tag{32}$$

Then it follows from (30) that

$$J_{\lambda\mu}v^{(\pm)\mu}=\hbar(i\pm B)v^{(\pm)}{}_\lambda. \tag{33}$$

Now according to (31), $v^{(\pm)}{}_\lambda$ is a 4-vector operator, so that

$$[v^{(\pm)}{}_\lambda,J_{\mu\nu}]=i\hbar(g_{\lambda\mu}v^{(\pm)}{}_\nu-g_{\lambda\nu}v^{(\pm)}{}_\mu) \tag{34}$$

and hence

$$[v^{(\pm)}{}_\lambda,\tfrac{1}{2}J_{\mu\nu}J^{\mu\nu}]=2i\hbar J_{\lambda\mu}v^{(\pm)\mu}+3\hbar^2v^{(\pm)}{}_\lambda. \tag{35}$$

Combining (28b), (33), and (35) we have

$$[v^{(\pm)}{}_\lambda,\ (1+B^2)]=(-1\mp 2iB)v^{(\pm)}{}_\lambda,$$

that is

$$(B\mp i)^2v^{(\pm)}{}_\lambda=v^{(\pm)}{}_\lambda B^2. \tag{36}$$

In Appendix A we show the validity of the (apparently) stronger result

$$Bv^{(\pm)}{}_\lambda=v^{(\pm)}{}_\lambda(B\pm i), \tag{37}$$

and in Appendix B that (37) implies with (32), the hermiticity of $v^{(\pm)}{}_\lambda$. It must be emphasized that (37) is *consistent* with the hermiticity of $v^{(\pm)}{}_\lambda$ and B, although formally it seems to imply that $v^{(\pm)}{}_\lambda$ shifts an eigenvector of B corresponding to a real eigenvalue β, to one corresponding to the complex eigenvalue $(\beta\pm i)$. The point is that B has no eigenvectors in $\mathcal{H}$, and *a fortiori*, none in the domain of $v^{(\pm)}{}_\lambda$. [A similar situation occurs in those unitary representations of the conformal group corresponding to massless particles, where the Hermitian dilatation generator D and translation generators P_λ satisfy $DP_\lambda=P_\lambda(D-i)$.]

The operators $v^{(\pm)}{}_\lambda$ have several remarkable properties which we now list, putting derivations in Appendix B, and they play a central role in what follows. One has

$$v^{(\pm)}{}_\lambda{}^\dagger=v^{(\pm)}{}_\lambda \quad \text{(Hermiticity)} \tag{38a}$$
$$v^{(\pm)}{}_\lambda v^{(\pm)\lambda}=0 \tag{38b}$$
$$v^{(\pm)}{}_\lambda v^{(\mp)\lambda}=-(B\mp i)/2B \tag{38c}$$
$$[v^{(\pm)}{}_\lambda,v^{(\pm)}{}_\mu]=0 \tag{38d}$$

$$v^{(\pm)}{}_\lambda v^{(\mp)}{}_\mu - v^{(\pm)}{}_\mu v^{(\mp)}{}_\lambda = \mp J_{\lambda\mu}/2\hbar B. \tag{38e}$$

We now tackle the problem posed in Sec. 3, seeking an expression for the operator b_λ in the form

$$b_\lambda = F^{(+)}(B)\, v^{(+)}{}_\lambda + F^{(-)}(B)\, v^{(-)}{}_\lambda, \tag{39}$$

where $F^{(\pm)}(B)$ is a Lorentz-scalar operator-valued function of B. We shall think of $F^{(\pm)}$ as an "analytic" function with, for example on suitable vectors in $\mathcal{H}$,

$$F^{(+)}(B) = \sum_{n=0}^{\infty} a_n (B-b)^n \tag{40}$$

for some complex numbers a_n and b. The Hermitian conjugate of $F^{(+)}$ is then

$$\sum_{n=0}^{\infty} a_n{}^*(B-b^*)^n,$$

which we write as $F^{(+)*}(B)$. Thus

$$F^{(\pm)}(B)^\dagger = F^{(\pm)*}(B). \tag{41}$$

In what follows, we repeatedly make use of relations like

$$F^{(\pm)}(B) v^{(+)}{}_\lambda = v^{(+)}{}_\lambda F^{(\pm)}(B+i),$$

which are taken to follow from (37) and (40).

Taking the Hermitian conjugate of (39), we have

$$\begin{aligned} b_\lambda{}^\dagger &= v^{(+)}{}_\lambda F^{(+)*}(B) + v^{(-)}{}_\lambda F^{(-)*}(B) \\ &= F^{(+)*}(B-i) v^{(+)}{}_\lambda + F^{(-)*}(B+i) v^{(-)}{}_\lambda \end{aligned}$$

so that b_λ is Hermitian if and only if

$$F^{(\pm)}(B) = F^{(\pm)*}(B \mp i). \tag{42}$$

Next we note from (39) that

$$\begin{aligned} b_\lambda b_\mu = {} & F^{(+)}(B) F^{(+)}(B-i) v^{(+)}{}_\lambda v^{(+)}{}_\mu \\ & + F^{(+)}(B) F^{(-)}(B-i) v^{(+)}{}_\lambda v^{(-)}{}_\mu \\ & + F^{(-)}(B) F^{(+)}(B+i) v^{(-)}{}_\lambda v^{(+)}{}_\mu \\ & + F^{(-)}(B) F^{(-)}(B+i) v^{(-)}{}_\lambda v^{(-)}{}_\mu. \end{aligned} \tag{43}$$

Then as a consequence of (38b, c) we have

$$\begin{aligned} b_\lambda b^\lambda = {} & -(B-i) F^{(+)}(B) F^{(-)}(B-i)/2B \\ & -(B+i) F^{(-)}(B) F^{(+)}(B+i)/2B, \end{aligned}$$

so that $b_\lambda b^\lambda = 1$ if and only if

$$\begin{aligned} & (B-i) F^{(+)}(B) F^{(-)}(B-i) + (B+i) F^{(+)}(B+i) F^{(-)}(B) \\ & = -2B. \end{aligned} \tag{44}$$

Furthermore, (43) also implies, with (38d, e), that

$$\begin{aligned} & [b_\lambda, b_\mu] \\ & = \left(-F^{(+)}(B) F^{(-)}(B-i) + F^{(+)}(B+i) F^{(-)}(B)\right) J_{\lambda\mu}/2\hbar B, \end{aligned}$$

so that $[b_\lambda, b_\mu] = 0$ if and only if

$$F^{(+)}(B) F^{(-)}(B-i) = F^{(+)}(B+i) F^{(-)}(B). \tag{45}$$

Combining (44) and (45) we have at once

$$F^{(+)}(B) F^{(-)}(B-i) = -1. \tag{46}$$

Thus a four-vector operator of the form (39) is Hermitian, with commuting components and unit length, if and only if (42) and (46) hold. [In particular this is so for a_λ itself, for which $F^{(+)}(B) = -F^{(-)}(B) = 1$.]

Turning now to the analog of the classical formula (25), we might try to impose any of

$$a_\lambda b_\mu - a_\mu b_\lambda = \alpha J_{\lambda\mu}, \tag{47a}$$

$$b_\mu a_\lambda - b_\lambda a_\mu = \alpha J_{\lambda\mu}, \tag{47b}$$

$$(a_\lambda b_\mu - a_\mu b_\lambda) + (b_\mu a_\lambda - b_\lambda a_\mu) = 2\alpha J_{\lambda\mu}. \tag{47c}$$

Considering firstly (47a), we note that

$$\begin{aligned} a_\lambda b_\mu &= (v^{(+)}{}_\lambda - v^{(-)}{}_\lambda)(F^{(+)}(B) v^{(+)}{}_\mu + F^{(-)}(B) v^{(-)}{}_\mu) \\ &= F^{(+)}(B-i) v^{(+)}{}_\lambda v^{(+)}{}_\mu + F^{(-)}(B-i) v^{(+)}{}_\lambda v^{(-)}{}_\mu \\ &\quad - F^{(+)}(B+i) v^{(-)}{}_\lambda v^{(+)}{}_\mu - F^{(-)}(B+i) v^{(-)}{}_\lambda v^{(-)}{}_\mu, \end{aligned}$$

so that in view of (38d, e)

$$a_\lambda b_\mu - a_\mu b_\lambda = \left(-F^{(-)}(B-i) - F^{(+)}(B+i)\right) J_{\lambda\mu}/2\hbar B. \tag{48}$$

Thus (47a) holds if and only if

$$F^{(+)}(B+i) + F^{(-)}(B-i) = -2\alpha\hbar B. \tag{49}$$

Multiplying both sides of this equation by $F^{(+)}(B)$, and noting (46) we have

$$F^{(+)}(B) F^{(+)}(B+i) + 2\alpha\hbar B F^{(+)}(B) = 1. \tag{50}$$

Taking the Hermitian conjugate of (50), we get

$$F^{(+)*}(B)\, F^{(+)*}(B-i) + 2\alpha\hbar B F^{(+)*}(B) = 1.$$

which, in view of (42), is equivalent to

$$F^{(+)}(B+i) F^{(+)}(B) + 2\alpha\hbar B F^{(+)}(B+i) = 1. \tag{51}$$

Then (50) and (51) imply

$$F^{(+)}(B) = F^{(+)}(B+i). \tag{52}$$

But then (50) and (52) imply

$$F^{(+)}(B) F^{(+)}(B) + 2\alpha\hbar B F^{(+)}(B) = 1 \tag{53}$$

and

$$F^{(+)}(B+i) F^{(+)}(B+i) + 2\alpha\hbar B F^{(+)}(B+i) = 1; \tag{54}$$

and (53) implies

$$F^{(+)}(B+i) F^{(+)}(B+i) + 2\alpha\hbar (B+i) F^{(+)}(B+i) = 1,$$

which is inconsistent with (54). Thus (47a) is inconsistent with (42) and (46).

The attempt to impose (47b) rather than (47a) leads to similar conclusions, and we turn now to the symmetric case (47c). Just as we derived (48), we find also that

$$b_\mu a_\lambda - b_\lambda a_\mu = -\left(F^{(+)}(B) + F^{(-)}(B)\right) J_{\lambda\mu}/2\hbar B,$$

so that (47c) holds if and only if

$$\left[F^{(-)}(B-i) + F^{(+)}(B+i) + F^{(+)}(B) + F^{(-)}(B)\right] = -4\alpha\hbar B, \tag{55}$$

or equivalently,

$$G(B) + G(B+i) = -2\alpha\hbar B, \tag{56}$$

where

$$2G(B) = F^{(+)}(B) + F^{(-)}(B-i). \tag{57}$$

Taking the Hermitian conjugate of (57) and using (42), we get

$$G^*(B) = G(B+i). \tag{58}$$

Multiplying by $F^{(+)}(B)$ in (57) and using (46) we get

$$F^{(+)}(B)F^{(+)}(B) - 2G(B)F^{(+)}(B) - 1 = 0,$$

so that

$$F^{(+)}(B) = G(B) + [1 + G^2(B)]^{1/2}, \tag{59}$$

where $[1 + G^2(B)]^{1/2}$ denotes some Lorentz-scalar square root of $[1 + G^2(B)]$.

Then (46) implies that

$$F^{(-)}(B - i) = G(B) - [1 + G^2(B)]^{1/2},$$

that is

$$F^{(-)}(B) = G(B + i) - [1 + G^2(B + i)]^{1/2}. \tag{60}$$

Conversely, if $G(B)$ satisfies (56) and (58), then $F^{(+)}(B)$ and $F^{(-)}(B)$, defined as in (59), (60), can be seen to satisfy (42), (46), and (55), and so to define via (39) a 4-vector operator b_λ with the required properties of hermiticity, unit length, commuting components, and satisfaction of (47c). Since (56) and (58) evidently do not uniquely determine $G(B)$, the solution to the problem at hand is not yet specified completely.

In order to remove this ambiguity, we now impose (27). From (32) and (39), we get with the help of (38b, c),

$$a_\lambda b^\lambda = [(B + i)F^{(+)}(B + i) - (B - i)F^{(-)}(B - i)]/2B$$

and

$$b_\lambda a^\lambda = [(B - i)F^{(+)}(B) - (B + i)F^{(-)}(B)]/2B,$$

so that (27) implies

$$(B + i)G(B + i) - (B - i)G(B) = -3i\alpha\hbar B. \tag{61}$$

Then (56) and (61) imply

$$G(B) = -\alpha\hbar(B - \tfrac{1}{2}i),$$

which is seen to be consistent with (58).

Substituting in (59), (60), we arrive at the expressions

$$F^{(\pm)}(B) = -\alpha\hbar(B \mp \tfrac{1}{2}i) \pm H^{(\pm)}(B), \tag{62}$$

where

$$H^{(\pm)}(B) = [1 + \alpha^2\hbar^2(B \mp \tfrac{1}{2}i)^2]^{1/2}. \tag{63}$$

Substituting from (62) in (39), and recalling the definition (31) of $v^{(\pm)}{}_\lambda$, we have finally

$$b_\lambda = [-\alpha + (H^{(+)}(B) - H^{(-)}(B))/2\hbar B]J_{\lambda\mu}a^\mu + [(3i\alpha\hbar B + (B - i)H^{(+)}(B) + (B + i)H^{(-}(B))/2B]a_\lambda. \tag{64}$$

There is a remaining ambiguity concerning the definition of the operator square roots $H^{(\pm)}(B)$ in (63) and (64). This reflects the fact that we have yet to impose the condition $b_0 \geqq 1$. An Hermitian 4-vector operator with unit length, commuting components, and satisfying (47c) can have either $b_0 \geqq 1$ or $b_0 \leqq -1$. The second possibility corresponds to a classical formula like (26) with a minus sign preceding the a_λ therein

We can guarantee $b_0 \geqq 1$ by choosing the square roots $H^{(\pm)}(B)$ so that (64) will yield (26) in the classical limit. In that limit, it is clear that in some sense which we need not make precise,

$$\hbar \sim 0, \quad B \sim +\infty, \quad \hbar^2B^2 \sim -\tfrac{1}{2}J^{\mu\nu}.$$

Then

$$H^{(+)}(B) \sim H^{(-)}(B) \sim [1 - \tfrac{1}{2}\alpha^2 J_{\mu\nu}J^{\mu\nu}]^{1/2}$$

and (26) is recovered from (64), *provided* the point $H^{(\pm)}(\beta)$ in the spectrum of $H^{(\pm)}(B)$, corresponding to the point β in the spectrum of B, has positive real part ($\sim |\alpha|\hbar\beta$) when $\beta \gg 0$. This is achieved by taking $H^{(\pm)}(\beta)$ to be the principal square root of $1 + \alpha^2\hbar^2(\beta \mp \frac{1}{2}i)^2$.

In other words, in the representation described in Appendix A, where B is realized as multiplication by the nonnegative quantity β, $H^{(\pm)}(B)$ will be realized as multiplication by the principal square root $[1 + \alpha^2\hbar^2(\beta \mp \frac{1}{2}i)^2]^{1/2}$. In this connection, it is worth mentioning that for $\alpha^2\hbar^2 \geqq 4$, the two curves $z^{(\pm)}(\beta) = [1 + \alpha^2\hbar^2(\beta \mp \frac{1}{2}i)^2]$, $\beta \geqq 0$, in the complex z plane meet the branch cut of the principal square root $z^{1/2}$ at $\beta = 0$. It *may* be that this means that b_λ as defined in (64) is not self-adjoint in such cases, but with our algebraic approach we cannot determine this. Note that $\alpha^2\hbar^2 < 4$ can be written in the very suggestive form

$$(mc)k > \tfrac{1}{2}\hbar.$$

5. CONCLUSION

We have derived for a spinless particle with nonzero rest mass m and positive energy, the analog in quantum mechanics of Dirac's formula (16) defining the point form of classical dynamics. Substituting $\alpha = 1/mck$, $a_\lambda = q_\lambda/k$, $b_\lambda = P_\lambda/mc$ in (64) we have

$$k^2P_\lambda = [-1 + mck(H^{(+)}(B) - H^{(-)}(B))/2\hbar B]J_{\lambda\mu}q^\mu + [(3i\hbar B + mck(B - i)H^{(+)}(B) + mck(B + i)H^{(-)}(B))/2B]q_\lambda, \tag{65}$$

where

$$H^{(\pm)}(B) = [1 + \hbar^2(B \mp \tfrac{1}{2}i)^2/m^2c^2k^2]^{1/2}, \tag{66}$$

By the same means, we have derived a formula for the 4-vector coordinate operator q_λ in terms of the generators of the inhomogeneous Lorentz group $\mathcal{P}$. Substituting $\alpha = -1/mck$, $a_\lambda = P_\lambda/mc$, $b_\lambda = q_\lambda/k$ in (64) we have

$$m^2c^2q_\lambda = [1 + mck(H^{(+)}(B) - H^{(-)}(B))/2\hbar B]J_{\lambda\mu}P^\mu + [(-3i\hbar B + mck(B - i)H^{(+)}(B) + mck(B + i)H^{(-)}(B))/2B]P_\lambda, \tag{67}$$

with $H^{(\pm)}(B)$ as in (66)

This 4-vector operator satisfies $q_\lambda q^\lambda = k^2$, $q_0 \geqq k > 0$, and has commuting components which are Hermitian. We have made implicity in the text certain reasonable but unproven assumptions about domains of definition of operators, and we certainly cannot claim to have proved the stronger condition of self-adjointness of q_λ. In particular, we have suggested that there is some question as to the self-adjointness of q_λ when one does not have

$$(mc)k > \tfrac{1}{2}\hbar.$$

The operator q_λ is the analogue in quantum mechanics of the coordinate 4-vector of the point where the world line of the classical particle meets the positive sheet of a two-sheeted hyperboloid, and as such certainly qualifies to be called a coordinate operator. It bears the same relation to this surface as the Newton–Wigner 3-vector operator does to an instant. Only transformations in the Euclidean subgroup of $\mathcal{P}$ leave an instant invari-

ant, and accordingly the Newton–Wigner operator transforms simply under this subgroup but not simply under Lorentz boosts. Similarly, the sheet of the hyperboloid is Lorentz invariant, and q_λ transforms simply under the homogeneous Lorentz group (as a 4-vector) but not simply under translations in space and time. In particular, the canonical relations

$$[q_r, P_s] = i\hbar\,\delta_{rs}$$

do *not* hold. We have so far been unable to evaluate the commutator $[q_\lambda, P_\mu]$ in terms of simpler expressions, in order to find the analog of the classical equation (14).

It could reasonably be argued that the formula (67) is so complicated that one cannot hope to manipulate readily or usefully with the operator q_λ. Our main purpose has been to indicate the existence of this 4-vector operator, which we have seen is defined by the conditions that it has Hermitian, commuting components, and satisfies

$$\begin{aligned} &q_\lambda q^\lambda = k^2, \quad q_0 \gtreqless k > 0, \\ &(q_\lambda P_\mu - q_\mu P_\lambda) + (P_\mu q_\lambda - P_\lambda q_\mu) = 2J_{\lambda\mu}, \\ &[q_\lambda, P^\lambda] = -3i\hbar. \end{aligned} \tag{68}$$

Given that, we hope it will prove possible to investigate its properties further (for example, to find the common generalized eigenvectors of its components in, say, the momentum representation) by other means.

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APPENDIX A

Chakrabarti, Levy-Nahas, and Seneor[18] have described the matrix elements of the operators a_λ in a "Lorentz basis" for the representation $(1, 0, +)$ of $\mathcal{P}$. This basis, in which B, $\frac{1}{2}J_{rs}J_{rs}$ and J_{12} are diagonalized is not a true basis, as it consists of nonnormalizeable vectors, but it can be used to define a realization of the underlying abstract structure. Then the Hilbert space is realized as the space of vectors

$$\begin{aligned} &\phi = (\phi_{00}(\beta),\ \phi_{11}(\beta),\ \phi_{10}(\beta),\ \phi_{1\text{-}1}(\beta),\ \phi_{22}(\beta)\cdots), \\ &\quad 0 \leqq \beta < \infty, \end{aligned}$$

where

$$\sum_{l,m} \left(\int_0^\infty |\phi_{lm}(\beta)|^2 d\beta \right) < \infty,$$

the sum being over $m = l,\ l-1, \ldots, -l$ for $l = 0, 1, 2\cdots$. The scalar product of two such vectors is

$$(\phi, \psi) = \sum_{l,m} \left(\int_0^\infty \phi^*_{lm}(\beta)\psi_{lm}(\beta) d\beta \right).$$

The results of Chakrabarti *et al.* [see in particular Eqs. (2.3), (2.18), (2.19), and (2.29) in Ref. 18] show that in this realization, the action of the operators a_0 and B is

$$\begin{aligned} (a_0\phi)_{lm}(\beta) &= [(l - i\beta)(l + i\beta + 1)/4\beta(\beta - i)]^{1/2}\phi_{lm}(\beta + i) \\ &\quad + [(l + i\beta)(l - i\beta + 1)/4\beta(\beta + i)]^{1/2}\phi_{lm}(\beta - i) \\ (B\phi)_{lm}(\beta) &= \beta\phi_{lm}(\beta). \end{aligned} \tag{A1}$$

Here the action of a_0 evidently presupposes certain analyticity properties of the functions $\phi_{lm}(\beta)$ for vectors ϕ in its domain. Although it is difficult to exhibit explicitly a common invariant dense domain of Hermiticity for a_0 and B, it is nevertheless clear from (A1) that

$$a_0 = u^{(+)}{}_0 - u^{(-)}{}_0 \tag{A2}$$

where, on suitable vectors ϕ

$$(u^{(\pm)}{}_0\phi)_{lm}(\beta) = \pm[(l \pm i\beta)(l \mp i\beta + 1)/4\beta(\beta \pm i)]^{1/2}\phi_{lm}(\beta \mp i)$$

and, consequently

$$Bu^{(\pm)}{}_0 = u^{(\pm)}{}_0(B \pm i). \tag{A3}$$

It follows from (A2) and (A3) that

$$u^{(\pm)}{}_0 = \pm\tfrac{1}{2}a_0 + \tfrac{1}{2}i[a_0, B]. \tag{A4}$$

Defining the 4-vector operator

$$u^{(\pm)}{}_\lambda = \pm\tfrac{1}{2}a_\lambda + \tfrac{1}{2}i[a_\lambda, B] \tag{A5}$$

so that

$$a_\lambda = u^{(+)}{}_\lambda - u^{(-)}{}_\lambda, \tag{A6}$$

we see from (A3) by covariance that

$$Bu^{(\pm)}{}_\lambda = u^{(\pm)}{}_\lambda(B \pm i). \tag{A7}$$

Since it then follows trivially that

$$(B \mp i)^2 u^{(\pm)}{}_\lambda = u^{(\pm)}{}_\lambda B^2 \tag{A8}$$

we see from (A6), (A8), (32), and (36) that $u^{(\pm)}{}_\lambda = v^{(\pm)}{}_\lambda$, and (37) is thus justified.

APPENDIX B

Once (37) is established, it follows using (32) that

$$v^{(\pm)}{}_\lambda = \pm\tfrac{1}{2}a_\lambda + \tfrac{1}{2}i[a_\lambda, B]. \tag{B1}$$

Since a_λ and B are Hermitian, it follows at once that $v^{(\pm)}{}_\lambda$ is also Hermitian; that is (38a) holds.

Now note from (B1) and (37) that

$$v^{(\pm)}{}_\lambda v^{(\pm)\lambda} = \pm\tfrac{1}{2}v^{(\pm)}{}_\lambda a^\lambda + \tfrac{1}{2}iv^{(\pm)}{}_\lambda a^\lambda B - \tfrac{1}{2}i(B \mp i)v^{(\pm)}{}_\lambda a^\lambda. \tag{B2}$$

But from (31)

$$\begin{aligned} v^{(\pm)}{}_\lambda a^\lambda &= (2\hbar B)^{-1}(J_{\lambda\mu}a^\mu a^\lambda - (i \mp B)\hbar a_\lambda a^\lambda) \\ &= -(i \mp B)/2B, \end{aligned} \tag{B3}$$

since the components of a_λ commute, and $a_\lambda a^\lambda = 1$. Combining (B2) and (B3) we have

$$v^{(\pm)}{}_\lambda v^{(\pm)\lambda} = 0,$$

establishing (38b). In a similar way, (38c) is deduced.

Again using (B1) and (37) we have

$$v^{(\pm)}{}_\lambda v^{(\pm)}{}_\mu = \pm\tfrac{1}{2}v^{(\pm)}{}_\lambda a_\mu + \tfrac{1}{2}iv^{(\pm)}{}_\lambda a_\mu B - \tfrac{1}{2}i(B \pm i)v^{(\pm)}{}_\lambda a_\mu. \tag{B4}$$

But from (31)

$$v^{(\pm)}{}_\lambda a_\mu = (2\hbar B)^{-1}(J_{\lambda\nu}a^\nu a_\mu - (i \mp B)\hbar\, a_\lambda a_\mu), \tag{B5}$$

so that

$$v^{(\pm)}{}_\lambda a_\mu - v^{(\pm)}{}_\mu a_\lambda = (2\hbar B)^{-1}(J_{\lambda\nu}a^\nu a_\mu - J_{\mu\nu}a^\nu a_\lambda). \tag{B6}$$

Now (24c) is equivalent to

$$J_{\lambda\nu}a_\mu + J_{\mu\lambda}a_\nu + J_{\nu\mu}a_\lambda = 0.$$

Contracting with a^ν from the right in this equation, and

noting that $a_\nu a^\nu = 1$, we obtain

$$J_{\lambda\nu}a^\nu a_\mu - J_{\mu\nu}a^\nu a_\lambda = J_{\lambda\mu}. \tag{B7}$$

Combining (B6) and (B7) we have

$$v^{(\pm)}{}_\lambda a_\mu - v^{(\pm)}{}_\mu a_\lambda = (2\hbar B)^{-1} J_{\lambda\mu},$$

and thus from (B4) that

$$v^{(\pm)}{}_\lambda v^{(\pm)}{}_\mu - v^{(\pm)}{}_\mu v^{(\pm)}{}_\lambda = 0,$$

establishing (38d). In a similar way, (38e) is deduced.

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Properties of the self dual equations for an SU(n) gauge theory

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The Yang equations for all self dual solutions of SU(r,s) gauge theory are exhibited in simple form. Algebraic and Bäcklund transformations of the solutions of these equations are derived. The Bäcklund transformations change an SU(r,s) solution into an SU($r-1$, $s+1$) solution.

Recently considerable progress has been made in understanding the classical structure of self-dual solutions to the SU(2) gauge theory.[1-5] Not only has an explicit solution been given for the Ward Atiyah lth ansatz in terms of $2l+1$ free fields, but also Bäcklund transformations and algebraic transformations have been found which change one ansatz into another. These transformations were discovered as transformations leaving invariant the three equations obtained by Yang which characterize the solutions of self-dual gauge theory.

In the present note, by extending Yang's treatment to the case of SU(r, s), $r+s=n$, gauge theory, which includes SU(n), we show that the equations of self-dual gauge theory may be expressed in a very simple and transparent form, which follow from a Lagrangian. The algebraic transformations of the solutions then follow almost automatically. There exist Bäcklund transformations β, which have the property of changing an SU(r, s) solution into an SU($r-1$, $s+1$) solution. The kth power ($k=1,\ldots,n-1$) of β is also a Bäcklund transformation while β is also a Bäcklund transformation while β^n is essentially the identity. These $n-1$ independent transformations are associated with the $n-1$ (nonidentical) cyclic permutations of order n, and have the appearance of an extended form of gauge transformation, but they are not gauge transformations. They are represented by nonlinear differential equations of first order.

In Sec. I we present Yang's equation and use the local isomorphism between SO(4), the Euclidean version of space–time rotations in four dimensions, and SU(2)×SU(2) to give the simplest form of the self-dual equations and the best choice of variables for the problem.

In Sec. II we present the equations in a manifestly gauge invariant way by introducing suitable variables. The topological quantum number is directly expressible in terms of this form.

In Sec. III we discuss in a complete manner all possible algebraic transformations of the solutions. These transformations are shown to correspond to equivalent classes of SL(n, C) matrices.

In Sec. IV we present the Bäcklund transformations we have found.

In Sec. V the formulas for the Bäcklund transformations are written explicitly for the case of SU(3).

An appendix fixes our notations and the connections between the different bases which are introduced.

I. YANG'S EQUATIONS AND SU(2) ⊗ SU(2)

The basic simplicity of Yang's derivation[5] of the equations of motion describing self-dual gauge fields in four-dimensional Euclidean space lies in the transformation of coordinates x^μ ($\mu=1,2,3,0$) to $y^a=(y,\bar{y},z,\bar{z})$ defined by

$$Y=\sqrt{2}\begin{bmatrix} y & -\bar{z} \\ z & \bar{y} \end{bmatrix}=x^0-ix^j\sigma_j. \tag{1.1}$$

This notation exhibits clearly the local isomorphism between SO(4) and SU(2)⊗ SU(2) since the Euclidean transformations are represented by

$$Y'=AYB, \tag{1.2}$$

where A and B are two independent two by two unitary unimodular matrices. In other words, an SO(4) vector x^μ transforms as a $(\frac{1}{2},\frac{1}{2})$ representation of SU(2)⊗ SU(2). Introducing also $y_a=(\bar{y},y,\bar{z},z)$ the invariant length of x^μ is

$$x^\mu x^\mu=\det Y=\tfrac{1}{2}y^a y_a=(y\bar{y}+z\bar{z}). \tag{1.3}$$

As shown in the appendix, in this frame the self-duality relations become

$$F_{yz}=F_{\bar{y}\bar{z}}=F_{y\bar{y}}+F_{z\bar{z}}=0, \tag{1.4}$$

where $F^{\mu\nu}$ is the antisymmetric gauge field tensor whose

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components take values in the (complexified) Lie algebra of SU(n) here written in the new variables. Introducing the further change of variables $p^a=(p,\bar{p},q,\bar{q})$

$$Z=\sqrt{2}\begin{bmatrix} p & -\bar{q} \\ q & \bar{p} \end{bmatrix}=\begin{bmatrix} \bar{y}+z & \bar{y}-\bar{z} \\ \bar{z}-y & \bar{z}+y \end{bmatrix}, \tag{1.5}$$

where Z transforms in exactly the same way as Y (1.2), the equations (1.4) can be expressed in the more symmetrical form

$$F_{yz}=F_{\bar{y}\bar{z}}=F_{p\bar{q}}=F_{\bar{p}\bar{q}}=0, \tag{1.6}$$

where only three of the above set of four equations are linearly independent. Under SU(2)$\otimes$ SU(2) an antisymmetrical tensor transforms as a $(1,0)+(0,1)$ representation and (1.6) expresses the self-duality as the absence of the (0, 1) components.

The first two sets of equations (1.6) imply

$$\begin{aligned} &A_y=-iD^{-1}D_{,y},\quad A_z=-iD^{-1}D_{,z}, \\ &A_{\bar{y}}=-iE^{-1}E_{,\bar{y}},\quad A_{\bar{z}}=-iE^{-1}E_{,\bar{z}}, \end{aligned} \tag{1.7}$$

where $D_{,a}$ represents the a derivative of the matrix D, of determinant one to guarantee that A be of zero trace. A gauge transformation on the theory corresponds to a transformation

$$D'=VDU,\quad E'=WET. \tag{1.8}$$

For a SU(n) theory, $U=T$ is an arbitrary y^a dependent unitary unimodular n by n matrix. The matrix $V(W)$ is a member of SL(n,C) which may depend upon $\bar{y}$ and $\bar{z}$ (y and z). Also

$$E=(D^+)^{-1} \tag{1.9}$$

can be chosen to ensure that $A_{\bar{y}}$ be the Hermitian conjugate of A_y and hence that A_μ be real fields.

The third set of equations, $F_{y\bar{y}}+F_{z\bar{z}}=0$, are the n^2-1 dynamical equations which remain to be solved to give the most general dual field.

The distinction we have made between E and D allows us to treat the more general case of a SU(r,s) ($r+s=n$) gauge theory. Indeed with the metric M diagonal with r plus ones' and s minus ones' the connection between D and E is

$$E=M(D^+)^{-1}M. \tag{1.10}$$

since in that case

$$A_{\bar{y}}=MA_y^+M. \tag{1.11}$$

Gauge transformations take then the form (1.8) with

$$\begin{aligned} &U=T, \\ &U^+MU=M, \\ &W=MV^{-1+}M. \end{aligned} \tag{1.12}$$

II. GAUGE INVARIANT EQUATIONS

We now show that Yang's equations can be cast in a gauge independent formulation. Introduce the matrix

$$P=DE^{-1}. \tag{2.1}$$

The last equations of (1.4) become upon multiplication by E on the right and by E^{-1} on the left

$$(PP^{-1}_{,\bar{y}})_{,y}+(PP^{-1}_{,\bar{z}})_{,z}=0 \tag{2.2}$$

$$(P^{-1}P_{,y})_{,\bar{y}}+(P^{-1}P_{,z})_{,\bar{z}}=0. \tag{2.3}$$

These equations can be derived from a Lagrangian which we are unable to express in terms of P however. We leave the discussion of the Lagrangian until the appendix.

It is obvious that (2.2) is invariant under the transformation

$$P'=VPW^{-1}, \tag{2.4}$$

where V and W are constant SL(2, C) matrices. There is another obvious invariance under

$$P'=(P^{-1})^T. \tag{2.5}$$

There are only n^2-1 linear independent equations among (2.2) since it follows from det $P=1$ that the trace of equation (2.2) is identically zero.

We conclude this section by giving an expression in terms of P for the topological invariant in the case of self-dual $F_{\mu\nu}$

$$\begin{aligned} T&=\frac{1}{16\pi^2}\int \mathrm{Tr}(F_{\mu\nu}\hat{F}_{\mu\nu})d^4x \\ &=\frac{1}{16\pi^2}\int \mathrm{Tr}(F_{y\bar{y}}F_{z\bar{z}}+F_{y\bar{z}}F_{\bar{y}z})dy\,dz\,d\bar{y}\,d\bar{z} \\ &=-\frac{1}{16\pi^2}\int \mathrm{Tr}\{(P_{,\bar{y}}P^{-1})_{,y}(P_{,\bar{z}}P^{-1})_{,z} \\ &\quad+(P_{,\bar{z}}P^{-1})_{,y}(P_{,\bar{y}}P^{-1})_{,z}\}dy\,dz\,d\bar{y}\,d\bar{z}, \end{aligned} \tag{2.6}$$

where $\hat{F}_{\mu\nu}$ is defined as usual by

$$\hat{F}_{\mu\nu}=\tfrac{1}{2}\epsilon_{\mu\nu\alpha\beta}F_{\alpha\beta}. \tag{2.7}$$

III. ALGEBRAIC TRANSFORMATIONS IN THE TRIANGULAR GAUGE

In what we will call the triangular gauge (Yang's R gauge) the matrix D is chosen as lower triangular with real diagonal elements. We will now show that in this gauge there are algebraic transformations on the elements of D which keep the new D triangular and are gauge transformations. Indeed given any SL(n,C) matrix V there is a unique SU(n) matrix U such that

$$D'=VDU \tag{3.1}$$

remains triangular.

Proof: Let

$$D'D'^+=VDD^+V^+. \tag{3.2}$$

This equation can be solved sequentially for the components of D' assumed to be lower triangular. The n^2-1 independent nonzero components of D' ($n-1$ diagonal and $n(n-1)$ off diagonal complex elements) are determined by the n^2-1 independent equations (3.2). Then $U=D^{-1}V^{-1}D'$ is unitary by (3.2).

The algebraic transformations from D to D' can be classified by classifying all the SL(n,C) transformations. Introduce the "translations" defined by lower triangular matrices with ones along the diagonal T and

the "dilations" C defined by diagonal matrices of determinant one. Then any SL(n, C) matrix can be written as

$$V = T_1 C_1 S_j T_2 C_2, \quad \det S_j = 1, \tag{3.3}$$

where S_j is uniquely defined by V and is one of the (up to a sign) permutation matrices. We recall that a permutation is represented by matrix with a one in every line and every column. One of the signs of S_j is adjusted in such a way as to make S_j of determinant one.

To every triangular matrix V, a translation or a dilation, corresponds the SU(n) unit matrix. To the $(n)! - 1$ nontrivial regular permutations (excluding the identity) correspond $(n)! - 1$ nontrivial matrices U_j. The $(n)! - 1$ special transformation obtained by

$$D'_j = V_j D U_j \tag{3.4}$$

are the special algebraic transformations which play a crucial role.

In the special case of SU(2) with

$$D = \frac{1}{\sqrt{f}} \begin{bmatrix} 1 & 0 \\ e & f \end{bmatrix} \tag{3.5}$$

$$E^{-1} = \frac{1}{\sqrt{f}} \begin{bmatrix} 1 & -g \\ 0 & f \end{bmatrix} \tag{3.6}$$

the Hermiticity implies (1.9)

$$g = -\bar{e} \tag{3.7}$$

and the algebraic transformation ($(n)! - 1 = 1$) is

$$\begin{aligned} f' &= f^{-1}, \\ e' &= g(f^2 - ge)^{-1}, \\ g' &= e(f^2 - ge)^{-1}. \end{aligned} \tag{3.8}$$

In this case the three remaining equations of motion are

$$\begin{aligned} & f^{-2}\{f(f_{,y\bar{y}} + f_{,z\bar{z}}) - f_{,y} f_{,\bar{y}} - f_{,z} f_{,\bar{z}} \\ & - e_{,y} g_{,\bar{y}} - e_{,z} g_{,\bar{z}}\} = 0, \\ & f^{-2}\{f(g_{,y\bar{y}} + g_{,z\bar{z}}) - 2g_{,\bar{y}} f_{,y} - 2g_{,\bar{z}} f_{,z}\} = 0, \\ & f^{-2}\{f(e_{,y\bar{y}} + e_{,z\bar{z}}) - 2e_{,y} f_{,\bar{y}} - 2e_{,z} f_{,\bar{z}}\} = 0. \end{aligned} \tag{3.9}$$

IV. BÄCKLUND TRANSFORMATIONS

With the notation of the preceding sections and of the appendix we will now try to define Bäcklund transformations, i.e., transformations which enable us to define D' and E' as solutions of our set of equations in terms of another set D and E which satisfies our equations. One set of matrices is defined from the other by a system of first-order differential equations, the integration conditions being a consequence of the self-duality conditions.

Set

$$\begin{aligned} & A'_p = R^{-1} A_p R, \quad A'_q = R^{-1} A_q R, \\ & A'_{\bar{p}} = S^{-1} A_{\bar{p}} S, \quad A'_{\bar{q}} = S^{-1} A_{\bar{q}} S, \end{aligned} \tag{4.1}$$

where R and S are constant matrices.

Now, if A_A satisfies the equations of motion (1.6) then automatically A'_A, as defined above, will satisfy the two equations

$$F_{pq} = F_{\bar{p}\bar{q}} = 0. \tag{4.2}$$

We now try to choose R and s so that the third independent equation is solved, so that A'_A are expressed in terms of D' and E' matrices and so that the defining equations are integrable.

Let R be the cyclic permuation matrix with nonzero elements

$$R_{j,j+1} = 1, \tag{4.3}$$

where the indices are defined modulo n. Let D be written

$$D = LF, \tag{4.4}$$

where L is lower triangular with one along the diagonal and F is purely diagonal real with elements a_j and has determinant one, and let

$$E^{-1} = F\hat{L}, \tag{4.5}$$

where L is upper diagonal [for SU(n) $\hat{L} = L^+$, for SU(r, s) $\hat{L} = ML^+M$, see (1.10)] with ones on the diagonal.

Using (4.4) to define the Bäcklund transformation the D' and E' defined implicitly by (4.1) satisfy

$$F'_{yz} = F'_{\bar{y}\bar{z}} = 0. \tag{4.6}$$

Indeed (4.1) implies

$$a'_j = a_{j+1} \quad (j \bmod n) \tag{4.7}$$

$$L'_{ij} = L_{i+1,j+1} \quad (n > i > j) \tag{4.8}$$

$$(F'^{-1} L'^{-1} L'_{,y} F')_{nj} = -(\hat{F} L_{,\bar{z}} \hat{L}^{-1} F^{-1})_{1,j+1} \quad (n > j) \tag{4.9}$$

From this then follows

$$(L'^{-1})_{ij} = (L^{-1})_{i+1,j+1} \quad (n > i > j), \tag{4.10}$$

and

$$((L'^{-1})_{nj})_{,y} = -(F^2 \hat{L}_{,\bar{z}} \hat{L}^{-1} F^{-2} L^{-1})_{1,j+1} \quad (n > j). \tag{4.11}$$

In order to find $(L'^{-1})_{nj}$ from (4.11) and from the (up to a sign analogous) expression which gives its z derivative in terms of the $\bar{y}$ derivative of $\hat{L}$, the right-hand side of (4.11) has to satisfy conditions of integrability. These conditions read

$$((F^2 \hat{L}_{,\bar{z}} \hat{L}^{-1} F^{-2} L^{-1})_{1,j+1})_{,z} + ((F^2 \hat{L}_{,\bar{y}} \hat{L}^{-1} F^{-2} L^{-1})_{1,j+1})_{,y} = 0. \tag{4.12}$$

Compare with

$$(F_{z\bar{z}} + F_{y\bar{y}})_{1,j+1} = 0, \tag{4.13}$$

then (4.12) is just (4.13) premultiplied by F and postmultiplied by $F^{-1}L^{-1}$. The matrix S is then found to be a matrix with nonzero elements

$$S_{i,i+1} = 1, \quad S_{n,1} = -1 \quad (n > i). \tag{4.14}$$

It is not difficult to show that the transformation β between D, E and D', E', just defined, changes the reality condition (1.10) from a SU(r, s) theory to a SU($r - 1$, $s + 1$) theory.

Further transformations may be found by iteration of

the β transformation. They will close on the cyclic group of order n. More precisely the nth power of β is essentially a translation as defined before.

By combining, in arbitrary order, the $(n)!-1$ special algebraic transformations of Sec. III the translations and dilation with the $n-1$ Bäcklund transformations defined by β^k $(k<n)$, one generates starting from any solution of the equations of motion an infinite set of independent solutions.

We have however not been able to prove that we have found all possible Bäcklund transformations[6] nor that we can exhaust all possible solutions of the equations starting from some simple set and applying our two types of transformations.

We emphasize that defined by (4.1) the Bäcklund transformations may look like gauge transformations, but in fact are not. This is due to the fact that under a permutation a triangular matrix does not retain its form. In the decomposition of $A_\rho\sqrt{2}=A_{\bar y}+A_z$ upper and lower triangular matrices appear so that $A^t_{\bar y}$ depends on both $A_{\bar y}$ and A_z in a nontrivial first-order nonlinear differential way.

V. EXPLICIT FORM OF THE EQUATIONS FOR THE CASE OF SU(3)

For the case of SU(2) the general results are given in Refs. 3 and 4. We here give the explicit formulae for the equations of motion and for the Bäcklund transformations in the case of SU(r,s) $(r+s=3)$. The algebraic transformations can be obtained by using the general results of Sec. III.

Take for D

$$D=\begin{bmatrix} a & 0 & 0\\ d & b & 0\\ e & f & c\end{bmatrix}. \tag{5.1}$$

Then L and $\hat L$ as defined by (4.4) and (4.5) are

$$L=\begin{bmatrix} 1 & 0 & 0\\ h & 1 & 0\\ k & l & 1\end{bmatrix}, \tag{5.2}$$

$$L=\begin{bmatrix} 1 & h & k\\ 0 & 1 & l\\ 0 & 0 & 1\end{bmatrix},$$

where $h=d/a$, etc.

In terms of these variables the Lagrangian

$$\begin{aligned}\mathcal{L}=&\,2\frac{a_{,y}a_{,\bar y}}{a^2}+2\frac{b_{,y}b_{,\bar y}}{b^2}+2\frac{c_{,y}c_{,\bar y}}{c^2}\\ &+\left(\frac{a}{b}\right)^2 h_{,y}\hat h_{,\bar y}+\left(\frac{b}{c}\right)^2 l_{,y}\hat l_{,\bar y}\\ &+\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})(\hat k_{,y}-\hat l\hat h_{,y})\\ &+\text{terms with } y\to z \text{ and } \bar y\to\bar z\end{aligned} \tag{5.3}$$

provides the nine equations of motion [the last term of (1.4)] where the symmetrization $(y\to z)$ and $(\bar y\to\bar z)$ is understood,

$$\left[2\frac{a_{,y}}{a}-\left(\frac{a}{b}\right)^2 h_{,y}\hat h-\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})(\hat k-\hat l\hat h)\right]_{,\bar y}=0, \tag{5.4b}$$

$$\left[2\frac{b_{,y}}{b}+\left(\frac{a}{b}\right)^2 h_{,y}\hat h-\left(\frac{b}{c}\right)^2 l_{,y}\hat l-\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})\hat l\hat h\right]_{,\bar y}=0 \tag{5.4b}$$

$$\left[2\frac{c_{,y}}{c}+\left(\frac{b}{c}\right)^2 l_{,y}\hat l+\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})\hat k\right]_{,\bar y}=0, \tag{5.4c}$$

$$\left[\left(\frac{a}{c}\right)^2(\hat k_{,\bar y}-\hat l\hat h_{,\bar y})\right]_{,y}=0, \tag{5.4d}$$

$$\left[\left(\frac{a}{b}\right)^2\hat h_{,\bar y}-\left(\frac{a}{c}\right)^2(\hat k_{,\bar y}-\hat l\hat h_{,\bar y})l\right]_{,y}=0, \tag{5.4e}$$

$$\left[\left(\frac{b}{c}\right)^2\hat l_{,\bar y}+\left(\frac{a}{c}\right)^2(\hat k_{,\bar y}-\hat l\hat h_{,\bar y})h\right]_{,y}=0, \tag{5.4f}$$

$$\left[\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})\right]_{,\bar y}=0 \tag{5.4g}$$

$$\left[\left(\frac{a}{b}\right)^2 h_{,y}+\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})\hat l\right]_{,\bar y}=0, \tag{5.4h}$$

$$\left[\left(\frac{b}{c}\right)^2 l_{,y}+\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y})\hat h\right]_{,\bar y}=0. \tag{5.4i}$$

Note that equations (5.4a, b, c) are not linearly independent.

There are two types of Bäcklund transformations:

(A) $a'=b,\quad b'=c,\quad c'=a,$

$h'=l,\quad \hat h=\hat l,$

$$k'_{,y}-l'l'_{,y}=-\left(\frac{a}{b}\right)^2\hat h_{,z},\quad k'_{,z}-l'h'_{,z}=\left(\frac{a}{b}\right)^2\hat h_{,\bar y}, \tag{5.5}$$

$$\hat k'_{,y}-\hat l'\hat h'_{,\bar y}=\left(\frac{a}{b}\right)^2 h_{,z},\quad \hat k'_{,z}-\hat l'\hat h'_{,\bar z}=-\left(\frac{a}{b}\right)^2 h_{,y},$$

$$l'_{,y}=-\left(\frac{a}{c}\right)^2(\hat k_{,z}-\hat l\hat h_{,z}),\quad l'_{,z}=\left(\frac{a}{c}\right)^2(\hat k_{,\bar y}-\hat l\hat h_{,\bar y}),$$

$$l'_{,\bar y}=\left(\frac{a}{c}\right)^2(k_{,z}-lh_{,z}),\quad \hat l'_{,\bar z}=-\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y}).$$

(B) $a'=c,\quad b'=a,\quad c'=b,$

$l'=h,\quad \hat l'=\hat h,$

$$k'_{,y}-l'h'_{,y}=-\left(\frac{b}{c}\right)^2\hat l_{,z},\quad k'_{,z}-l'h'_{,z}=\left(\frac{b}{c}\right)^2\hat l_{,\bar y}, \tag{5.6}$$

$$\hat k'_{,\bar y}-\hat l'\hat h'_{,\bar y}=\left(\frac{b}{c}\right)^2 l_{,z},\quad \hat k'_{,\bar z}-\hat l'\hat h'_{,\bar z}=-\left(\frac{b}{c}\right)^2 l_{,y},$$

$$h'_{,y}=-\left(\frac{a}{c}\right)^2(\hat k_{,z}-\hat l\hat h_{,z}),\quad h'_{,z}=\left(\frac{a}{c}\right)^2(\hat k_{,\bar y}-\hat l\hat h_{,\bar y}),$$

$$\hat h'_{,\bar y}=\left(\frac{a}{c}\right)^2(k_{,z}-lh_{,z}),\quad \hat h'_{,\bar z}=-\left(\frac{a}{c}\right)^2(k_{,y}-lh_{,y}).$$

Evidently (5.6) is the iteration of (5.5) if no integration parameters are introduced and the cube of each trans-

formation is the identity. It is seen that the integration parameters are equivalent to translations.

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APPENDIX

In this appendix, for completeness, we list the precise formulae connecting the x^μ basis to the y^a basis and to the p^a basis.

$$\begin{aligned}
&\sqrt{2}A^y = A^0 - iA^3 = A_{\bar{y}}\sqrt{2}, \quad \sqrt{2}y = x^0 - ix^3,\\
&\sqrt{2}A^{\bar{y}} = A^0 + iA^3 = A_y\sqrt{2}, \quad \sqrt{2}\bar{y} = x^0 + ix^3,\\
&\sqrt{2}A^z = A^2 - iA^1 = A_{\bar{z}}\sqrt{2}, \quad \sqrt{2}z = x^2 - ix^1,\\
&\sqrt{2}A^{\bar{z}} = A^2 + iA^1 = A_z\sqrt{2}, \quad \sqrt{2}\bar{z} = x^2 + ix^1,
\end{aligned} \tag{A1}$$

$$F_{ab} = A_{b,a} - A_{a,b} + i[A_a, A_b]. \tag{A2}$$

Indeed for the derivatives one has the dual transformations

$$\partial_a X = \frac{\partial X}{\partial y^a} = X_{,y^a}, \quad \partial^a X = \frac{\partial X}{\partial_{y_a}} \tag{A3}$$

associated with the nondiagonal metric (1.3).

Analogously [see (1.5)]

$$\begin{aligned}
&\sqrt{2}A^b = A^{\bar{y}} + A^z = A_{\bar{p}}\sqrt{2},\\
&\sqrt{2}A^{\bar{b}} = A^y + A^{\bar{z}} = A_p\sqrt{2},\\
&\sqrt{2}A^q = A^{\bar{z}} - A^y = A_{\bar{q}}\sqrt{2},\\
&\sqrt{2}A^{\bar{q}} = A^z - A^{\bar{y}} = A_q\sqrt{2}.
\end{aligned} \tag{A4}$$

There are formulas analogous to (A2) and (A3) in this basis.

The connection between the gauge fields in the two bases $F^{\mu\nu}$ and F_{ab} is as follows:

$$\begin{aligned}
&F_{\bar{y}y} = iF^{03},\\
&F_{\bar{z}z} = iF^{21},\\
&F_{\bar{y}z} = \tfrac{1}{2}(F^{02} + F^{31} + iF^{01} - iF^{32}),\\
&F_{y\bar{z}} = \tfrac{1}{2}(F^{02} + F^{31} - iF^{01} + iF^{32}),\\
&F_{yz} = \tfrac{1}{2}(F^{02} - F^{31} + iF^{01} + iF^{32}),\\
&F_{\bar{y}\bar{z}} = \tfrac{1}{2}(F^{02} - F^{31} - iF^{01} - iF^{32}).
\end{aligned} \tag{A5}$$

Self-duality implies

$$F^{\mu\nu} = \tfrac{1}{2}\epsilon^{\mu\nu\rho\sigma}F^{\rho\sigma}, \tag{A6}$$

i.e.,

$$F^{01} = F^{23}, \quad F^{02} = F^{31}, \quad F^{03} = F^{12} \tag{A7}$$

and in the other bases

$$F_{yz} = F_{\bar{y}\bar{z}} = F_{y\bar{y}} + F_{z\bar{z}} = 0. \tag{A8}$$

Finally

$$\begin{aligned}
F_{pq} &= \tfrac{1}{2}(F_{yz} + F_{\bar{y}\bar{z}} + F_{y\bar{y}} + F_{z\bar{z}}),\\
F_{\bar{p}\bar{q}} &= \tfrac{1}{2}(F_{yz} + F_{\bar{y}\bar{z}} - F_{y\bar{y}} - F_{z\bar{z}}).
\end{aligned} \tag{A9}$$

This proves (1.6) and shows that the four equations are not linearly independent.

The Lagrangian

In terms of the decomposition of D and E given by (4.4) and (4.5), the self-dual equations can be derived from the Lagrangian

$$\begin{aligned}
\mathcal{L} &= 2\mathrm{tr}(F_{,y}F_{,\bar{y}}F^{-2}) + \mathrm{tr}(L^{-1}L_{,y}F^2\hat{L}_{,\bar{y}}\hat{L}^{-1}F^{-2})\\
&\quad + \text{terms with } y \to z,\ \bar{y} \to \bar{z}
\end{aligned} \tag{A10}$$

by varying with respect to $F, L, \hat{L}$. This Lagrangian can be written in the alternative form

$$\mathcal{L} = \tfrac{1}{2}\mathrm{tr}(A_y + A_y^T)(A_{\bar{y}} + A_{\bar{y}}^T) + y \to z, \tag{A11}$$

where A^T denotes the transpose of A. In this form the gauge dependence of the Lagrangian is manifest. This equivalence is highly nontrivial and depends upon the fact that L is lower triangular and $\hat{L}$ is upper triangular.

Note added in proof: There has subsequently appeared a paper by M. F. Atiyah, N. J. Hitchin, V. G. Drinfeld, and Y. I. Manin, Phys. Lett. A 65, 185 (1978), giving an algebraic method of solution for self dual fields.

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Beam propagation in focusing media with random-axis misalignments: Second- and higher-order moments[a)]

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A novel statistical technique which allows the asymptotic evaluation of second- and higher-order averaged observables related to the stochastic complex parabolic equation is applied to the problem of beam propagation in a focusing medium characterized by random-axis misalignments. Analytical and numerical results concerning on- and off-axis statistics (e.g., the variance of intensity fluctuations, modal power transfer, the probability distribution density of the log-irradiance, etc.) are presented, and comparisons are made with previously reported findings.

1. INTRODUCTION

In the quasioptical regime, the propagation of beamed signals along the z direction in focusing media with random-axis misalignments is described exceedingly well by the stochastic complex parabolic equation[1,2]

$$\frac{i}{k}\frac{\partial}{\partial z}\psi(\mathbf{x},z;\alpha)=-\frac{1}{2k^2}\nabla_{\mathbf{x}}^2\psi(\mathbf{x},z;\alpha)+V(\mathbf{x},z;\alpha)\psi(\mathbf{x},z;\alpha),\quad z>0, \tag{1.1a}$$

$$V(\mathbf{x},z;\alpha)=\tfrac{1}{2}g^2[\mathbf{x}-\mathbf{a}\delta H(z;\alpha)]^2,\quad \mathbf{x}\in R^2, \tag{1.1b}$$

$$\psi(\mathbf{x},0;\alpha)=\psi_0(\mathbf{x}). \tag{1.1c}$$

Here, k is a reference wavenumber, g is a spatial frequency (units: radians/meter), and $\mathbf{a}$ is a fixed vector quantity. The potential field given in (1.1b) corresponds to a parabolically focusing medium whose equilibrium axis is perturbed via the zero-mean, z-dependent, real random function $\delta H(z;\alpha)$. The latter, as well as the slowly varying, complex, random, amplitude function $\psi(\mathbf{x},z;\alpha)$, depends on a parameter $\alpha\in A$, (A,F,P) being an underlying probability measure space.

It is our goal in this exposition to examine the boundary-value problem (1.1) in an unbounded (with respect to $\mathbf{x}$) domain. It should be pointed out, however, that this idealized problem provides a good approximation to the forward propagation of low-order modes in a fiber lightguide having a parabolically graded refraction index, with random-axis misalignment of microbending.[3,4] It can also give some insight into the problem of forward propagation of low-order acoustic modes near an idealized, randomly perturbed, underwater sound channel axis, provided that transverse (with respect to z) satistical fluctuations due to internal waves can be ignored.

There exist physical situations which require that the initial condition (1.1c) be random (e.g., aberrations in a lens through which a laser beam passes before it enters into the random medium). However, a generalization of the discussion in this paper to account for such an initially partially coherent beam presents no fundamental difficulties. It is, also, relatively straightforward to account for random deformations along the channel axis of the more general form $\delta\mathbf{H}(z;\alpha)$, where $\delta\mathbf{H}(z;\alpha)$ is a zero-mean, vector-valued, real random function.

The problem (1.1) has already been investigated by Besieris *et al.*[5] from the point of view of a quantum mechanical harmonic oscillator whose equilibrium position is randomly perturbed.[6] This was done using a kinetic approach at the level of second-order satistical moments. Marcuse (cf. Ref. 3) has also studied an initial-boundary-value problem closely resembling (1.1). His problem (related to fiber-optical propagation) is more realistic than (1.1). As a result, his approach (a modal analysis) is more difficult to justify with estimates of accuracy. The only carefully derived results to date dealing with higher-order statistics of the problem (1.1) are those reported by McLaughlin.[7] Using the diffusion approximation (cf. Refs. 8–10), he has studied the average intensity and the intensity fluctuations on the beam axis, as well as the decay of mean power from the fundamental mode of the unperturbed focusing medium, and mean power transitions to higher modes.

It is our intent to study (1.1) by means of a new satistical technique which allows the asymptotic evaluation of second- and higher-order statistical observables without having to derive first equations for second- or higher-order coherence functions. It will be shown that in the special case where $\delta H(z;\alpha)$ in (1.1) is a wide-sense stationary, δ-correlated, Gaussian random process, a certain class of even moments of the wavefunction $\psi(\mathbf{x},z;\alpha)$ can be computed exactly. More importantly, it will be shown that these quantities can be computed asymptotically (e.g., in the long-range regime), even under realistic assumptions about the satistical fluctuations of the medium. Our main findings will be compared to those of previous workers, especially McLaughlin's (cf. Ref. 7). We shall obtain, in addition, several new results, such as off-axis statistics, the variance connected with beam wandering, the probability distribution density function of the log irradiance, etc.

The structure of the paper can be outlined as follows: A basic conservation law pertaining to the stochastic parabolic equation (1.1) is developed in Sec. 2. A fundamental ansatz on which the proposed technique is based is then introduced in Sec. 3 for the general case of two-

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dimensional beam propagation in a parabolically focusing medium with random-axis misalignments. The one-dimensional version of this problem is discussed in Sec. 4. Finally, following an analysis of the basic satistical problem (cf. Sec. 5), several new results linked to second- and higher-order observables are computed in Secs. 6 and 7.

2. BASIC CONSERVATION LAW

Corresponding to the stochastic parabolic equation (1.1), let

$$i(\mathbf{x},z;\alpha)=\psi^*(\mathbf{x},z;\alpha)\psi(\mathbf{x},z;\alpha) \tag{2.1}$$

and

$$\mathbf{j}(\mathbf{x},z;\alpha)=\frac{i}{2k}[\psi(\mathbf{x},z;\alpha)\nabla_{\mathbf{x}}\psi^*(\mathbf{x},z;\alpha)-\psi^*(\mathbf{x},z;\alpha)\nabla_{\mathbf{x}}\psi(\mathbf{x},z;\alpha)] \tag{2.2}$$

denote the *intensity* (or irradiance) and *intensity flux densities*, respectively. By virtue of the self-adjointness of the operator $-(1/2k^2)\nabla_{\mathbf{x}}^2+(1/2)g^2[\mathbf{x}-\mathbf{a}\delta H(z;\alpha)]^2$ in (1.1), we have the following conservation law:

$$\frac{\partial}{\partial z}i(\mathbf{x},z;\alpha)+\nabla_{\mathbf{x}}\cdot\mathbf{j}(\mathbf{x},z;\alpha)=0 \quad \forall\ \alpha\in A. \tag{2.3}$$

As a consequence, the total intensity $I(z;\alpha)$, defined by

$$I(z;\alpha)=\int_{R^2}d\mathbf{x}\,i(\mathbf{x},z;\alpha), \tag{2.4}$$

is conserved for every realization $\alpha\in A$, viz.,

$$\frac{d}{dz}I(z;\alpha)=0, \tag{2.5}$$

or

$$I(z;\alpha)=I(0;\alpha)=\int_{R^2}d\mathbf{x}\,\psi^*(\mathbf{x},0;\alpha)\psi(\mathbf{x},0;\alpha). \tag{2.6}$$

In the sequel, we shall assume that $I(0;\alpha)$ is normalized to unity for every realization $\alpha\in A$.

We define, next, a vector $\mathbf{s}(\mathbf{x},z;\alpha)$ by the relationship

$$\mathbf{s}(\mathbf{x},z;\alpha)=i(\mathbf{x},z;\alpha)\hat{\mathbf{z}}+\mathbf{j}(\mathbf{x},z;\alpha), \quad \mathbf{z}\equiv\mathbf{z}/|\mathbf{z}|. \tag{2.7}$$

The conservation law (2.3) can be rewritten in terms of $\mathbf{s}(\mathbf{x},z;\alpha)$ as follows:

$$\nabla\cdot\mathbf{s}(\mathbf{x},z;\alpha)=0, \quad \nabla=\nabla_{\mathbf{x}}+(\partial/\partial z)\hat{\mathbf{z}}. \tag{2.8}$$

From physical considerations, $\mathbf{s}(\mathbf{x},z;\alpha)$ may be interpreted as a *power flux density*. On the strength of the divergence theorem, one has the identity

$$\int\int_V\int\nabla\cdot\mathbf{s}(\mathbf{x},z;\alpha)dV=\int_{S_c}\mathbf{s}(\mathbf{x},z;\alpha)\cdot\hat{\mathbf{n}}dA=0, \tag{2.9}$$

where V is the volume bounded by a regular closed surface S_c and $\hat{\mathbf{n}}$ is a unit outwardly directed normal vector. From a more practical point of view, the power intercepted by a detector (indicated by an open S_0) can be written as follows:

$$\int_{S_0}\mathbf{s}(\mathbf{x},z;\alpha)\cdot\hat{\mathbf{n}}dA. \tag{2.10}$$

3. THE FUNDAMENTAL ANSATZ

In the stochastic parabolic equation (1.1) we make a change of the transverse (with respect to z) spatial variable corresponding to a "moving" coordinate system,

$$\mathbf{y}(z;\alpha)=\mathbf{x}-\mathbf{u}(z;\alpha), \tag{3.1}$$

and represent the wavefunction $\psi(\mathbf{x},z;\alpha)$ in the form

$$\psi(\mathbf{x},z;\alpha)=\phi[\mathbf{y}(z;\alpha),z]\exp\{ik[\dot{\mathbf{u}}(z;\alpha)\cdot\mathbf{y}(z;\alpha)+\gamma(z;\alpha)]\}, \tag{3.2}$$

where $\mathbf{u}(z;\alpha)$ and $\gamma(z;\alpha)$ are as yet unspecified random functions. The dot over $\mathbf{u}(z;\alpha)$ in (3.2) designates a derivative with respect to z. To avoid unnecessary complexity in notation, we shall not write the arguments of $\mathbf{y},\mathbf{u}$, and γ out explicitly, unless there is ambiguity.

Our next step is to substitute (3.2) into (1.1) and carry out the indicated operations. This procedure leads to the following expression:

$$\begin{aligned}\frac{i}{k}\frac{\partial}{\partial z}\phi=&-\frac{1}{2k^2}\nabla_{\mathbf{y}}^2\phi+\tfrac{1}{2}g^2\mathbf{y}^2\phi\\&+(\ddot{\mathbf{u}}+g^2\mathbf{u}-g^2\mathbf{a}\,\delta H)\cdot\mathbf{y}\phi\\&+(\dot{\gamma}-\tfrac{1}{2}\dot{u}^2+\tfrac{1}{2}g^2u^2-g^2\mathbf{u}\cdot\mathbf{a}\,\delta H+\tfrac{1}{2}g^2a^2\delta H^2)\phi.\end{aligned} \tag{3.3}$$

We require that the terms within the parentheses on the right-hand side of (3.3) vanish. This condition gives rise to the following relationships:

$$\text{(i)}\ \frac{i}{k}\frac{\partial}{\partial z}\phi(\mathbf{y},z)=\frac{1}{2k^2}\nabla_{\mathbf{y}}^2\phi(\mathbf{y},z)+\tfrac{1}{2}g^2\mathbf{y}^2\phi(\mathbf{y},z), \tag{3.4}$$

$$\text{(ii)}\ \ddot{\mathbf{u}}(z;\alpha)+g^2\mathbf{u}(z;\alpha)=g^2\mathbf{a}\delta H(z;\alpha), \tag{3.5}$$

$$\text{(iii)}\ \dot{\gamma}(z;\alpha)=\tfrac{1}{2}\dot{u}^2-\tfrac{1}{2}g^2u^2+g^2\mathbf{u}\cdot\mathbf{a}\delta H-\tfrac{1}{2}g^2a^2\delta H^2. \tag{3.6}$$

It is seen that within the framework of this formulation, the new wavefunction $\phi(\mathbf{y},z)$ satisfies the parabolic equation characterizing the unperturbed focusing medium. It should be noted, however, that ϕ is a random function by virtue of its implicit dependence on $\mathbf{u}(z;\alpha)$, viz., $\phi=\phi[\mathbf{x}-\mathbf{u}(z;\alpha),z]$, which, in turn, satisfies the Langevin-type equation (3.5).

To proceed with our analysis, we shall need appropriate initial conditions for $\mathbf{u}$ and $\dot{\mathbf{u}}$. Toward this end, we set $z=0$ on both sides of (3.2):

$$\psi_0(\mathbf{x})=\phi(\mathbf{x}-\mathbf{u}_0,0)\exp\{ik[\dot{\mathbf{u}}_0\cdot(\mathbf{x}-\mathbf{u}_0)+\gamma_0]\}, \tag{3.7}$$

where $\mathbf{u}_0,\dot{\mathbf{u}}_0$, and γ_0 are respectively the values of $\mathbf{u}(z;\alpha)$, $\dot{\mathbf{u}}(z;\alpha)$, and $\gamma(z;\alpha)$ at $z=0$. From (3.6), one has

$$\gamma(z;\alpha)=\int_0^z d\zeta(\tfrac{1}{2}\dot{u}^2-\tfrac{1}{2}g^2u^2+g^2\mathbf{u}\cdot\mathbf{a}\delta H-\tfrac{1}{2}g^2a^2\delta H^2)+c, \tag{3.8}$$

where c is a constant of integration. Choosing the initial conditions $\mathbf{u}_0=\dot{\mathbf{u}}_0=0$, it follows, then, from (3.7) and (3.8) that

$$\psi_0(\mathbf{x})=\phi_0(\mathbf{x})\exp(ikc), \tag{3.9}$$

where $\phi_0(\mathbf{x})=\phi(\mathbf{x},0)$. The phase term $\exp(ick)$ plays an unimportant role in the evaluation of a large class of "even" moments of the wavefunction ψ; it will, therefore, be omitted by taking $c=0$. We have, then, finally,

$$\psi_0(\mathbf{x})=\phi_0(\mathbf{x}). \tag{3.10}$$

Thus, given the initial value $\psi_0(\mathbf{x})$ for the stochastic parabolic equation (1.1), the correct initial condition for the "deterministic" parabolic equation (3.4) is

$$\phi(\mathbf{y},0)\equiv\phi_0(\mathbf{y})=\psi_0(\mathbf{y}). \tag{3.11}$$

Our procedure in the sequel can be outlined as

follows: The parabolic equation (3.4) for the unperturbed medium, with the boundary condition (3.11), will be solved first for the wavefunction ϕ. The latter is a functional of the random function $u(z;\alpha)$ via the relationship $\phi = \phi[\mathbf{x} - \mathbf{u}(z;\alpha), z]$. This solution for ϕ will, be used in the expression (3.2) for the original wavefunction $\psi(\mathbf{x}, z;\alpha)$. This wavefunction is, in turn, a functional of $\mathbf{u}(z;\alpha), \mathring{\mathbf{u}}(z;\alpha)$, and $\delta H(z;\alpha)$ because of its dependence on ϕ and the presence of the exponential factor in (3.2). Our ultimate goal will be to obtain statistical moments of the random wavefield $\psi(\mathbf{x}, z;\alpha)$ which are linked with physical observables.

Before we proceed any further, we wish to point out that the statistical technique outlined in this section has been motivated by the work of Papanicolaou *et al.*[11] and McLaughlin (cf. Ref. 7). Using "key representations" which are similar to—but distinct from—our basic ansatz (3.2), they have studied the propagation of a Gaussian beam in a randomly perturbed strongly focusing medium, and have derived detailed information, especially in connection with beam-axis statistics, which would have been difficult to obtain by other methods. In the special case of a deterministic perturbation, viz., $\delta H(z;\alpha) \to \delta H(z)$, our "key representation" (3.2) is an extension of a well-known method in quantum mechanics. Ter Haar,[12] for example, has used it to determine the motion of an one-dimensional harmonic oscillator under the action of an externally applied force. Along the same vein, Svin'in[13] has recently applied this technique to the study of the Brownian motion of an one-dimensional, damped, quantum mechanical harmonic oscillator in an external field. Conceptually, we feel that our technique is also close to recently formulated methods based on the operator Langevin equation (cf. Ref. 14; see, also, remarks in Ref. 13) and Feynman path integration (cf. Refs. 15,16). This is an important conjecture which we hope to substantiate in the future.

4. SPECIALIZATION TO THE ONE–DIMENSIONAL CASE

To avoid unnecessary complexity which may obscure our main contributions, we shall limit our subsequent work to the one-dimensional version of the stochastic parabolic equation (1.1), viz.,

$$\frac{i}{k}\frac{\partial}{\partial z}\psi(x,z;\alpha) = -\frac{1}{2k^2}\frac{\partial^2}{\partial x^2}\psi(x,z;\alpha) + \tfrac{1}{2}g^2[x - a\delta H(z;\alpha)]^2\psi(x,z;\alpha), \quad z>0, \tag{4.1a}$$

$$\psi(x,0;\alpha) = \psi_0(x). \tag{4.1b}$$

Corresponding to (3.1), (3.2), (3.4)– (3.6), (3.8), and (3.11), we have, then, the relations

$$y = x - u(z;\alpha), \tag{4.2}$$

$$\psi(x,z;\alpha) = \phi[y(z;\alpha), z]\exp\{ik[\mathring{u}(z;\alpha)y(z;\alpha) + \gamma(z;\alpha)]\}, \tag{4.3}$$

$$\frac{i}{k}\frac{\partial}{\partial z}\phi(y,z) = -\frac{1}{2k^2}\frac{\partial^2}{\partial y^2}\phi(y,z) + \tfrac{1}{2}g^2y^2\phi(y,z), \quad z>0, \tag{4.4a}$$

$$\phi(y,0) = \phi_0(y) = \psi_0(y), \tag{4.4b}$$

$$\ddot{u}(z;\alpha) + g^2u(z;\alpha) = g^2a\delta H(z;\alpha), \quad z>0, \tag{4.5a}$$

$$u(0;\alpha) = \mathring{u}(0;\alpha) = 0, \tag{4.5b}$$

$$\gamma(z;\alpha) = \int_0^z d\xi\,(\tfrac{1}{2}\mathring{u}^2 - \tfrac{1}{2}g^2u^2 + g^2ua\delta H - \tfrac{1}{2}g^2a^2\delta H^2). \tag{4.6}$$

Consider, next, the parabolic equation (4.4) for the unperturbed medium. This problem is isomorphic to the Schrödinger equation for an one-dimensional quantum mechanical harmonic oscillator whose solution is well known.[17] Let $G(y,y',z)$ be the Green's function associated with (4.4). In this case, it is given explicitly as follows:

$$G(y,y',z) = (gk/2\pi i\,\sin gz)^{1/2} \times \exp[-(gk/2i\sin gz)(y^2\cos gz - 2yy' + y'^2\cos gz)]. \tag{4.7}$$

This expression provides a link between the wavefunction $\phi(y,z), z>0$, and the boundary condition $\phi_0(y)$:

$$\phi(y,z) = \int_{-\infty}^{\infty} dy'\,G(y,y',z)\phi_0(y'). \tag{4.8}$$

In order to evaluate the wavefunction $\phi(y,z)$ explicitly, we shall have to decide on a specific boundary condition $\psi_0(x)$ and, hence, $\phi_0(y)$. For simplicity, let us choose the fundamental mode corresponding to the parabolic equation for the background focusing medium, viz.,

$$\psi_0(x) = (gk/\pi)^{1/4}\exp[-(1/2)gkx^2]. \tag{4.9}$$

This initial configuration is normalized to unity [cf. Eq. (2.6)]. In light of the identity $\phi_0(y) = \psi_0(y)$, expressions (4.7)– (4.9) lead to the wavefunction

$$\phi(y,z) = (gk/\pi)^{1/4}\exp[-(1/2)gky^2]\exp[-\tfrac{1}{2}igz]. \tag{4.10}$$

This, of course, is the "ground state" wavefunction ("stationary state") of the parabolic equation (4.4).

We introduce, next, (4.10) into our fundamental relation (4.3):

$$\psi(x,z;\alpha) = (gk/\pi)^{1/4}\exp[-\tfrac{1}{2}gky^2]\exp[-\tfrac{1}{2}igz]\exp[ik(\dot{u}y + \gamma)]. \tag{4.11}$$

This constitutes a solution to the original stochastic complex parabolic equation (4.1) for every realization $\alpha \in A$. In general, the computation of the ensemble average of an arbitrary functional of $\psi(x,z;\alpha)$ requires the joint probability density function of the random functions $u(z;\alpha), \dot{u}(z;\alpha)$, and $\gamma(z;\alpha)$. The latter can be found from the analysis of the following set of coupled first-order, nonlinear, stochastic, ordinary differential equations:

$$\dot{u}(z;\alpha) = v(z;\alpha), \tag{4.12a}$$

$$\dot{v}(z;\alpha) + g^2u(z;\alpha) = g^2a\delta H(z;\alpha), \quad z>0, \tag{4.12b}$$

$$u(0;\alpha) = v(0;\alpha) = 0, \tag{4.12c}$$

$$\dot{\gamma}(z;\alpha) = \tfrac{1}{2}v^2(z;\alpha) - \tfrac{1}{2}g^2u^2(z;\alpha) + g^2au(z;\alpha)\delta H(z;\alpha) - \tfrac{1}{2}g^2a^2\delta^2H(z;\alpha), \quad z>0, \tag{4.13a}$$

$$\gamma(0;\alpha) = 0. \tag{4.13b}$$

It is important, however, to note that expressions of the form $\{\psi^*(x_1,z;\alpha)\psi^*(x_2,z;\alpha)\cdots\psi^*(x_m,z;\alpha)(\psi(x_1',z;\alpha) \times\psi(x_2',z;\alpha)\cdots\psi(x_m',z;\alpha)\}$, linked to a large class of important averaged physical observables (cf. Sec. 6 *et seq.*), are functionals only of $u(z;\alpha)$ and $\dot{u}(z;\alpha)$. Since the latter are governed solely by the Langevin-type, linear, stochastic, ordinary differential equation (4.5)

[cf., also, Eq. (4.12)], our task of computing a large number of physically important moments of the wave-function $\psi(x, z;\alpha)$ can be accomplished provided the joint probability density function of the random functions $u(z;\alpha)$ and $\dot{u}(z;\alpha)$ is available. This problem is considered in detail in the next section.

5. ANALYSIS OF THE BASIC STATISTICAL PROBLEM

The second-order, Langevin-type, stochastic ordinary differential equation (4.5) may be recast into the form

$$\frac{d}{dz}v(z;\alpha)+g^2u(z;\alpha)=g^2a\delta H(z;\alpha), \tag{5.1a}$$

$$\frac{d}{dz}u(z;\alpha)=v(z;\alpha), \tag{5.1b}$$

$$u(0;\alpha)=v(0;\alpha)=0. \tag{5.1c}$$

This problem is closely related to the Brownian motion of a randomly forced, classical, harmonic oscillator.

The "fine-grained" density, or classical "phase-space" distribution function, associated with (5.1) is introduced next as follows:

$$f_c(u,v,z;\alpha)=\delta[u-u(z;\alpha)]\delta[v-v(z;\alpha)], \tag{5.2a}$$

$$f_c(u,v,0;\alpha)=\delta(u)\delta(v). \tag{5.2b}$$

It obeys the continuity, or Liouville equation, which reads[18]

$$\frac{\partial}{\partial z}f_c(u,v,z;\alpha)=Lf_c(u,v,z;\alpha); \tag{5.3a}$$

$$Lf_c(u,v,z;\alpha)=-v\frac{\partial}{\partial u}f_c(u,v,z;\alpha)+\theta f_c(u,v,z;\alpha); \tag{5.3b}$$

$$\theta f_c(u,v,z;\alpha)=\left[g^2u\frac{\partial}{\partial v}-g^2a\delta H(z;\alpha)\frac{\partial}{\partial v}\right]f_c(u,v,z;\alpha). \tag{5.3c}$$

We shall embark next on a statistical analysis of (5.3). Using only the first-order smoothing approximation (cf. Refs. 19,20; see, also, Refs. 21 and 5), we obtain the following kinetic equation for the ensemble average of the density function:

$$\left(\frac{\partial}{\partial z}+v\frac{\partial}{\partial u}-g^2u\frac{\partial}{\partial v}\right)E\{f_c(u,v,z;\alpha)\}$$
$$=g^4a^2\frac{\partial}{\partial v}\left[\int_0^z d\zeta\Gamma(\zeta)\left(\frac{\sin g\zeta}{g}\frac{\partial}{\partial u}+\cos g\zeta\frac{\partial}{\partial v}\right)\right.$$
$$\times E\left\{f_c\left(u\cos g\zeta-\frac{1}{g}v\sin g\zeta,\ v\cos g\zeta\right.\right.$$
$$\left.\left.\left.+gu\sin g\zeta, z-\zeta;\alpha\right)\right\}\right]. \tag{5.4}$$

In deriving this expression it has been assumed that $\delta H(z;\alpha)$ is a zero-mean, wide-sense stationary random process, with correlation function $\Gamma(\zeta)=E\{\delta H(z;\alpha)\,\delta H(z-\zeta;\alpha)\}$. The kinetic equation (5.4) is uniformly valid in range. The right-hand side of (5.4) contains generalized operators (nonlocal, with space "memory") in phase space.

For a random process $\delta H(z;\alpha)$ which is δ-correlated in range, viz., $\Gamma(\zeta)=S\delta(\zeta)$, where S is a constant, the integration over ζ in (5.4) can be carried out explicitly. The resulting transport equation is

$$\left(\frac{\partial}{\partial z}+v\frac{\partial}{\partial u}-g^2u\frac{\partial}{\partial v}\right)E\{f_c(u,v,z;\alpha)\}$$
$$=D\frac{\partial^2}{\partial v^2}E\{f_c(u,v,a;\alpha)\}, \tag{5.5}$$

where $D=g^4a^2S$. If, in addition to the above assumptions, $\delta H(z;\alpha)$ is a Gaussian random process, (5.5) is the *exact* statistical equation for $E\{f(u,v,z,\alpha)\}$. This can be established by means of the Donsker–Furutsu–Novikov functional formalism.[22–24] In the long-range Markovian approximation (cf. Ref. 25; see, also, Refs. 21b and 5), (5.4) reduces to the simpler transport equation

$$\left(\frac{\partial}{\partial z}+v\frac{\partial}{\partial u}-g^2u\frac{\partial}{\partial v}\right)E\{f_c(u,v,z;\alpha)\}$$
$$=D_1\frac{\partial^2}{\partial v^2}E\{f_c(u,v,z;\alpha)\}+D_2\frac{\partial^2}{\partial u\partial v}E\{f_c(u,v,z;\alpha)\}. \tag{5.6}$$

The diffusion coefficients are given by the expressions

$$D_1=g^4a^2\int_0^\infty d\zeta\,\Gamma(\zeta)\cos g\zeta, \tag{5.7a}$$

$$D_2=g^3a^2\int_0^\infty d\zeta\,\Gamma(\zeta)\sin g\zeta. \tag{5.7b}$$

The quantity $E\{f_c(u,v,z;\alpha)\}$ is nonnegative; as such, provided that it is normalized to unity, it can be considered as the joint probability distribution density of u and v. A requirement of our statistical formulation (cf. Sec. 4) is that $E\{f_c(u,v,z;\alpha)\}$ be known explicitly. In general, no exact solution seems to be possible for the kinetic equation (5.4) [augmented by the boundary condition $E\{f_c(u,v,0;\alpha)\}=\delta(u)\delta(v)$]; this, however, is not the case for the Fokker–Planck equations (5.5) and (5.6), as it will be shown below.

The Fokker–Planck equation (5.5) has been studied extensively (cf., e.g., Refs. 26 and 27). Its exact solution is a two-dimensional Gaussian distribution in u and v.

Let

$$\Sigma=E\{[\mathbf{w}(z;\alpha)-E\{\mathbf{w}(z;\alpha)\}][\mathbf{w}(z;\alpha)-E\{\mathbf{w}(z;\alpha)\}]^T\} \tag{5.8}$$

be the autocovariance matrix of the two-dimensional vector process $\mathbf{w}(z;\alpha)=[u(z;\alpha),\ v(z;\alpha)]$. It is given explicitly as follows:

$$\Sigma=\{\sigma_{ij}^2\},\quad i,j=1,2, \tag{5.9a}$$

$$\sigma_{11}^2=D[(z/g^2)-(1/2g^3)\sin 2gz], \tag{5.9b}$$

$$\sigma_{12}^2=\sigma_{21}^2=(D/g^2)\sin^2 gz, \tag{5.9c}$$

$$\sigma_{22}^2=D[z+(1/2g)\sin 2gz]. \tag{5.9d}$$

In deriving (5.9), use has been made of the fact that $E\{u\}=E\{v\}=0$, and hence, $E\{\mathbf{w}\}=0$. Accounting for this property, the general form of the desired normal distribution density function is

$$E\{f_c(\mathbf{w},z;\alpha)\}\equiv F(\mathbf{w},z)=(2\pi)^{-1}(\det\Sigma)^{-1/2}\exp(-\tfrac{1}{2}\mathbf{w}^T\Sigma^{-1}\mathbf{w}), \tag{5.10}$$

where Σ^{-1} is the inverse of the covariance matrix. More explicitly,

$$F(\mathbf{w},z)=(2\pi)^{-1}(\det\Sigma)^{-1/2}$$
$$\times\exp\left[-\frac{1}{2}\frac{1}{\det\Sigma}\left(\sigma_{22}^2u^2+\sigma_{11}^2v^2-2\sigma_{12}^2uv\right)\right], \quad (5.11)$$

where the σ_{ij}^2, $i,j=1,2$, are the entries of the covariance matrix [cf. Eqs. (5.9b)–(5.9d)] and

$$\det\Sigma=(D^2/g^2)z^2-(D^2/g^4)\sin^2gz. \quad (5.12)$$

Finally, the "marginal" distribution density functions of the random functions $u(z;\alpha)$ and $v(z;\alpha)$ can be readily found from (5.10):

$$F(u,z)=\int_{-\infty}^{\infty}dvF(v,v,z)=(2\pi)^{-1/2}\sigma_{11}^{-1}$$
$$\times\exp\left(-\frac{1}{2}\frac{1}{\sigma_{11}^2}u^2\right), \quad (5.13)$$
$$F(v,z)=\int_{-\infty}^{\infty}duF(u,v,z)=(2\pi)^{-1/2}\sigma_{22}^{-1}$$
$$\times\exp\left(-\frac{1}{2}\frac{1}{\sigma_{22}^2}v^2\right). \quad (5.14)$$

The more complicated Fokker–Planck equation (5.6) based on the long-range Markovian approximation is a variant of Kramers' equation (cf. Ref. 28). As such, it can be integrated by the method of characteristics. Its solution constitutes a two-dimensional normal distribution of the form (5.11), with covariance matrix

$$\Sigma=\{\sigma_{ij}^2\}, \quad i,j=1,2, \quad (5.15a)$$
$$\sigma_{11}^2=(D_2/g^2)\sin^2gz+D_1[(z/g^2)-(1/2g^3)\sin2gz], \quad (5.15b)$$
$$\sigma_{12}^2=\sigma_{21}^2=(D_2/2g)\sin2gz+(D_1/g^2)\sin^2gz, \quad (5.15c)$$
$$\sigma_{22}^2=D_1[z+(1/2g)\sin2gz]-D_2\sin^2gz. \quad (5.15d)$$

Several general results presented in the following two sections hold for both Fokker–Planck equations (5.5) and (5.6). This is due to the fact that the solutions to these equations, i.e., the respective joint probability distribution density functions, have the same functional form [cf. Eq. (5.11)]. For the sake of simplicity, however, many specific analytic and numerical results are based on the assumption that $\delta H(z;\alpha)$ is a wide-sense stationary, δ-correlated random process.

6. SECOND-ORDER OBSERVABLES

A. Basic second-order moments

We set as our first task the computation of the *mean intensity* $E\{i(x,z;\alpha)\}$, where $i(x,z;\alpha)=\psi^*(x,z;\alpha)\psi(x,z;\alpha)$ is the irradiance function [cf. Eq. (2.1)]. Toward this end, we note from (4.11) that

$$i(x,z;\alpha)=(gk/\pi)^{1/2}\exp\{-gk[x-u(z;\alpha)]^2\}. \quad (6.1)$$

Since the last quantity is a functional only of $u(z;\alpha)$,

$$E\{i(x,z;\alpha)\}=\int_{\infty}^{\infty}du\,i(x,u)F(u,z), \quad (6.2)$$

where $F(u,z)$ is the marginal probability density function given in (5.13). The integration in (6.2) can be performed easily, yielding

$$E\{i(x,z;\alpha)\}=\pi^{-1/2}[gk/(1+2gk\sigma_{11}^2)]^{1/2}$$
$$\times\exp\{-[gk/(1+2gk\sigma_{11}^2)]x^2\}. \quad (6.3)$$

On the beam axis (i.e., $x=0$), (6.3) specializes to

$$E\{i(0,z;\alpha)\}=\pi^{-1/2}[gk/(1+2gk\sigma_{11}^2)]^{1/2}. \quad (6.4)$$

Since $\sigma_{11}^2(z)>0$, $\forall\, z>0$ [cf. (5.9b)], it is seen that the on-axis mean intensity decreases monotonically as a function of the range z. This is due to the transfer of mean power from the fundamental mode to higher modes, a subject that will be considered in detail later on.

The *mean centroid* of the beam, defined by

$$X(z)=\int_{-\infty}^{\infty}dx\,xE\{i(x,z;\alpha)\}, \quad (6.5)$$

is zero for all z since the integrand is an odd function of x.

A measure of the *spreading of the beam* can be found by using the definition

$$\tfrac{1}{2}\sigma_x^2(z)=\int_{-\infty}^{\infty}dx\,[x-X(z)]^2\,E\{i(x,z;\alpha)\}. \quad (6.6)$$

It turns out that

$$\sigma_x^2(z)=(1+2gk\sigma_{11}^2)/gk. \quad (6.7)$$

Introducing (6.7) into (6.3), the mean intensity can be written more succinctly as follows:

$$E\{i(x,z;\alpha)\}=[\pi\sigma_x^2(z)]^{-1/2}\exp[-x^2/\sigma_x^2(z)]. \quad (6.8)$$

Comparing (6.8) with the initial intensity, viz.,

$$i(x,0;\alpha)=(gk/\pi)^{1/2}\exp(-gkx^2), \quad (6.9)$$

it is seen that the mean intensity remains Gaussian for $z>0$. Since $\psi_0(x)$ is taken to be the fundamental mode of the unperturbed problem, $i(x,z)=(gk/\pi)^{1/2}\exp(-gkx^2)$ in the absence of random perturbations. In this case, the original beam would not spread at all. In the presence of random fluctuations, however, the variance of the transverse coordinate x changes from $(gk)^{-1}$ to the quantity $\sigma_x^2(z)$ given in (6.7).

If the expression for σ_{11}^2 given in (5.9b) is substituted in (6.7), one has

$$\sigma_x^2(z)=[1+2gkD(z/g^2-\sin2gz/2g^3)]/gk. \quad (6.10)$$

In terms of the dimensionless quantities

$$\zeta=gz, \quad c=kD/g^2. \quad (6.11)$$

Eq. (6.10) can be brought into a form convenient for numerical investigation. Specifically,

$$\sigma_x^2(\zeta;c)gk=1+c(2\zeta-\sin2\zeta). \quad (6.12)$$

A plot of this expression versus ζ, with c (a dimensionless measure of the strength of the fluctuations) as a parameter, is shown in Fig. 1. The monotonic increase of the beam spreading is clearly evident.

The intensity flux density defined in (2.2) can be written more compactly as

$$j(x,z;\alpha)=\mathrm{Re}[-(i/k)\psi^*(x,z;\alpha)(\partial/\partial x)\psi(x,z;\alpha)]. \quad (6.13)$$

Using (4.11) and performing the operations indicated in (6.13), we obtain

$$j(x,z;\alpha)=(gk/\pi)^{1/2}v(z;\alpha)\exp\{-gk[x-u(z;\alpha)]^2\}, \quad (6.14)$$

a functional of both $u(z;\alpha)$ and $v(z;\alpha)$. The *mean intensity flux density* is, therefore, given by

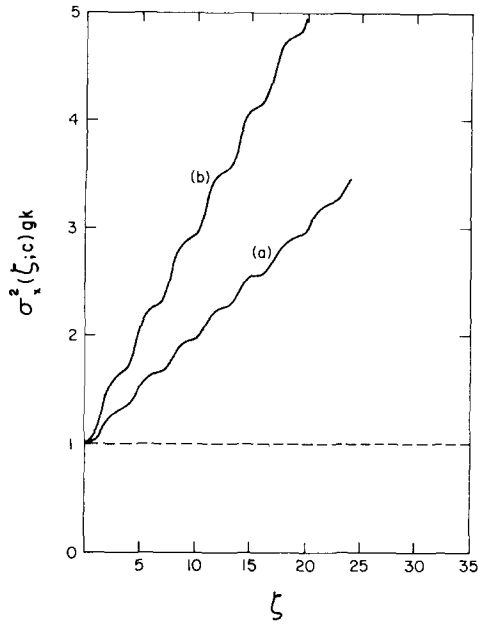

FIG. 1. Variance of transverse beam displacements. (a) $c=0.05$; (b) $c=0.1$.

$$E\{j(x,z;\alpha)\}=\int_{-\infty}^{\infty}du\int_{-\infty}^{\infty}dv\,j(x,u,v)F(u,v,z), \tag{6.15}$$

where $F(u,v,z)$ is the joint probability density function in (5.11). In this case, the integration in (6.15) can be performed without difficulty. The final result is

$$E\{j(x,z;\alpha)\}=2\pi^{-1/2}\sigma_{12}^2[gk/(1+2gk\sigma_{11}^2)]^{3/2}\times\exp\{-[gk/(1+2gk\sigma_{11}^2)]x^2\}. \tag{6.16}$$

As a consequence of the conservation law (2.3) which holds for every realization $\alpha\in A$, one has by inspection the relation

$$\frac{\partial}{\partial z}E\{i(x,z;\alpha)\}+\frac{\partial}{\partial x}E\{j(x,z;\alpha)\}=0. \tag{6.17}$$

The latter means that the total mean intensity is conserved, i.e.,

$$\frac{d}{dz}\left[\int_{-\infty}^{\infty}dx\,E\{i(x,z;\alpha)\}\right]=0. \tag{6.18}$$

The conservation law (6.17) can be found by taking the ensemble average of the one-dimensional version of (2.7). Alternatively, it can be obtained by combining our results for $E\{i(x,z;\alpha)\}$ and $E\{j(x,z;\alpha)\}$ given in (6.3) and (6.16), respectively.

Having established both $E\{i(x,z;\alpha)\}$ and $E\{j(x,z;\alpha)\}$, we are in a position to compute one more observable: the *mean power flux density* [cf. Eq. (2.7)]. Specifically

$$E\{\mathbf{s}(x,z;\alpha)\}=E\{i(x,z;\alpha)\}\hat{\mathbf{z}}+E\{j(x,z;\alpha)\}\hat{\mathbf{x}}. \tag{6.19}$$

On the basis of a statement made earlier (cf. Sec. 2), the quantity

$$\int_{S_0}\int E\{\mathbf{s}(x,z;\alpha)\}\cdot\hat{\mathbf{n}}\,dA \tag{6.20}$$

can be interpreted as the *total mean power* intercepted by a detector characterized by the open surface S_0.

We shall undertake next the computation of the *spatial mutual coherence function* $E\{\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha)\}$. We form first the quantity $\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha)$ using the expression for $\psi(x,z;\alpha)$ in (4.11):

$$\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha)=(gk/\pi)^{1/2}\exp\{-\tfrac{1}{2}gk[[x_2-u(z;\alpha)]^2+[x_1-u(z;\alpha)]^2]\}\times\exp[-ikv(z;\alpha)(x_2-x_1)]\equiv m[x_2,x_1,u(z;\alpha),v(z;\alpha)]. \tag{6.21}$$

Its ensemble average is given by

$$E\{\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha)\}=\int_{-\infty}^{\infty}du\int_{-\infty}^{\infty}dv\,m(x_2,x_1,u,v)F(u,v,z). \tag{6.22}$$

The integration can be performed exactly, yielding the following expression for the spatial mutual coherence function:

$$\begin{aligned}E\{\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha)\}&=\pi^{-1/2}[gk/(1+2gk\sigma_{11}^2)]^{1/2}\exp[-\tfrac{1}{2}gk(x_2^2+x_1^2)]\\&\times\exp\{\tfrac{1}{2}[(gk\sigma_{11})^2/(1+2gk\sigma_{11}^2)](x_2+x_1)^2\}\\&\times\exp[-\tfrac{1}{2}k^2(\sigma_{12}^4/\sigma_{11}^2)(1+2gk\sigma_{11}^2)^{-1}(x_2-x_1)^2]\\&\times\exp[-\tfrac{1}{2}k^2(\det\Sigma/\sigma_{11}^2)(x_2-x_1)^2]\\&\times\exp[-ikgk\sigma_{21}^2(1+2gk\sigma_{11}^2)^{-1}(x_2^2-x_1^2)].\end{aligned} \tag{6.23}$$

In the special case that x_2 and x_1 coalesce, i.e., $x_2=x_1=x$, the spatial mutual coherence must coincide with the mean intensity found earlier [cf. Eq. (6.3)]. A simple calculation shows that this is, indeed, the case.

B. Modal power transfer

The unperturbed $[\delta H(z;\alpha)\to 0]$ parabolic equation (4.1) is characterized by a set of modes $h_p(x)$, $p=0,1,2,\cdots$, satisfying the eigenvalue problem

$$-\frac{1}{2k^2}\frac{d^2}{dx^2}h_p(x)+\tfrac{1}{2}g^2x^2h_p(x)=E_ph_p(x). \tag{6.24}$$

It is well known (cf. e.g., Ref. 29) that

$$E_p=g(p+\tfrac{1}{2})/k \tag{6.25}$$

and

$$h_p(x)=2^{-p/2}(p!)^{-1/2}(gk/\pi)^{1/4}\exp(-\tfrac{1}{2}gkx^2)H_p[(gk)^{1/2}x]. \tag{6.26}$$

Here, $H_p(\xi)$ denotes the *pth* Hermite polynomial, viz.,

$$H_p(\xi)=(-1)^p\exp(\xi^2)(d^p/d\xi^p)\exp(-\xi^2). \tag{6.27}$$

The eigenfunctions given in (6.26) are orthonormal, i.e.,

$$\int_{-\infty}^{\infty}dx\,h_{p'}(x)h_p(x)=\delta_{p'p}. \tag{6.28}$$

The boundary condition $\psi_0(x)$ specified in (4.9) is the fundamental mode $h_0(x)$. This follows easily from (6.26).

We shall determine next the portion of the beam which remains in the fundamental mode. The complex amplitude of the fundamental mode is defined by

$$q_0(z;\alpha)=\int_{-\infty}^{\infty}dx\,\psi(x,z;\alpha)h_0(x). \tag{6.29}$$

The quantity of interest is the ensemble average of the

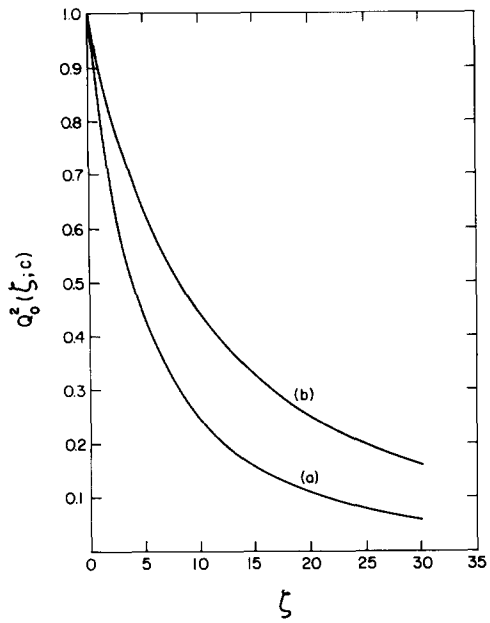

FIG. 2. Decay of mean power in the fundamental mode. (a) $c=0.1$; (b) $c=0.05$.

absolute square of $q_0(z;\alpha)$, viz.,

$$Q_0^2(z)\equiv E\{|q_0(z;\alpha)|^2\}. \tag{6.30}$$

We note, first, that

$$|q_0(z;\alpha)|^2=\exp(-\tfrac{1}{2}gku^2)\exp[-\tfrac{1}{2}(k/g)v^2]. \tag{6.31}$$

Integrating this quantity over u and v, with the joint probability density $F(u,v,z)$ as a weight, we find

$$Q_0^2(z)=[1+gk\sigma_{11}^2+(k/g)(\sigma_{22}^2+gk\det\Sigma)]^{-1}. \tag{6.32}$$

In the absence of random fluctuations, $\sigma_{11}^2\to 0$, $\sigma_{22}^2\to 0$, and $\det\Sigma\to 0$; hence, $Q_0^2(z)\to 1$, $\forall z$. In other words, the power remains entirely in the fundamental mode. On the other hand, the general expression (6.32) shows how power (in a mean sense) leaks out of the excited fundamental mode into higher modes.

Using the expressions for σ_{11}^2, σ_{22}^2, and $\det\Sigma$ [cf. Eqs. (5.9b), (5.9d), and (5.12), respectively] into (6.32), $Q_0^2(z)$ can be written as

$$Q_0^2(\zeta;c)=[1+2c\zeta+c^2(\zeta^2-\sin^2\zeta)]^{-1} \tag{6.33}$$

in terms of the dimensionless quantities ζ and c [cf. Eq. (6.11)]. A plot of $Q_0^2(\zeta;c)$ versus ζ, with c as a parameter, is shown in Fig. 2.

Analogously to (6.30), we define the expected modal power transfered from the fundamental mode at $z=0$ to the pth mode at distance z as follows:

$$Q_p^2(z)=E\{|q_p(z;\alpha)|^2\}, \tag{6.34}$$

where $q_p(z;\alpha)$ is the pth-order complex amplitude function, viz.,

$$q_p(z;\alpha)=\int_{-\infty}^{\infty}dx\,\psi(x,z;\alpha)h_p(x). \tag{6.35}$$

The square modulus $|q_p(z;\alpha)|^2$ required in (6.34) is found to be

$$|q_p(z;\alpha)|^2=2^{-p}(p!)^{-1}[(k/g)v^2+gku^2]^p \times\exp[-\tfrac{1}{2}(k/g)v^2]\exp(-\tfrac{1}{2}gku^2). \tag{6.36}$$

Finally,

$$Q_p^2(z)=2^{-p}(p!)^{-1}(gk)^p(2\pi)^{-1}(\det\Sigma)^{-1/2}(\pi/a)^{1/2}(\pi/a')^{1/2} \times\sum_{s=0}^{p}\sum_{p=0}^{s}\binom{p}{s}g^{-2s}(2s)!\,(b'/a)^{2s}[l!\,(2s-2l)!\,]^{-1} \times(a/4b'^2)^l[2(p-l)-1]!!/(2a')^{p-l}, \tag{6.37a}$$

where

$$a=\tfrac{1}{2}[(k/g)+(\sigma_{11}^2/\det\Sigma)], \tag{6.37b}$$

$$a'=\tfrac{1}{2}[gk+(gk\sigma_{11})^2+(k\sigma_{22})^2+gk^3\det\Sigma](gk\sigma_{11}^2+k^2\det\Sigma)^{-1} \tag{6.37c}$$

$$b'=\tfrac{1}{2}(\sigma_{12}^2/\det\Sigma). \tag{6.37d}$$

Particular values of modal power transfer functions can be obtained from the general expression (6.37) by restricting the values of the index p. Setting $p=0$, for example, specializes (6.37) to the quantity $Q_0^2(z)$ found earlier. For $p=1$, on the other hand, one has

$$Q_1^2(z)=\tfrac{1}{2}[gk\sigma_{11}^2+(k/g)\sigma_{22}^2+2k^2\det\Sigma] \times[1+gk\sigma_{11}^2+(k/g)(\sigma_{22}^2+gk\det\Sigma)]^{-3/2}, \tag{6.38}$$

a relationship exhibiting how mean power is transfered from the fundamental mode to the first one. Since, σ_{11}^2, σ_{22}^2, and $\det\Sigma$ become zero at the boundary $z=0$, it follows that $Q_1^2(0)=0$. This, of course, is expected since at $z=0$ all the mean power is stored in the fundamental mode.

In the special case that $\delta H(z;\alpha)$ is δ-correlated, $Q_1^2(z)$ can be written in the dimensionless form

$$Q_1^2(\zeta;c)=[c\zeta+c^2(\zeta^2-\sin^2\zeta)][1+2c\zeta+c^2(\zeta^2-\sin^2\zeta)]^{-3/2}. \tag{6.39}$$

A plot of $Q_1^2(\zeta;c)$ versus ζ for two values of the parameter c is shown in Fig. 3. The average power contained in the first mode rises from zero to a maximum, and, then, decays monotonically to zero as $\zeta\to\infty$. It is, also, seen that the position of the maximum, as well as the rate of decay, depends on the strength of the random fluctuations.

Qualitatively, one would expect the same general behavior for the average modal power transfer from the fundamental mode of $z=0$ to the pth mode at distance z. The rate of transfer, however, would depend on the order of the mode.

C. Degree of coherence

Given the random wavefunction $\psi(x,z;\alpha)$, the *degree of coherence*, $D(z)$, is defined as follows:

$$D^2(z)=\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dx_1\,|E\{\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha)\}|^2. \tag{6.40}$$

It can be calculated by using the expression for the spatial mutual coherence [cf. Eq. (6.23)]. The final result is

$$D^2(z)=[1+2gk\sigma_{11}^2+2(k/g)(\sigma_{22}^2+2gk\det\Sigma)]^{-1/2}. \tag{6.41}$$

For a random process $\delta H(z;\alpha)$ which is δ-correlated, (6.41) assumes the following dimensionless form:

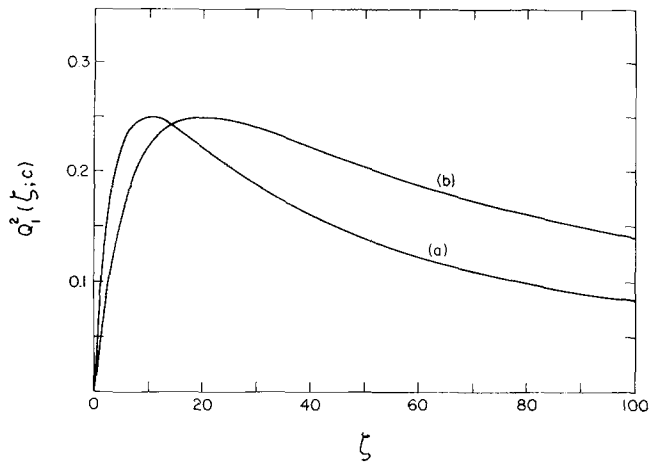

FIG. 3. Mean power transfer to the first mode. (a) $c=0.1$; (b) $c=0.05$.

$$D^2(\zeta;c)=[1+4c\zeta+4c^2(\zeta^2-\sin^2\zeta)]^{-1/2}. \tag{6.42}$$

The latter is shown graphically in Fig. 4.

The degree of coherence is a measure of the irreversible loss of coherence due to the presence of random fluctuations in the medium. At $z=0$, $D(z)=1$, i.e., the beam is coherent. As the range z is increased, there is a loss of coherence, i.e., $D(z)<1$, and finally, $D(z)\to 0$ as $z\to\infty$, i.e., the beam is rendered completely incoherent.

In the absence of random fluctuations in the medium, $D^2(z)$ and, hence, $D(z)$ would be conserved, i.e., $D(z)=D(0)=1$, $\forall\, z$. If the beam were partially coherent at $z=0$ due, for example, to aberrations in a focusing optical system, then $D(0)<1$. In this case, $D(z)\leq D(0)$, $\forall\ z\geq 0$, the equality holding for a nonrandom medium.

The degree of coherence defined in (6.40) is by no means the only quantity exhibiting the irreversibility due to the random fluctuations in the medium. Another quantity which describes this irreversible loss of coherence (or information) is the H-function used in statistical mechanics.[30] This function is intimately related to the thermodynamic (or information-theoretic) concept of entropy. To construct an appropriate definition for the H-function, we shall require a few preliminary results.

A two (transverse)-point field density function is introduced first as follows in terms of the wavefunction $\psi(x,z;\alpha)$:

$$\rho(x_2,x_1,z;\alpha)=\psi^*(x_2,z;\alpha)\psi(x_1,z;\alpha). \tag{6.43}$$

The "phase-space" analog of the density function is provided by the Wigner distribution density function which is defined as follows[31]:

$$f(x,\theta,z;\alpha)=\frac{k}{2\pi}\int_{-\infty}^{\infty}dy\ e^{ik\theta y}\rho(x+\tfrac{1}{2}y,x-\tfrac{1}{2}y,z;\alpha). \tag{6.44}$$

This quantity is real, but not necessarily positive everywhere. It can be shown (cf. Appendix A of Ref. 5; also, Ref. 32), in general, that $|f(x,\theta,z;\alpha)|\leq(k/\pi)$ for any realization $\alpha\in A$. Provided that $f(x,\theta,z;\alpha)$ is normalized to unity, this means that the Wigner distribution density function is different from zero in a region of which the volume in phase space is at least equal to (π/k). Hence, $f(x,\theta,z;\alpha)$ can never be sharply localized in z and θ. This situation is reminiscent of the quantum mechanical uncertainty principle. It is also analogous to the ambiguity arising in Fourier optics,[33,34] and the radar ambiguity discussed originally by Woodward.[35]

The mean Wigner distribution density function can be determined by ensemble-averaging both sides of (6.44):

$$E\{f(x,\theta,z;\alpha)\}=\frac{k}{2\pi}\int_{-\infty}^{\infty}dy\ e^{ik\theta y}E\{\rho(x+\tfrac{1}{2}y,x-\tfrac{1}{2}y,z;\alpha)\}. \tag{6.45}$$

The quantity $E\{\rho(x+\frac{1}{2}y,x-\frac{1}{2}y,z;\alpha)\}$ in the integrand is simply the spatial mutual coherence function [cf. Eq. (6.23)] expressed in terms of "center of mass" and difference coordinates. Taking this into consideration, we find that

$$\begin{aligned}E\{f(x,\theta,z;\alpha)\}&=(k/\pi)[1+2gk\sigma_{11}^2+2(k/g)(\sigma_{22}^2+2gk\det\Sigma)]^{-1/2}\\&\times\exp\{-(k/g)(1+2gk\sigma_{11}^2)[1+2gk\sigma_{11}^2+2(k/g)\\&\times(\sigma_{22}^2+2gk\det\Sigma)]^{-1}\\&\times[\theta-2gk\sigma_{11}^2(1+2gk\sigma_{11}^2)^{-1}x]^2\}\exp\{-[gk/(1+2gk\sigma_{11}^2)]x^2\}.\end{aligned} \tag{6.46}$$

The H-function is defined next in terms of the mean Wigner distribution density function as follows:

$$H(z)=\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}d\theta\,E\{f'(x,\theta,z;\alpha)\}\ln E\{f'(x,\theta,z;\alpha)\}. \tag{6.47}$$

Here, $f'(x,\theta,z;\alpha)=f(x,\theta,z;\alpha)/k$. It has already been pointed out that the Wigner distribution density function (and, hence, its ensemble average), although real, may not necessarily be positive everywhere. Consequently, the definition of the H-function in (6.47) cannot possibly be valid in general, by virtue of the logarithmic term which is not defined for negative values of $E\{f(x,\theta,z;\alpha)\}$. [It is this specific difficulty which is surmounted by the

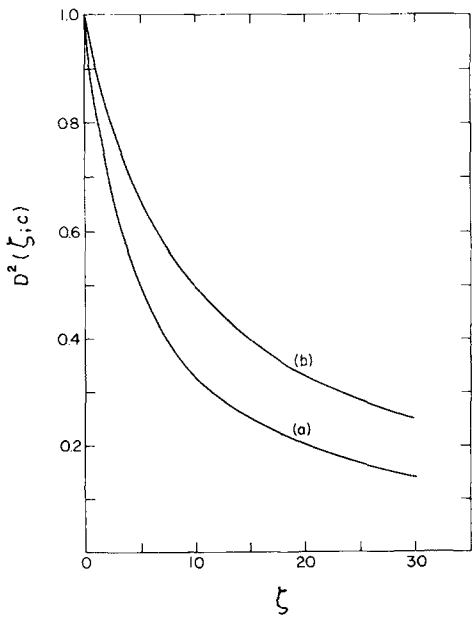

FIG. 4. Variation of the square of the degree of coherence. (a) $c=0.1$; (b) $c=0.05$.

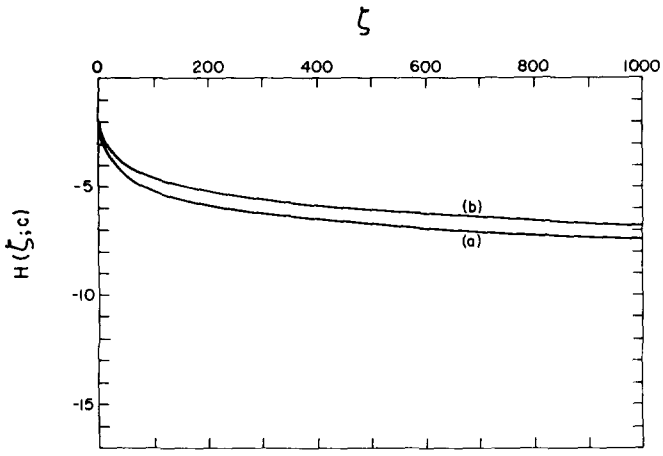

FIG. 5. Axial variation of the H-function. (a) $c=0.1$; (b) $c=0.05$.

definition of the degree of coherence given in (6.40)]. However, for the particular problem under consideration here, $f(x,\theta,z;\alpha)$ (and, hence, its ensemble average) is nonnegative. This can be easily seen by inspecting the explicit solution for $E\{f(x,\theta,z;\alpha)\}$ given in (6.46). We are, therefore, fully justified in using the definition (6.47). Carrying out the operations indicated on the right-hand side of (6.47) results in the following expression for the H-function:

$$H(z)=\ln[D^2(z)/\pi]-1. \tag{6.48}$$

Interestingly, it is a functional of the square of the degree of coherence determined earlier [cf. Eq. (6.41)].

An important property characterizing $H(z)$ is subsumed in the *H-theorem*, viz.,

$$(d/dz)H(z)\leq 0, \tag{6.49}$$

which is widely used in statistical mechanics (see, e.g., Ref. 30). The validity of this theorem follows readily from the result (6.48) for $H(z)$, in conjunction with the expression for the degree of coherence, $D(z)$, given in (6.41) and the specific forms of $\sigma_{11}^2,\sigma_{22}^2$, and $\det\Sigma$ derived in Sec. 5.

The entropy, $S(z)$, is defined as the negative H-function. Corresponding to the H-theorem (6.49), we have, then,

$$(d/dz)S(z)\geq 0. \tag{6.50}$$

This relation is a manifestation of the second law of thermodynamics, and states that the total entropy of the system (resp. beam) cannot decrease.

The H-function in (6.48) can be written in terms of the dimensionless quantities ζ and c as follows:

$$H(\zeta;c)=\ln\{\pi^{-1}[1+4c\zeta+4c^2(\zeta^2-\sin^2\zeta)]^{-1/2}\}-1. \tag{6.51}$$

The latter is depicted in Fig. 5. The non-increasing property of the H-function incorporated into the H-theorem is clearly evident in this plot.

D. Effective coherence distance

We shall close this section by defining and computing a characteristic scale called the *effective coherence distance*. [In the case of a two-dimensional problem (circular beam), this characteristic scale is referred to as the "effective coherence radius" of the beam (cf. Ref. 36)]. This quantity is intimately related to the angular width of the beam.

Let us begin by integrating $E\{\psi^*(x+\frac{1}{2}y,z;\alpha)\}\psi(x-\frac{1}{2}y,z;\alpha)\}$ over x. The result is

$$\gamma(y,z)\equiv\int_{-\infty}^{\infty}dx\,E\{\psi^*(x+\tfrac{1}{2}y,z;\alpha)\psi(x-\tfrac{1}{2}y,z;\alpha)\}$$
$$=\exp\{-\tfrac{1}{2}[\tfrac{1}{2}gk+k^2\sigma_{22}^2]y^2\}. \tag{6.52}$$

The effective coherence distance, y_e, is defined as that value of y at which $\gamma(y,z)$ has become e times smaller than $\gamma(0,z)$, viz.,

$$\gamma(y_e,z)=e^{-1}\gamma(0,z). \tag{6.53}$$

It is clear from (6.52) that $\gamma(z,z)=1$. Hence,

$$\gamma(y_e,z)=e^{-1}. \tag{6.54}$$

The desired quantity y_e can be easily determined by taking the natural logarithm of (6.54):

$$y_e(z)=[2^{-1}(2^{-1}gk+k^2\sigma_{22}^2)]^{-1/2}. \tag{6.55}$$

The corresponding dimensionless quantity $y_e(\zeta;c)$ is plotted in Fig. 6 for two values of the parameter c. It has the value of unity at the initial boundary, and decreases monotonically to zero as $\zeta\to\infty$.

7. HIGHER-ORDER MOMENTS

A. Fourth-order moments

We consider first the *correlation of the field intensity at two tranverse points*, viz., $E\{i(x_2,z;\alpha)i(x_1,z;\alpha)\}$. Using the expression found earlier for $i(x,z;\alpha)$ [cf. Eq. (6.1)], we have

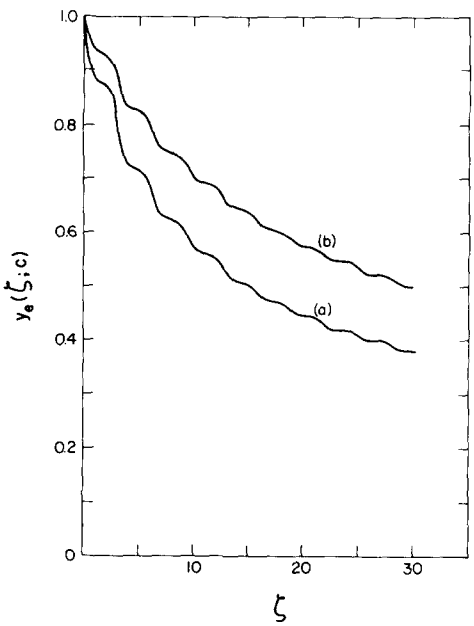

FIG. 6. Effective coherence distance of the beam (a) $c=0.1$; (b) $c=0.05$.

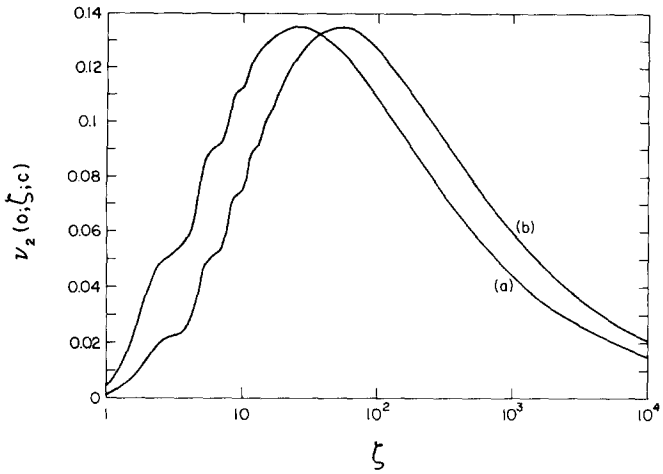

FIG. 7. Variance of on-axis intensity fluctuations. (a) $c=0.1$; (b) $c=0.05$.

$$i(x_2,z;\alpha)i(x_1,z;\alpha)=(gk/\pi)\exp\{-gk[x_2-u(z;\alpha)]^2\} \times\exp\{-gk[x_1-u(z;\alpha)]^2\}, \tag{7.1}$$

from which, upon averaging over the probability density function $F(u,v,z)$, we obtain

$$E\{i(x_2,z;\alpha)i(x_1,z;\alpha)\}=(gk/\pi)(1+4gk\sigma_{11}^2)^{-1/2} \times\exp\{-gk[(1+2gk\sigma_{11}^2)/(1+4gk\sigma_{11}^2)](x_2^2+x_1^2)\} \times\exp\{4\sigma_{11}^2[(gk)^2/(1+4gk\sigma_{11}^2)]x_1x_2\}. \tag{7.2}$$

As an illustration of a physical situation which requires the special fourth-order moment given in (7.2), consider the problem of "beam wandering." Associated with the stochastic parabolic equation (4.1), we define the "centroid" of the beam by

$$x(z;\alpha)=\int_{-\infty}^{\infty}dx\,x\,i(x,z;\alpha),\quad \forall\,\alpha\in A. \tag{7.3}$$

(As explained earlier, we assume that the total intensity is normalized to unity for each realization $\alpha\in A$.) The mean centroid, $X(z)$, of the beam has already been defined [cf. Eq. (6.5)] and found to be equal to zero. It is interesting, however, to consider also the variance of the random function $x(z;\alpha)$, viz.,

$$\mathrm{var}\{x(z;\alpha)\}=E\{[x(z;\alpha)-X(z)]^2\} =\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dx_1\,x_2x_1\,E\{i(x_2,z;\alpha)i(x_1,z;\alpha)\}. \tag{7.4}$$

Introducing (7.2) into the last equation and carrying out the integration we find

$$\mathrm{var}\{x(z;\alpha)\}=\sigma_{11}^2, \tag{7.5}$$

an expression which vanishes at $z=0$ and becomes unbounded as $z\to\infty$. This behavior is a manifestation of the instability of the beam due to the presence of random-axis misalignments.

Setting $x_2=x_1=x$, (7.2) reduces to the *intensity autocorrelation function*

$$E\{i^2(x,z;\alpha)\}=(gk/\pi)(1+4gk\sigma_{11}^2)^{-1/2} \times\exp\{-2[gk/(1+4gk\sigma_{11}^2)]x^2\}. \tag{7.6}$$

This result can be used in conjunction with the expression for the mean intensity [cf. Eq. (6.3)] in order to compute the *variance* (or *fluctuation*) *of the intensity*:

$$E\{[i(x,z;\alpha)-E\{i(x,z;\alpha)\}]^2\}\equiv\nu_2(x,z) =(gk/\pi)\{(1+4gk\sigma_{11}^2)^{-1/2}\exp\{-2[gk/(1+4gk\sigma_{11}^2)]x^2\} -(1+2gk\sigma_{11}^2)^{-1}\exp\{-2[gk/(1+2gk\sigma_{11}^2)]x^2\}\}. \tag{7.7}$$

Figure 7 shows the behavior of the on-axis fluctuations of intensity $\nu_2(0,\zeta;c)$ for two values of the parameter c. As expected from physical considerations, $\nu_2(0,\zeta,c)$ vanishes at the plane of the source ($\zeta=0$). It is also seen, however, that $\nu_2(0,\zeta,c)$ decays monotonically to zero as $\zeta\to\infty$, after it rises to a maximum at an intermediate range. On- and off-axis intensity fluctuations are shown graphically in Fig. 8. Here, $\nu_2(\zeta;c;d)$ is plotted versus ζ for one value of c and five values of the new dimensionless parameter $d=(gk)^{1/2}x$. In general, one might expect that for fixed values of the range ζ and the strength of the random fluctuations (incorporated into the parameter c), $\nu_2(\zeta;c;d)$ would decrease monotonically as d was increased. This is definitely not the case, as it is clearly shown in Fig. 8. Specifically, for $\zeta=10$ and $c=0.1$, $\nu_2(\zeta;c;d)$ increases for values of d up to about 0.75, and decreases for higher values of this parameter. A plausible explanation of this "anomalous" behavior could be the "elastic" influence of the background deterministic focusing medium.

B. Higher-order moments

Statistical moments beyond the fourth order level can be calculated without too much difficulty. For example,

$$E\{i^n(x,z;\alpha)\}=(gk/\pi)^{n/2}(1+2ngk\sigma_{11}^2)^{-1/2} \times\exp\{-n[gk/(1+2ngk\sigma_{11}^2)]x^2\}, \tag{7.8}$$

where n is a positive integer. Furthermore,

$$E\{i^n(x_2,z;\alpha)i^n(x_1,z;\alpha)\}=(gk/\pi)^n(1+4ngk\sigma_{11}^2)^{-1/2} \times\exp\{-ngk[(1+2ngk\sigma_{11}^2)/(1+4ngk\sigma_{11}^2)](x_2^2+x_1^2)\} \times\exp\{4\sigma_{11}^2[(ngk)^2/(1+4ngk\sigma_{11}^2)]x_1x_2\}. \tag{7.9}$$

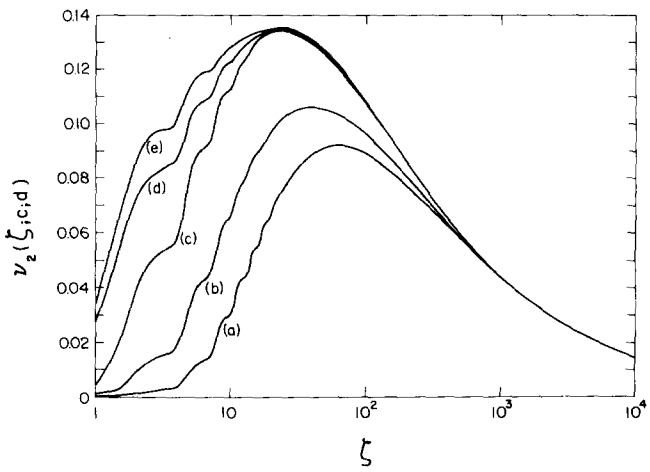

FIG. 8. Variance of on-and off-axis intensity fluctuations. (a) $d=2.25$; (b) $d=2$; (c) $d=0$ (on-axis); (d) $d=0.5$; (e) $d=0.75$. All curves are computed for $c=0.1$.

Finally, analogously to (7.7), we find that

$$E\{[i^n(x,z;\alpha) - E\{i^n(x,z;\alpha)\}]^2\} = \nu_{2n}(x,z)$$
$$= (gk/\pi)^n[(1+4ngk\sigma_{11}^2)^{-1/2}\exp\{-2n[gk/(1+4ngk\sigma_{11}^2)]x^2\}$$
$$-(1+2ngk\sigma_{11}^2)^{-1}\exp\{-2n[gk/(1+2ngk\sigma_{11}^2)]x^2\}]. \quad (7.10)$$

C. Probability density function of the log irradiance

The probability density function $p(i)$ of the intensity (or irradiance) $i=\psi^*\psi$ can be expressed in terms of the moments $E\{i^\nu(x,z;\alpha)\}$ as follows:

$$p(i) = (2\pi i)^{-1}\int_{-i\infty-\epsilon}^{i\infty-\epsilon} d\nu\, i^{-\nu-1}(x,z;\alpha)E\{i^\nu(x,z;\alpha)\}, \quad (7.11)$$

where ϵ is an infinitesimal positive number. The conditions for the applicability of (7.11), viz., that $E\{i^\nu(x,z;\alpha)\} \leq \exp(\nu E_c)$, $\nu\sim\infty$, E_c being a real constant, and $E\{i^\nu(x,z;\alpha)\}$ be analytic on the right half-plane of ν [satisfied by our expression given in (7.8)], are fully discussed in Refs. 37 and 38.

We introduce, next, the definitions $E=\ln[i(x,z;\alpha)/i_0]$, $i_0=(gk/\pi)^{1/2}$, $E_0=gkx^2$, and $\sigma_E=2gk\sigma_{11}^2$. (We have kept here unaltered the notation introduced by Furutsu in Ref. 37.) We have, then,

$$p(E) = p(i)(d/dE)i$$
$$= (2\pi i)^{-1}\int_{-i\infty-\epsilon}^{i\infty-\epsilon} d\nu\,(1+\nu\sigma_E)^{-1/2}$$
$$\times\exp\{-\nu[(1+\nu\sigma_E)^{-1}E_0 - E]\}. \quad (7.12)$$

The contour integration can be carried out, with the result

$$p(E) = \begin{cases} 0, & E>0, \quad (7.13a) \\ (-\pi E\sigma_E)^{-1/2}\exp[(E-E_0)/\sigma_E]\cos h2[(-EE_0)^{1/2}/\sigma_E], & \\ E<0, & \quad (7.13b) \end{cases}$$

(7.13a) being a direct consequence of the analyticity of the integrand in (7.12) on the right half-plane of ν. The probability density function $p(E)$ of the log irradiance is nonnegative; furthermore, it satisfies the normalization property

$$\int_{-\infty}^{0} dE\, p(E) = 1. \quad (7.14)$$

On the beam axis ($x=0$ or, equivalently, $E_0=0$), (7.13) reduces to the simpler form

$$p(E) = \begin{cases} 0, & E>0, \quad (7.15a) \\ (-\pi E\sigma_E)^{-1/2}\exp(E/\sigma_E), & E<0. \quad (7.15b) \end{cases}$$

Having established an analytical expression for $p(E)$, various moments of the log irradiance can be found by direct integration. For example,

$$M_1 \equiv E\{E\} = \int_{-\infty}^{0} dE\, E\, p(E) = -(\tfrac{1}{2}\sigma_E + E_0) \quad (7.16)$$

and

$$M_2 \equiv E\{(E-E\{E\})^2\}$$
$$= \int_{-\infty}^{0} dE\,(E-E\{E\})^2 p(E) = \tfrac{1}{2}\sigma_E^2 + 2E_0\sigma_E \quad (7.17)$$

for the general case, i.e., $x\neq 0$. Higher-order moments of the log irradiance can be computed in the same manner.

Furutsu and Furuhama (cf. Ref. 38) have suggested an alternative method for calculating log-irradiance moments. Their technique can be briefly outlined as follows. The nth moment of E is given by

$$E\{E^n\} = \int_{\infty}^{0} dE\, E^n p(E) = -n/(2\pi i)^{-1}\int_{-i\infty-\epsilon}^{i\infty-\epsilon} d\nu\,\nu^{-n-1}f(\nu), \quad (7.18)$$

where

$$f(\nu) = (\nu\sigma_E+1)^{-1/2}\exp[-\nu E_0/(\nu\sigma_E+1)]. \quad (7.19)$$

The last expression, however, is analytic for $\mathrm{Re}(\nu) > -\epsilon$ and tends to zero as $|\nu|\to\infty$. Therefore, the second integral on the right-hand side of (7.18) can be carried out by a clockwise contour integration around the pole $\nu=0$. Moreover, in the vicinity of this pole,

$$f(\nu) = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}E\{E^n\}\nu^n, \quad (7.20)$$

and the log-irradiance moments $E\{E^n\}$, $n=1,2,\ldots$, can be obtained by matching (7.20) with the Taylor series expansion of $f(\nu)$ around $\nu=0$.

D. Saturation phenomena

Consider the expression

$$\sigma_G^{(n)} = [\ln(E\{i^{2n}(x,z;\alpha)\}/[E\{i^n(x,z;\alpha)\}]^2)]^{1/2}. \quad (7.21)$$

where n is a positive integer. Using a result obtained earlier in this section [cf. Eq. (7.8)], as well as the notation introduced in the previous subsection, we may write in the place of (7.21)

$$\sigma_G^{(n)} = [\ln((1+n\sigma_E)(1+2n\sigma_E)^{-1/2}$$
$$\times\exp\{[2n^2E_0\sigma_E/(1+2n\sigma_E)(1+n\sigma_E)]\})]^{1/2}. \quad (7.22)$$

For the special cases $n=1$ and $n=2$, we have, respectively,

$$\sigma_G^{(1)} = (\ln\{(1+\sigma_E)(1+2\sigma_E)^{-1/2}$$
$$\times\exp[2E_0\sigma_E/(1+2\sigma_E)(1+\sigma_E)]\})^{1/2} \quad (7.23)$$

and

$$\sigma_G^{(2)} = (\ln\{(1+2\sigma_E)(1+4\sigma_E)^{-1/2}$$
$$\times\exp[8E_0\sigma_E/(1+4\sigma_E)(1+2\sigma_E)]\})^{1/2}. \quad (7.24)$$

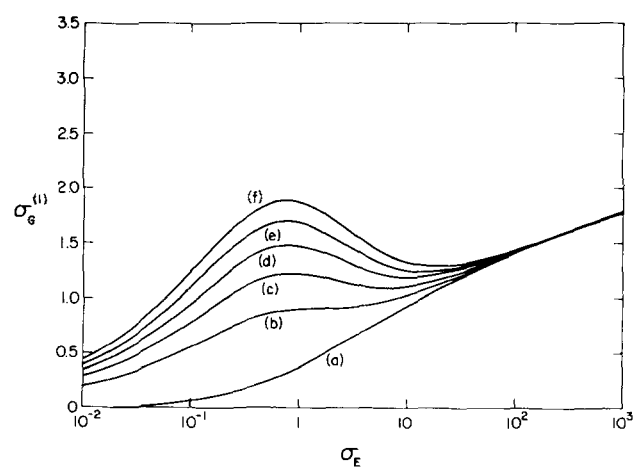

FIG. 9. $\sigma_G^{(1)}$ as a function of σ_E, with E_0 as a parameter. (a) $E_0=0$; (b) $E_0=2$; (c) $E_0=4$; (d) $E_0=6$; (e) $E_0=8$; (f) $E_0=10$.

The quantity $\sigma_G^{(1)}$ given in (7.23)—the square of which would be the variance of the log irradiance provided that the probability density function $p(E)$ were assumed to be log-normal—is plotted in Fig. 9 against σ_E for various values of the dimensionless parameter E_0. It is clear from this graph that $\sigma_G^{(1)}$ saturates for values of σ_E close to 0.8.

Saturation phenomena associated with the scintillation of waves propagating in turbulent media have been known experimentally. Various theoretical predictions (based for the most part on numerical solutions of the equation for the second moment of irradiance) have, also, been made (cf., e.g., Refs. 39 and 40). Theoretical results very similar to those reported in this paper have been published by Furutsu and Furuhama (cf. Ref. 38) for the special case of a beam propagating in a deterministically flat (homogeneous) medium, with additively superimposed random fluctuations. The latter are characterized by a simplified (quadratic) Kolmogorov spectrum.

In contradistinction to $\sigma_G^{(1)}$, the variance of log irradiance M_2 [cf. Eq. (7.17)] does not exhibit any saturation. This quantity is shown graphically in Fig. 10. An explanation for this behavior of M_2 has been provided by Furutsu and Furuhama (cf. Ref. 38; also, remarks made in the previous paragraph). The variance of log irradiance M_2 does not saturate since it contains many higher-order moments of the irradiance $E\{i^\nu(x,z;\alpha)\}$, and the higher the order ν is, the earlier the saturation starts. This situation is partially depicted in Fig. 11, where $\sigma_G^{(2)}$ [cf. Eq. (7.24)] is plotted versus σ_E for various values of the parameter E_0. A direct comparison of this graph with the analogous one for $\sigma_G^{(1)}$ (cf. Fig. 9) shows that the range of values of σ_E for which $\sigma_G^{(2)}$ saturates is approximately centered around 0.4, Qualitatively, one would expect that this "shifting to the left" of the values of σ_E at saturation would continue as the superscript index in σ_G assumes larger and larger values, i.e., $\sigma_G^{(3)}, \sigma_G^{(4)}$, etc.

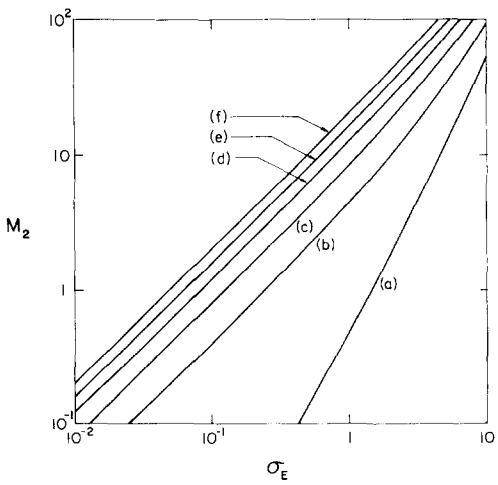

FIG. 10. Variance of the log irradiance. (a) $E_0=0$; (b) $E_0=2$; (c) $E_0=4$; (d) $E_0=6$; (e) $E_0=8$; (f) $E_0=10$.

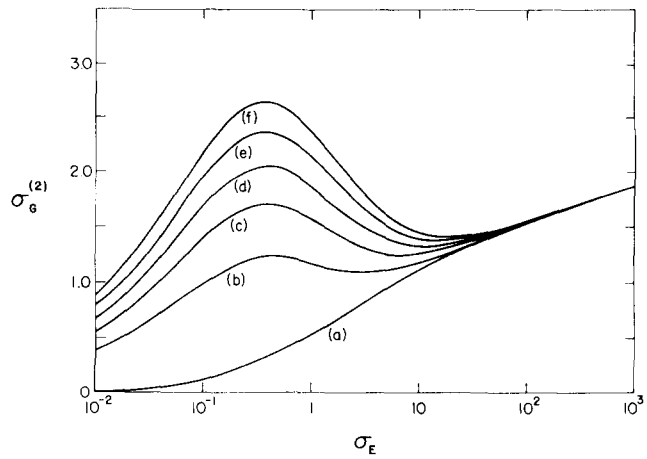

FIG. 11. $\sigma_G^{(2)}$ as a function of σ_E, with E_0 as a parameter. (a) $E_0=0$; (b) $E_0=2$; (c) $E_0=4$; (d) $E_0=6$; (e) $E_0=8$; (f) $E_0=10$.

8. CONCLUDING REMARKS

The statistical technique expounded in this paper is based on the fundamental ansatz introduced in Sec. 3. This ansatz constitutes essentially an embedding process: Through the transformations (3.1) and (3.2), the stochastic parabolic equation (1.1) is brought into an one-to-one correspondence with the parabolic equation (3.4) characterizing the unperturbed focusing medium, together with a set of stochastic nonlinear ordinary differential equations [cf. Eqs. (3.5) and (3.6)] which account for the statistical fluctuations in the medium. The basic statistical analysis of the original stochastic partial differential equation is thus simplified significantly since it can now be performed at the level of a set of stochastic ordinary differential equations the mathematical theory of which is already highly developed (cf., e.g., Refs. 8—10).

Conceptually, we feel that the proposed statistical technique, although distinct, is closely related to recently formulated methods based on functional path integration (cf. Refs. 14—16). Similarly to the functional path integration methods, our technique has the distinct advantage that it works on a *global* rather than a *local* level making, thus, easier the algorithmic derivation of asymptotic solutions to higher-order statistical moments.

There seems to exist another important connection between our statistical approach and the path integral technique: The latter can be used to derive systematically *ansätze* (analogous to the one postulated in Sec. 3 of the paper) which can account for more realistic randomly perturbed channels. We are presently investigating along these lines the problem of beam propagation in a focusing medium whose unperturbed frequency is randomly modulated (cf., also, Ref. 11). Proceeding along the same vein, we also hope to make some progress with the more difficult problem of beam propagation in a medium whose parabolically graded deterministic profile is additively perturbed by x- and z-dependent random fluctuations.

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Some results on automorphisms of affine algebraic groups

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We study the group of automorphisms Aut(G) of a given group G from the groups of automorphisms (supposed known) of some of its subgroups; basic results are applied to topological groups and widely developed inside the Borel–Chevalley theory of linear groups; affine algebraic complete groups are studied in detail.

INTRODUCTION

Our purpose in this paper is to improve and to extend to topological groups the basic results about groups of automorphisms obtained in the study of extensions of the connected Poincaré group.[10] In mathematical physics, the construction of a symmetry group for a given physical system is often formulated in terms of coupling two groups; to solve this problem, mathematical tools are supplied by extension theory or by unification theory. In this paper, we are essentially concerned with extension theory of groups and, more precisely, with splitting extensions also called semidirect products; that because this structure arises in many important cases, e.g., in physic, the symmetry group of a free particle in nonrelativistic, Schrödinger-quantum mechanics, the Poincaré group, are semidirect products; it is a well-known fact that many space groups are splitting extensions of crystallographic point group by a lattice group; these latter as the Lorentz group are linear groups; this is, among other, the reason why the Borel–Chevalley theory of linear groups is the framework of this work. The first part of this paper is devoted to the study of Aut(G), the group of automorphisms of a group G, when $G=K\times_\theta H$ is a semidirect product; the most interesting case happens when the normal subgroup K is characteristic; the following sections concern the automorphisms of topological groups, particularly affine algebraic groups and their completude.

I. THE AUTOMORPHISMS OF A SEMIDIRECT PRODUCT

Let G be a group; throughout this paper Aut(G) [resp. Int(G)] denotes the group of all automorphisms (resp. the group of inner automorphisms) of G. If $x\in G$, F_x is the inner automorphism $F_x(g)=xgx^{-1}$, for every $g\in G$.

A. The case of abstract groups

Let $G=K\times_\theta H$ be the semidirect product of the abstract groups K and H, where θ is the homomorphism from H into Aut(K) defining G. For every $\Gamma\in H$, put $\theta(\Gamma)=\Gamma^\sim$, then the product of two elements (a,Γ), (b,Λ) of G is $(a,\Gamma)(b,\Lambda)=(a\cdot\Gamma^\sim(b),\Gamma\Lambda)$. The unit e (or 1) of G is $e=(1,1)$ where 1 is the unit element of K (resp. H); the inverse of $(a,\Gamma)\in G$ is $(a,\Gamma)^{-1}=((\tilde{\Gamma}^{-1}(a))^{-1},\Gamma^{-1})$, then K is a normal subgroup of G and we have the splitting exact sequence

$1\to K\to G\to H\to 1$, K (resp. H) will be identified with the subgroup $K\times\{1\}$ (resp. $\{1\}\times H$) of G.

B. The automorphisms of $G=K\times_\theta H$

Let $F\in\mathrm{Aut}(G)$, then $\forall a\in K$, $\exists!(b,\Lambda)\in G, H(a,1)=(b,\Lambda)$; putting $b=f(a)$ and $\Lambda=\alpha(a)$, we define the maps $f: K\to K$ and $\alpha: K\to H$; on the other hand, $\forall\Gamma\in H$, $\exists!(C,\Delta)\in G$, $F(1,\Gamma)=(C,\Delta)$; writing as above $C=\varphi(\Gamma)$ and $\Delta=\Phi(\Gamma)$, we define two other maps $\varphi: H\to K$ and $\Phi: H\to H$.

(a) *Properties and relations*

$\forall F\in\mathrm{Aut}(G)$, $\forall a,b\in K$, $(ab,1)=(a,1)(b,1)$; then $F(ab,1)=F((a,1)(b,1))$. Whence $(f(ab),\alpha(ab))=(f(a)\alpha(a)^\sim(f(b)),\alpha(a),\alpha(b))$ and, by identification, we get

$$f(ab)=f(a)\alpha(a)^\sim(f(b)),\ \forall a,b\in K, \tag{1}$$

$$\alpha(ab)=\alpha(a)\alpha(b),\ \forall a,b\in K; \tag{2}$$

it follows from (2) that α is a groups morphism. On the other hand, we have $\forall F\in\mathrm{Aut}(G)$, $\forall\Gamma,\Lambda\in H$, $(1,\Gamma\Lambda)=(1,\Gamma)(1,\Lambda)$; then $F(1,\Gamma\Lambda)=F((1,\Gamma)(1,\Lambda))$; whence $(\varphi(\Gamma\Lambda),\Phi(\Gamma\Lambda))=(\varphi(\Gamma)\Phi(\Gamma)^\sim(\varphi(\Lambda)),\Phi(\Gamma)\Phi(\Lambda))$; from this, we deduce by identification

$$\varphi(\Gamma\Lambda)=\varphi(\Gamma)\Phi(\Gamma)^\sim(\varphi(\Lambda)),\quad\forall\Gamma,\Lambda\in H, \tag{3}$$

$$\Phi(\Gamma\Lambda)=\Phi(\Gamma)\Phi(\Lambda),\quad\forall\Gamma,\Lambda\in H. \tag{4}$$

Then Φ is an endomorphism of the group H; since an element $(a,\Gamma)\in G$ has a unique decomposition of the form $(a,\Gamma)=(a,1)(1,\Gamma)$, we have $F(a,\Gamma)=F((a,1)(1,\Gamma))$, therefore $\forall(a,\Gamma)\in G$ but $(f(a)\alpha(a)^\sim(\varphi(\Gamma)),\alpha(a)\Phi(\Gamma))$; $\forall a\in K,\forall\Gamma\in H$ $(1,\Gamma)(a,1)=(\Gamma(a)^\sim,\Gamma)$, so that $F((1,\Gamma)(a,1))=F(\Gamma^\sim(f(a)),\Gamma)$, so

$$(\varphi(\Gamma)\cdot\Phi(\Gamma)^\sim(f(a)),\Phi(\Gamma)\alpha(a))=(f(\Gamma^\sim(a)\alpha(\Gamma^\sim(a))^\sim(\varphi(\Gamma)),\alpha(\Gamma^\sim(a))\Phi(\Gamma))),$$

then we obtain

$$f(\Gamma^\sim(a)\alpha(\Gamma^\sim(a))^\sim(\varphi(\Gamma)))=\varphi(\Gamma)\Phi(\Gamma)^\sim(f(a)),\quad\forall(a,\Gamma)\in G, \tag{5}$$

$$\alpha(\Gamma^\sim(a))\Phi(\Gamma)=\varphi(\Gamma)\Phi(\Gamma)^\sim(f(a)),\quad\forall(a,\Gamma)\in G. \tag{6}$$

It follows from these formulas that every automorphism of $G=K\times_\theta H$ can be identified with a quadruplet (f,α,φ,Φ) of maps defined as above, verifying the six previous relations and related by the latter.

Proposition 1.1 (Nai-Chao Hsu[1]): Let $G=K\times_\theta H$ be a semidirect product of groups, and (f,α,φ,Φ) a quadruplet of maps such that $f: K\to K$, $\alpha: K\to H$, $\varphi: H\to K$, $\Phi: H\to H$. If

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the six previous relations are satisfied and if: $\forall\ (b,\Lambda)\in G$, $\exists\ (a,\Gamma)\in G$ such that

$$b=f(a)\alpha(a)^{\sim}(\varphi(\Gamma)),\quad \Gamma=\alpha(a)\Phi(\Gamma), \tag{7}$$

then, there is an unique automorphism F of G defined by $F=(f,\alpha,\varphi,\Phi)$. We shall call *fundamental relations* the seven previous relations. We deduce from these results that there is a canonical bijection from $\mathrm{Aut}(G)$ onto the set of quadruplets (f,α,φ,Φ) defined as above and satisfying the fundamental relations; we shall identify an automorphism of G with such a quadruplet when we need it.

(*b*) *The case of a direct product*

When $G=K\times_{\theta}H$ is a direct product, the morphism θ is trivial, then for $\Gamma\in H$, $\Gamma^{\sim}=\mathbf{1}_K$, where $\mathbf{1}_K$ is the identity map of K it follows from (1) and (3) that f and φ are group morphisms; thus, in this case, the elements of a quadruplet $(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$ are all group morphisms; it is convenient to use the Nai-Chao Hsu matrixial notation.

If $F=(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$, put

$$F=\begin{pmatrix} f & \varphi \\ \alpha & \Phi \end{pmatrix},$$

then,

$$\forall(a,\Gamma)\in G,\ F(a,\Gamma)=\begin{pmatrix} f & \varphi \\ \alpha & \Phi \end{pmatrix}\begin{pmatrix} a \\ \Gamma \end{pmatrix}=\begin{pmatrix} f(a) & \varphi(\Gamma) \\ \alpha(a) & \Phi(\Gamma) \end{pmatrix}.$$

Let $F_1=(f_1,\alpha_1,\varphi_1,\Phi_1)$, $F_2=(f_2,\alpha_2,\varphi_2,\Phi_2)\in\mathrm{Aut}(G)$, it is easy to establish that

$$F_2F_1=\begin{pmatrix} f_2 & \varphi_2 \\ \alpha_2 & \Phi_2 \end{pmatrix}\begin{pmatrix} f_1 & \varphi_1 \\ \alpha_1 & \Phi_1 \end{pmatrix}$$

$$=\begin{pmatrix} f_2f_1\otimes\varphi_2\alpha_1 & f_2\varphi_1\otimes\varphi_2\Phi_1 \\ \alpha_2f_1\otimes\Phi_2\alpha_1 & \alpha_2\varphi_1\otimes\Phi_2\Phi_1 \end{pmatrix},$$

where $fg=f\circ g$ is the law composition of maps and $f\otimes g$ is defined by $(f\otimes g)(u)=f(u)g(u)$.

Since $G=K\times H$ is a direct product, $\forall\ (a,\Gamma)\in G$, $(a,\Gamma)=(a,1)(1,\Gamma)=(1,\Gamma)(a,1)$. Hence, if $F=(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$,

$$F(a,\Gamma)=(f(a)\varphi(\Gamma),\alpha(a)\Phi(\Gamma))$$

$$=(\varphi(\Gamma)f(a),\Phi(\Gamma)\alpha(a)),$$

and therefore, $\forall\ (a,\Gamma)\in G\ \varphi(\Gamma)f(a)=f(a)\varphi(\Gamma)$ and $\alpha(a)\Phi(\Gamma)=\Phi(\Gamma)\alpha(a)$; denote by $Z_K(\mathrm{Im}f)$ [resp. $Z_H(\mathrm{Im}\Phi)$] the centralizer of the image of f (resp. of Φ) in K (resp. in H), Then:

Proposition 1.2: Let $G=K\times H$ be a direct product of groups, $F=(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$. Then

$$\mathrm{Im}(\alpha)\subset Z_H(\mathrm{Im}\Phi),\quad \mathrm{Im}(\varphi)\subset Z_K(\mathrm{Im}f).$$

We shall investigate now the automorphism group of $G=K\times_{\theta}H$, where the normal subgroup K is also characteristic (i.e., invariant under all automorphisms of G).

(*c*) *When K is a characteristic subgroup of G*

Let $G=K\times_{\theta}H$ be a semidirect product, with K characteristic. If $F=(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$, $\alpha(a)=1$, $\forall\ a\in K$, and the fundamental relation (1) implies that f is an endomorphism of K.

Proposition 1.3: Let $G=K\times_{\theta}H$ be a semidirect product of groups if the subgroup K is characteristic; then an automorphism F of G can be represented by $F=(f,\varphi,\Phi)$, where $f\in\mathrm{Aut}(K)$, $\Phi\in\mathrm{Aut}(H)$.

Proof: Since K is characteristic, f is the restriction of F to K. Then $f\in\mathrm{Aut}(K)$. Put

$$F=\begin{pmatrix} f & \varphi \\ 0 & \Phi \end{pmatrix},$$

where 0 is the trivial morphism from K into H; then the inverse of F is

$$F^{-1}=\begin{pmatrix} f' & \varphi' \\ 0 & \Phi' \end{pmatrix}.$$

We have

$$\begin{pmatrix} f & \varphi \\ 0 & \Phi \end{pmatrix}\begin{pmatrix} f' & \varphi' \\ 0 & \Phi \end{pmatrix}=\begin{pmatrix} f & \varphi' \\ 0 & \Phi' \end{pmatrix}\begin{pmatrix} f & \varphi \\ 0 & \Phi \end{pmatrix}$$

$$=\begin{pmatrix} \mathbf{1}_K & 0 \\ 0 & \mathbf{1}_H \end{pmatrix}.$$

Whence

$$\begin{pmatrix} ff' & f\varphi'\otimes\varphi\Phi' \\ 0 & \Phi\Phi' \end{pmatrix}=\begin{pmatrix} ff' & f'\varphi\otimes\varphi'\Phi \\ 0 & \Phi\Phi' \end{pmatrix}$$

$$=\begin{pmatrix} \mathbf{1}_K & 0 \\ 0 & \mathbf{1}_H \end{pmatrix}.$$

Therefore $ff'=f'f=\mathbf{1}_K$ and $\Phi\Phi'=\Phi'\Phi=\mathbf{1}_H$, then $\Phi\in\mathrm{Aut}(H)$.

Corollary 1.1: Let $G=K\times H$ be a direct of groups; if K and H are characteristic subgroups of G, then $\mathrm{Aut}(G)=\mathrm{Aut}(K)\times\mathrm{Aut}(H)$ (direct product).

Corrolary 1.2: Let $G=K\times H$ be a direct product of groups; if K is a characteristic subgroup without center, then $\mathrm{Aut}(G)=\mathrm{Aut}(K)\times\mathrm{Aut}(H)$ (direct product).

Proof: Using Corollary 1.1 above, we just have to prove that H is also a characteristic subgroup. If $F=(f,\varphi,\Phi)\in\mathrm{Aut}(G)$, then $\mathrm{Im}f=K$ (from Proposition 1.3), so $Z_K(\mathrm{Im}f)=\{1\}$ and $\mathrm{Im}(\varphi)=\{1\}$ (by Proposition 1.2), hence H is a characteristic subgroup of G.

II. ON THE GROUPS OF AUTOMORPHISMS OF AFFINE ALGEBRAIC GROUPS

The purpose of this section is the study of the group $\mathrm{Aut}(G)$ when G is a given affine algebraic group via the groups of automorphisms (supposed known) of some invariants: maximal tori, Borel subgroups, etc.

A. Notations and recollections

Let K denote a commutative field; an *affine K-algebra* is a K-algebra of finite type and an *affine algebraic K-group* or *affine algebraic group over K* is:

(i) An algebraic affine variety G, i.e., G is the set $\mathrm{Spm}(A)$ of maximal ideals of some reduced affine K-algebra, endowed with the Zariski topology.

(ii) G is a topological group, i.e., G is a group and the map $(x,y)\mapsto xy^{-1}$ is a morphism of affine varieties of $G\times G$ in G.

Throughout this section K denotes a commutative algebraically closed field and all affine algebraic groups are K-groups. Let G be an affine algebraic group, then G is isomorphic to a closed subgroup of $\mathrm{GL}_n(K)$ for some positive integer n; G^0 denotes the connected component (of the unit 1) of G; put G_u (resp. G_s) for the set of unipotent (resp. semisimple) elements of G.

Recall that an abstract group is locally nilpotent (resp. locally solvable) if every subgroup of G of finite type is nilpotent (resp. solvable); an algebraic group is nilpotent (resp. solvable) if and only if the underlying abstract group is nilpotent (resp. solvable) [see Ref. 2, (2.4) or Ref. 3, exposé 3, théoréme 3].

B. The case of nilpotent or locally nilpotent affine algebraic groups

Theorem 2.1: Let G be a nilpotent or locally nilpotent affine algebraic group, then $\mathrm{Aut}(G)=\mathrm{Aut}(G_u)\times\mathrm{Aut}(G_s)$ (direct product).

Proof: It is well known (see Borel[2] or Chevalley[3] for the connected case, and Sprunenko and Tyskevic[4] for the locally nilpotent case) that G_u and G_s are closed subgroups of G and $G=G_u\times G_s$ (direct product); then it suffices to prove that G_u and G_s are characteristic subgroups of G. Assume $F=(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$, then, from Sec. I B(b), f,α,φ,Φ are group morphisms; the conservation theorem for unipotent and semisimple elements implies the triviality of α and φ so then G_u and G_s are characteristic. Hence from Proposition 1.3, Corollary 1.1, $\mathrm{Aut}(G)=\mathrm{Aut}(G_u)\times\mathrm{Aut}(G_s)$.

C. The case of connected locally solvable affine algebraic groups

The structure of connected solvable affine algebraic groups is well known. Moreover, a theorem due to Zassenhaus (see Ref. 5) states that a locally solvable affine algebraic group is solvable. Thus if G is a connected locally solvable affine algebraic group, $G=G_u\times_\theta T$ (semidirect product). Where T is a maximal torus, G_u is a normal subgroup and θ is defined by $\theta(t)=t^\sim=F_t$, $\forall\ t\in T$, i.e., $t^\sim(x)=txt^{-1}$, fo every x of G_u. Assuming that $F=(f,\alpha,\varphi,\Phi)\in\mathrm{Aut}(G)$, it follows from the conservation theorem of unipotent elements that α is trivial, hence G_u is a characteristic subgroup of G and any automorphism F of G can be identified with a triplet $F=(\phi,\varphi,\Phi)$ where $f\in\mathrm{Aut}(G_u)$ and $\Phi\in\mathrm{Aut}(T)$.

Theorem 2.2: If $G=G_u\times_\theta T$ is a connected locally solvable affine algebraic group, then $\mathrm{Aut}(G)=\mathrm{Int}(G)\cdot[\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)]_\theta$, where $\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)$ is a direct product and $[\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)]_\theta$ is the subgroup of $\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)$ whose elements (f,Φ) are related by the fundamental relations.

Proof: Denote by $\mathscr{C}$ the set of maximal tori of G; from the conjugation theorem of maximal tori in G, $\mathrm{Aut}(G)$ acts transitively (on the left) on $\mathscr{C}$; put $S(T)$ for the isotropy group of $T\in\mathscr{C}$, in $\mathrm{Aut}(G)$. Since $\forall\ T\in\mathscr{C}$, $F(T)\in\mathscr{C}$. there is $x\in G$ such that $xF(T)x^{-1}=T$; then $F\in\mathrm{Int}(G)\cdot S(T)$; since $G=G_u\times_\theta T$, $F\in S(T)\Longleftrightarrow F=(f,\Phi)$, where $f\in\mathrm{Aut}(G_u)$, $\Phi\in\mathrm{Aut}(T)$; hence $S(T)\subset[\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)]_\theta$; the converse inclusion is obvious; therefore $S(T)=[\mathrm{Aut}(G_u)\times\mathrm{Aug}(T)]_\theta$ and

$$\mathrm{Aut}(G)=\mathrm{Int}(G)\cdot[\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)]_\theta.$$ QED

Remark: Let $(f,\Phi)\in[\mathrm{Aut}(G_u)\times\mathrm{Aut}(T)]_\theta$. It is easy to check that $\forall\ b\in G_u$, $\forall\ \Gamma\in T$, $f(\Gamma^\sim(b))=\Phi(\Gamma)^\sim(f(b))$. Then $f\circ\Gamma^\sim=\Phi^\sim\circ f$, $\forall\ \Gamma\in T$; hence if $f=\mathbb{1}_{G_u}$ $(\mathbb{1}_{G_u},\Phi)\in\mathrm{Aut}(G)$ if $\Phi(\Gamma)^\sim=\Gamma^\sim$, $\forall\ \Gamma\in T$; i.e., if $\theta\circ\Phi=\theta$. Doing the same with $\Phi=\mathbb{1}_T$ it appears that $(f,\mathbb{1}_T)\in\mathrm{Aut}(G)$ if $f\circ\Gamma^\sim=\Gamma^\sim\cdot f$, $\forall\ \Gamma\in T$; i.e., if $f\in Z(\mathrm{Im}(\theta))$, the centralizer of $\mathrm{Im}(\theta)$ in $\mathrm{Aug}(G_u)$.

D. The general case

Our study of the group $\mathrm{Aut}(G)$, where G is a connected affine algebraic group proceeds via the groups of automorphisms of its Borel subgroups; the key to this method is Steinberg's theorem.

Theorem (Steinberg[6]: 7–2): Every epimorphism of an affine algebraic group G fixes a Borel subgroup (see also Ref. 7, 2.7).

Theorem 2.3: Let G be a connected affine algebraic group, B (resp. T) a Borel subgroup of G (resp. a maximal torus of B), $S(B,T)$ the isotropy group of the pair (B,T) in $\mathrm{Aut}(G)$; then $\mathrm{Aut}(G)=\mathrm{Int}(G)S(B,T)$.

This result was earlier obtained for connected semisimple affine algebraic groups by Chevalley (Ref. 3, Exposé 17). It stays true for any connected affine algebraic group.

Proof: Let $\mathscr{B}$ (resp. $\mathscr{C}$) be the set of Borel subgroups (resp. maximal tori) of G; it follows from the conservation and the conjugation theorems that $\mathrm{Aut}(G)$ acts transitively (on the left) on $\mathscr{B}$ and $\mathscr{C}$; denote by $S(B)$ [resp. $S(T)$] the isotropy group of $B\in\mathscr{B}$ (resp. $T\in\mathscr{C}$) in $\mathrm{Aut}(G)$; then $S(B,T)=S(B)\cap S(T)$; let $F\in\mathrm{Aut}(G)$ since $F(B)\in\mathscr{B}$; there is $x\in G$ such that $xF(B)x^{-1}=B$, then $F_x\circ F\in S(B)$ and $F_x\circ F(T)$ is a maximal torus of B, hence there is $b\in B$ such that $bF_x\circ F(T)b^{-1}=T$, then $F_{bx}\circ F(T)=T$; therefore, $F_{bx}\circ F\in S(B,T)$ and $F\in\mathrm{Int}(G)S(B,T)$; then $\mathrm{Aut}(G)=\mathrm{Int}(G)\cdot S(B,T)$.

Remark: Replace in the proof above $S(B,T)$ by $S(B)$ or $S(T)$, then we have

$$\mathrm{Aut}(G)=\mathrm{Int}(G)\cdot S(B)$$
$$=\mathrm{Int}(G)\cdot S(T).$$

The theorem of conjugation for Borel subgroups (resp. maximal tori) of G shows that the previous relation does not depend on the Borel subgroups [resp. the maximal torus resp. the pair (B,T) considered].

The limitations of our method appear clearly here. We have no criterion of lifting to $\mathrm{Aut}(G)$ an automorphism F of a Borel subgroup, which fixes a maximal torus. Let us nevertheless show how to use this method.

III. APPLICATIONS

In this section, our aim is to illustrate by means of some examples our previous assertions.

A. The automorphisms of the connected Poincaré group

Let $\mathbb{R}$ denotes the field of real numbers and $GL_4(\mathbb{R})$ the general linear group of 4×4 matrices over $\mathbb{R}$. Denote by L the general Lorentz group, i.e.,

$$L=\{\Lambda\in GL_4(\mathbb{R}) \mid {}^t\Lambda J\Lambda = J\},$$

where

$$J=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}$$

is the matrix of the real quadratic form $Q(x)=x_1^2+x_2^2+x_3^2-x_4^2$, $\forall\, x=(x_1,x_2,x_3,x_4)\in\mathbb{R}^4$, and ${}^t\Lambda$ is the transpose of $\Lambda\in GL_4(\mathbb{R})$; let $\Lambda=(\lambda_{ij})\in L$; then

(a) $\det(\Lambda)=\pm 1$,

(b) $\lambda_{14}^2+\lambda_{24}^2+\lambda_{34}^2-\lambda_{44}^2=-1$.

The connected component L^0 of the identity of L is

$$L^0=\{\Lambda:\Lambda\in L \mid \det(\Lambda)=1,\ \lambda_{44}\geqslant 1\}.$$

1. The general Poincaré group (or general inhomogeneous Lorentz group[8])

The general Poincaré group is the semidirect product $P=T\times_\theta L$, where T is the group of translations of the affine Euclidean space $\mathbb{R}^4$ and $\theta: L\to \mathrm{Aut}(T)$ is the canonical injection. The composition law in P is given by $(a,\Gamma)(b,\Lambda)=(a+\Gamma(b),\Gamma\Lambda)$, $\forall\,(a,\Gamma),(b,\Lambda)\in P$ and the identity 1 of P is $1=(0,1)$. P is a real Lie group whose connected component of e is $P^0=T\times_\theta L^0$.

Our pourpose is to determinate the group of automorphisms of the topological group P^0. $\mathrm{Aut}(P)$ and $\mathrm{Aut}(P^0)$ are well known (see for instance Ref. 9); in Ref. 10 some slight modifications were introduced in this proof; the latter is given here with some readjustments.

2. The automorphisms of the topological group P

Let $F\in\mathrm{Aut}(P^0)$, then $F=(f,\alpha,\varphi,\Phi)$; since T is a normal subgroup of P^0, so is $F(T)$ in P^0; then $\alpha(T)=F(T)\cap L^0$ is an Abelian normal subgroup of L^0, but L^0 is simple (see Wigner,[8] p. 167). Therefore, $\alpha(T)=1$ since T is Abelian. It follows from this that T is a characteristic subgroup of P^0, then a characteristic subgroup of P. Hence every automorphism F of P has the form $F=(f,\varphi;\Phi)$.

Properties and relations:

(1) $\mathbb{R}$ *linearity of* f: f is continuous because it is the restriction of F to T; $\forall\, n\in\mathbb{N}$, $\forall\, a\in T$, $f(na)=nf(a)$. Then by a standard argument f is $\mathbb{Q}$ linear, then $\mathbb{R}$ linear ($\mathbb{N}$ and $\mathbb{Q}$ are respectively the monoid of positive integers and the field of rational numbers).

(2) *Characterization of* Φ: $\forall\, a\in T$, $\forall\,\Gamma\in L$, $f\Gamma(f^{-1}(a))=f\Gamma f^{-1}(a)$ we deduce from the fundamental relation (5), $\forall\, a\in T$, $\forall\,\Gamma\in L$, $f\Gamma f^{-1}(a)=\Phi(\Gamma)(a)$; Hence $\forall\,\Gamma\in L$, $\Phi(\Gamma)=f\Gamma f^{-1}$; the automorphism Φ of L is then induced by the inner automorphism F_f of $GL_4(\mathbb{R})$; on the other hand, for every $f\in\mathcal{N}$, there is $F=(f,\Phi)\in\mathrm{Aut}(P)$ defined by $F(a,\Gamma)=(f(a),\Phi(\Gamma))$, $\forall\,(a,\Gamma)\in P$ and $\Phi(\Gamma)=f\Gamma f^{-1}$, $\forall\,\Gamma\in L$.

(3) *Characterization of* φ: Since -1 is central, we have $\Phi(-1)=-1$ and, for the same reason, $(-1)\Gamma=\Gamma(-1)$; the fundamental relation (3) implies that

$$\varphi(-1\cdot\Gamma)=\varphi(-1)+\Phi(-1)(\varphi(\Gamma))$$
$$=\varphi(\Gamma)+\Phi(\Gamma)(\varphi(-1));$$

then we have

$$\varphi(-1)-\varphi(\Gamma)=\varphi(\Gamma)+\Phi(\Gamma)(\varphi(-1));$$

hence

$$2\varphi(\Gamma)=\varphi(-1)-\Phi(\Gamma)(\varphi(-1)),$$

for all $\Gamma\in L$; put $\varphi(-1)=2a_0$ for some $a_0\in T$; then $2\varphi(\Gamma)=2a_0-2\Phi(\Gamma)(a_0)$, whence for all Γ of L $\varphi(\Gamma)=(1-f\Gamma f^{-1})(a_0)$; therefore the automorphism F depends only on f and a_0;

$$\forall\,(a,\Gamma)\in P,\ F(a,\Gamma)=(f(a)+a_0-f\Gamma f^{-1}(a_0),f\Gamma f^{-1})$$
$$=(a_0,1)(f(a),,f\Gamma f^{-1})(a_0,1)^{-1}$$
$$=F_{a_0}\circ(f,F_f)(a,\Gamma);$$

since the center of P is trivial, every $a_0\in T$ determines an unique inner automorphism F_{a_0} of P and every $(a_0,f)\in T\times\mathcal{N}$ determines clearly an unique automorphism of P verifying the relations just above; assume, $(a_0,f),(a_0',f')\in T\times\mathcal{N}$, then the product rule is $(a_0',f')(a_0,f)=(a_0'+f'(a_0),ff')$; therefore, $\mathrm{Aut}(P)=T\times_\theta\mathcal{N}$ is a semidirect product where θ is the canonical injection of $\mathcal{N}$ in $GL_4(\mathbb{R})$.

3. The automorphisms of P^0

The center of P^0 is trivial and every $F\in\mathrm{Aut}(P^0)$ has the form $F=(f,\varphi,\Phi)$ (see Sec. III B 2); then we conclude as above that

(i) f is $\mathbb{R}$ linear and normalizes L^0 in $GL_4(\mathbb{R})$,

(ii) $\Phi(\Gamma)=f\Gamma f^{-1}$, $\forall\,\Gamma\in L^0$,

We can lift F to an automorphism of P by setting $\Phi(-1)=-1$, $\varphi(-1)=2a_0$, $a_0\in T$; then we get $\mathrm{Aut}(P^0)=T\times_\theta N$, where N is the normalizer of L^0 in $GL_4(\mathbb{R})$ and $\theta: N\to GL_4(\mathbb{R})$ is the canonical injection.

We have proved that $\mathrm{Aut}(P)=T\times_t\mathcal{N}$.

4. The structure of $\mathcal{N}$

$\forall\, A\in\mathcal{N}$, $\forall\,\Gamma\in L$, $A\Gamma A^{-1}\in L$, then ${}^t(A\Gamma A^{-1})J(A\Gamma A^{-1})=J$, whence ${}^t\Gamma{}^tAJA\Gamma={}^tAJA$; since ${}^t\Gamma=J\Gamma^{-1}J$, we have ${}^t\Gamma{}^tAJA\Gamma=J\Gamma^{-1}J{}^tAJA\Gamma$, hence $J^{-1}J{}^tAJA\Gamma={}^tAJA$ and therefore $J{}^tAJA\Gamma=\Gamma J{}^tAJA$, $\forall\,\Gamma\in L$, $\forall\, A\in\mathcal{N}$, then $J{}^tAJA\in Z_{GL_4(\mathbb{R})}(L)$: the centralizer of L in $GL_4(\mathbb{R})$. Since the previous representation of L in $GL_4(\mathbb{R})$ is irreducible (see Ref. 11), we conclude that $J{}^tAJA=\lambda I$, where $\lambda\in\mathbb{R}^*$ and I is the unit of $GL_4(\mathbb{R})$, then ${}^tAJA=\lambda J$, $\forall\, A\in\mathcal{N}$. Conversely, if

$A\in GL_4(\mathbb{R})$ is such that $\exists\,\lambda\in\mathbb{R}$, ${}^tAJA=\lambda J$, then, $\forall\,\Gamma\in L$,

$$
\begin{aligned}
{}^t(A\Gamma A^{-1})J(A\Gamma A^{-1}) &= {}^tA^{-1}\Gamma^tAJA\Gamma A^{-1}\\
&= \lambda\,{}^tA^{-1}JA^{-1}\\
&= J.
\end{aligned}
$$

Hence $A\Gamma A^{-1}\in L$ and $A\in\mathcal{N}$, whence $\mathcal{N}=\{A\in GL_4(\mathbb{R})\mid\exists\lambda\in\mathbb{R}, {}^tAJA=\lambda J\}$; denote by ψ the map $\mathcal{N}\to\mathbb{R}^*I$ defined by $\psi(A)=\lambda I$ where λ is such that ${}^tAJA=\lambda J$; clearly ψ is an endomorphism of $\mathcal{N}$ and $\ker(\psi)=L$; then $\mathcal{N}/L\simeq\mathrm{Im}(\psi)$, whence $\mathcal{N}=\mathrm{Im}(\psi)\times L$ (direct product); then $\forall\,A\in\mathcal{N}$, $\exists\,(\lambda,\mu)\in\mathbb{R}^{*2}$ $\exists\,\Gamma\in L$ such that $A=\lambda\Gamma$ and ${}^tAJA=\mu J$, from this we get $\lambda^2\,{}^t\Gamma J\Gamma=L^2J=\mu J\Rightarrow\mu=\lambda^2>0$, therefore $\mathrm{Im}\psi=\{\lambda^2 I\mid\lambda\in\mathbb{R}_+^*\}$, where $\mathbb{R}_+^*$ is a multiplicative group of positive real numbers. Then $\mathcal{N}=\mathbb{R}_+^*L$.

5. *T is a characteristic subgroup of* $\mathbf{T}\times_1\mathcal{N}$

Let $F=(f,\alpha,\varphi,\Phi)$ be an automorphism of $T\times_t\mathcal{N}$; $\alpha(T)$ is a normal Abelian subgroup of $\mathcal{N}$ then central; hence $\forall$ $t\in T$, $\exists\,\lambda\in\mathbb{R}^*$, $\alpha(t)=\lambda I$. It follows from the fundamental relation (6) that

$$\forall\,\Gamma\in\mathcal{N},\ \forall\,t\in T,\ \alpha(\Gamma(t))\Phi(\Gamma)=\Phi(\Gamma)\alpha(t)=\lambda\Phi(\Gamma).$$

Then $\forall\,t\in T$, $\exists\,\lambda\in\mathbb{R}^*$, $\alpha(\Gamma(t))=\lambda I$, $\forall\,\Gamma\in\mathcal{N}$; so $\alpha(-t)=\alpha(t)^{-1}=\lambda I$, hence $\lambda^2=1$ whence $\lambda=\pm1$. Since $2I\in\mathcal{N}$ and $\alpha(a+a)=\alpha(a)^2$, we get $\alpha(2I(a))=\lambda^2=\lambda$; this implies that $\lambda=1$. Then $\forall\,t\in T$, $\alpha(t)=1$, so the morphism α is trivial and therefore T is a characteristic subgroup.

6. *$P=T\times_i L$ is a characteristic subgroup of $T\times_i\mathcal{N}$*

If we work with $T\times_t\mathcal{N}$ in place of $T\times_i L$ in the previous results, we get $\Phi(\Gamma)=f\Gamma f^{-1}$, $\forall\,\Gamma\in\mathcal{N}$. Let $\Gamma\in L$; there is $\lambda\in\mathbb{R}_+^*$ and $\Lambda\in L$ such that $\Phi(\Gamma)=f\Gamma f^{-1}=\lambda\Lambda$; then $\det(f\Gamma f^{-1})=\lambda^4\det(\Lambda)$, so $\lambda^4=1$. Therefore, L is Φ stable, and this implies that the restriction to $T\times_i L$ of an automorphism F of $T\times_t\mathcal{N}$ is an automorphism of $T\times_i L$. Then $P=\mathrm{Int}(P)$ is a characteristic subgroup of $\mathrm{Aut}(P)$, then $\mathrm{Aut}(G)$ is complete by a well known result.

Remark: We have proved in Sec. III 4 that $\mathcal{N}=\mathbb{R}_+^*L$. It is interesting to study $\mathrm{Aut}(\mathcal{N})$. It is easy to show that $\mathbb{R}_+^*$ is a characteristic subgroup of $\mathcal{N}$; then every automorphism F of $\mathcal{N}$ has the form $F=(f,\varphi,\Phi)$, with $f\in\mathrm{Aut}(\mathbb{R}_+^*)$, $\Phi\in\mathrm{Aut}(L)$, and $\varphi\in\mathrm{Hom}(L,\mathbb{R}_+^*)$ is known (see Bourbaki,[12] chap. V, p. 34, $n^0$1), L^0 is a characteristic subgroup of L, and L^0 is isomorphic to $SL_2(\mathbb{C})/(\pm I)$, where $\mathbb{C}$ is the field of complex numbers. The isomorphism is defined from the spinorial representation of $SL_2(\mathbb{C})$ into L^0 (see Naimark[11]). From these we can determine $\mathrm{Aut}(L)$ (which is known) and then $\mathrm{Aut}(\mathcal{N})$.

B. The group $\mathbb{H}$

K denotes an algebraically closed field of characteristic 0. $K^*=K-\{0\}$; the multiplicative group of K putting $GL_2=GL_2(K)$ for the general linear group of 2×2 matrices over K. GL_2 is a connected reductive group. Let $\mathbb{H}$ be the subgroup of GL_2 of matrices

$$h=\begin{pmatrix}a & b\\ 0 & 1\end{pmatrix},\quad a\in K^*,\quad b\in K\ .$$

1. *It is easy to see that $\mathbb{H}$ is a connected solvable subgroup of $\mathbb{GL}_2$*

Our aim is to prove that $\mathbb{H}$ is algebraically complete, i.e., its center is trivial and all its algebraic automorphisms are inner. Let $\mathbb{B}$ be the subgroup of GL_2 of upper triangular matrices and $\mathbb{B}_u=\mathbb{U}_2$ its unipotent subgroup ($\mathbb{U}_2$ consists of upper triangular matrices whose all eigenvalues are equal to 1). $\mathbb{U}_2$ is a closed connected Abelian subgroup of $\mathbb{B}$.

2. *$\mathbb{H}=\mathbb{U}_2\times\mathbb{S}$ (semidirect product, where $\mathbb{S}$ is a one-dimensional torus)*

Indeed, $\forall\,h\in\mathbb{H}$,

$$h=\begin{pmatrix}a & b\\ 0 & 1\end{pmatrix}=\begin{pmatrix}1 & b\\ 0 & 1\end{pmatrix}\begin{pmatrix}a & 0\\ 0 & 1\end{pmatrix}.$$

Put

$$\mathbb{S}=\left\{s=\begin{pmatrix}\alpha & 0\\ 0 & 1\end{pmatrix}\mid\alpha\in K^*\right\},$$

then $\mathbb{S}$ is a subgroup of $\mathbb{H}$ and the map

$$\alpha\mapsto\begin{pmatrix}\alpha & 0\\ 0 & 1\end{pmatrix}$$

from K^* onto $\mathbb{S}$ is an isomorphism of algebraic groups. Then $\mathbb{S}$ is a (one-dimensional) torus. Let $\mathbb{D}_2$ be the diagonal subgroup of GL_2; $\mathbb{D}_2$ is a two-dimensional torus. $\mathbb{S}$ is a subtorus of $\mathbb{D}_2$, and a maximal torus of $\mathbb{H}$ which normalizes $\mathbb{U}_2$; then $\mathbb{H}=\mathbb{U}_2\times\mathbb{S}$ (semidirect product).

3. *$\mathbb{S}$ has no center*

This is easy to verify. $\mathbb{H}$ is connected since $\mathbb{U}_2$ and $\mathbb{S}$ are so.

4. *The algebraic automorphisms of $\mathbb{H}$*

We have $\mathrm{Aut}(\mathbb{H})=\mathrm{Int}(\mathbb{H})\cdot(\mathrm{Aut}(\mathbb{U}_2)\times\mathrm{Aut}(\mathbb{S}))_\Theta$ by Theorem 2.2; every automorphism F of $\mathbb{H}$ has the form $F=F_h(f,\Phi)$, $h\in\mathbb{H}$, $f\in\mathrm{Aut}(\mathbb{U}_2)$, $\Phi\in\mathrm{Aut}(\mathbb{S})$; f and Φ being related by the fundamental relations. The map

$$b\mapsto\begin{pmatrix}1 & b\\ 0 & 1\end{pmatrix}$$

is an algebraic isomorphism of K (identified with the additive algebraic group $\mathbb{G}_a$) onto $\mathbb{U}_2$; since every algebraic automorphism of K has the form $x\mapsto\lambda x$, with $\lambda\in K^*$ (see Ref. 3, exposé 9, Lemma 1, or Ref. 13, chap. V, paragraph 23-D). Any automorphism of $\mathbb{U}_2$ has the form

$$\begin{pmatrix}1 & b\\ 0 & 1\end{pmatrix}=u\mapsto f(u)=\begin{pmatrix}1 & \lambda b\\ 0 & 1\end{pmatrix},\quad\text{with }\lambda\in K^*.$$

On the other hand (from Ref. 3, exposé 11, page 4), the group of algebraic automorphisms of the torus $\mathbb{S}$ can be identified with the group $\mathrm{Aut}(X_*(\mathbb{S}))$ of the discrete multiplicative group $X_*(\mathbb{S})$ of one-parameter subgroup; since $\mathbb{S}$ is one-dimensional, $X_*(\mathbb{S})$ is isomorphic to $\mathbb{Z}$, the ring of rational integers. Then $\mathrm{Aut}(X_*(\mathbb{S}))$ is of order 2, whence $\mathrm{Aut}(\mathbb{S})=\{1_{\mathbb{S}},i\}$, where i is defined by $i(s)=s^{-1}$, for all s of $\mathbb{S}$. It follows from this that $\mathrm{Aut}(\mathbb{U}_2)\times\mathrm{Aut}(\mathbb{S})=\{(f,1_{\mathbb{S}}),(f,i)_f\in\mathrm{Aut}(\mathbb{U}_2)\}$. Since $\mathbb{U}_2$ is

Abelian, if $(f,\Phi)\in(\mathrm{Aut}(\mathbb{U}_2)\times(\mathrm{Aut}(\mathbb{S}))_\theta$, then $f(s^\sim(b))=\Phi(s)^\sim(f(b))$ for all $b\in\mathbb{U}_2$ and $s\in\mathbb{S}$. But $\forall\, b\in\mathbb{U}_2$, $\forall\, s\in\mathbb{S}$, $\theta(s)(b)=s^\sim(b)=sbs^{-1}$, therefore $\forall\, b\in\mathbb{U}_2$, $\forall\, s\in\mathbb{S}$, $f(sbs^{-1})=\Phi(s)f(b)\Phi(s)^{-1}$. Put

$$\sigma=\begin{pmatrix}s & 0\\ 0 & 1\end{pmatrix},\quad \beta=\begin{pmatrix}1 & b\\ 0 & 1\end{pmatrix}.$$

We have

$$f(\sigma\beta\sigma^{-1})=\begin{pmatrix}1 & \lambda sb\\ 0 & 1\end{pmatrix},\quad \lambda\in K^*,\quad \Phi(s)f(B)\Phi(s)^{-1}$$

$$=\begin{pmatrix}1 & \lambda\Phi(s)b\\ 0 & 1\end{pmatrix}.$$

Hence by identification, $\forall\, s\in\mathbb{S}$, $\Phi(s)=s$. Then $\Phi=1_{\mathbb{S}}$ and therefore $(\mathrm{Aut}(\mathbb{U}_2)\times\mathrm{Aut}(\mathbb{S}))_\theta=\{f,1_{\mathbb{S}})/f\in\mathrm{Aut}(\mathbb{U}_2)\}$, whence $\mathrm{Aut}(\mathbb{H})=\mathrm{Int}(\mathbb{H})$ and we have the following.

Proposition 3.1: $\mathbb{H}$ is a connected solvable algebraically complete group.

IV. COMPLETUDE OF AFFINE ALGEBRAIC GROUPS

Throughout this section, the ground field is algebraically closed with characteristic 0.

A. Definitions and generalities

Definition: We call an affine algebraic group algebraically complete if it has the following two properties:

(i) Its center is trivial,

(ii) All its algebraic automorphisms are inner.

Example:

(1°) Let n be a positive integer, and $\mathbf{O}_{2n+1}(K)=\{A\in\mathrm{GL}_{2n+1}/{}^tA_A=I\}$, the orthogonal group of $(2n+1)\times(2n+1)$ matrices over K. The subgroup $\mathrm{SO}_{2n+1}(K)=\{A\in\mathbf{O}_{2n+1}(K)/\det(A)=1\}$ is algebraically complete.

(2°) We have proved in Sec. III that

$$\mathbb{H}=\left\{\begin{pmatrix}a & b\\ 0 & 1\end{pmatrix}/a\in K^*,\ b\in K\right\}$$

is algebraically complete.

A nilpotent affine group cannot be algebraically complete since the penultimate group of its descending central series is a nontrivial central subgroup.

Proposition 4.1: Let $G=K\times H$ be a direct product of affine algebraically complete groups. If K and H are closed in G, then G is algebraically complete if and only if K (or H) is a characteristic subgroup of G.

Proof: Obvious.

Proposition 4.2: Let A be an affine algebraically complete group. If A is a closed normal subgroup of an affine algebraic group G, then

(a) A is a direct factor;

(b) G is connected and algebraically complete if and only if

(i) A and $Z_G(A)$; its centralizer in G, are connected,

(ii) A or $Z_G(A)$ is a characteristic subgroup of G,

(iii) $Z_G(A)$ is algebraically complete.

Proof: (a) It is a well-known fact for abstract groups; the proof is the same for affine groups (see Ref. 14).

(b) Follows from (a) and the proposition above.

Corollary 4.1: Any extension E of an affine algebraically complete group G by an affine group H is trivial [this can be also deduced from the fact that $\mathrm{Aut}(G)/\mathrm{Int}(G)$ is trivial (see Ref. 15, tome 2, chap. XII)].

Corollary 4.2: Let $C=A/B$ be a factor group, where A and B are affine algebraically complete groups such that B is a closed characteristic subgroup of A. Then C is algebraically complete.

Corollary 4.3: Let G be an affine algebraic group. If G^0 the connected component of the identity is algebraically complete, then $G=G^0\times H$ (direct product), where H is a finite group.

This follows from the previous proposition and from the fact that G^0 has finite index in G.

B. Conservative groups

Let G be an affine algebraic K-group, let $A=K[G]$ be the Hopf algebra of regular functions on G, and $\mathrm{Aut}(G)$ the group of algebraic automorphisms of G. $\mathrm{Aut}(G)$ acts on A by $(\alpha,f)\mapsto f\circ\alpha$. Then A is a right $\mathrm{Aut}(G)$ module.

Definition: G is called a conservative group if, for every $f\in A$, the K-subspace of A spanned by $(f\circ\alpha)_{\alpha\in\mathrm{Aut}(G)}$ is finite-dimensional (conservative groups were introduced in Ref. 16 by Hochschild and Mostow; the following facts are credited to them).

Assume G is an affine algebraic K-group. If the center of G^0 is finite [or equivalently if the centralizer $Z_G(G^0)$ of G^0 in G is finite], then

(i) $\mathrm{Aut}(G)$ is an affine algebraic group;

(ii) The map $X:\mathrm{Aut}(G)\times G\to G$, defined by $X(F,g)=F(g)$ is a polynomial map;

(iii) The canonical map $G\to\mathrm{Int}(G)$ that sends $g\in G$ onto F_g is a morphism of affine algebraic groups.

Proposition 4.3: Assume G is an affine algebraic group, A and B are isomorphic subgroups of $\mathrm{Aut}(G)$ such that $\mathrm{Int}(G)\subset A\cap B$, and μ is an isomorphism of A onto B such that $\mu(\mathrm{Int}(G))=\mathrm{Int}(G)$. If the centralizer $Z_G(G^0)$ of G^0 in G is trivial, then the isomorphism μ is induced by an inner automorphism of $\mathrm{Aut}(G)$.

Proof: Denote by $Z(G)$ the center of G; $Z_G(G^0)=\{1\}$ implies $Z(G)=\{1\}$; hence we have the hypothesis of a well known result in the case of abstract groups (see Plotkin,[17] 5-1-3) but in the affine algebraic case, we need the following lemma.

Lemma (Hochschild[18]: Proposition 2.1): Let G be an

affine algebraic group, $\lambda : G \to \mathrm{Int}(G)$ the canonical map that sends f onto F_g; put $G_0 = \lambda(G^0)$.

(i) If $Z_G(G^0)$ is finite, then $Z_{\mathrm{Aut}(G)}(G^0)$ is finite and acts trivially on G^0.

(ii) If $Z_G(G^0)$ is trivial, so is $Z_{\mathrm{Aut}(G)}(G_0)$.

With these assumptions, $\mathrm{Aut}(G)$, $\mathrm{Aut}(G^0)$, and $\mathrm{Aut}(\mathrm{Aut}(G))$ are affine algebraic groups. Denote by ν the restriction of μ to $\mathrm{Int}(G)$; then $\nu \in \mathrm{Aut}((\mathrm{Int}(G))$. Identifying $\mathrm{Int}(G)$ [resp. $\mathrm{Aut}(G)$] with G [resp. $\mathrm{Int}(\mathrm{Aut}(G))$], there is $\varphi \in \mathrm{Aut}(G)$ such that $\nu = F_\varphi | \mathrm{Int}(G)$, restriction of F_φ to $\mathrm{Int}(G)$. Let us show now that $\mu = F_\varphi | A$, $\forall\, \alpha \in A$, $\forall\, \psi \in \mathrm{Int}(G)$, $\alpha\psi\alpha^{-1} \in \mathrm{Int}(G)$, whence $\mu(\alpha\psi\alpha^{-1}) = F_\varphi(\alpha\psi\alpha^{-1})$. Then $\mu(\alpha)\mu(\psi)\mu(\alpha)^{-1} = F_\varphi(\alpha)\varphi\psi\varphi^{-1}F_\varphi(\alpha)^{-1}$. Hence $\mu(\alpha)\varphi\psi\varphi^{-1}\mu(\alpha)^{-1} = F_\varphi(\alpha)\varphi\psi\varphi^{-1}F_\varphi(\alpha)^{-1}$. From this we have $\varphi^{-1}F_\varphi(\alpha)^{-1}\mu(\alpha)\varphi \in Z_{\mathrm{Aut}(G)}(\mathrm{Int}(G)) = (1_G)$. Then $F_\varphi(\alpha) = \mu(\alpha)$, $\forall\, \alpha \subset A$; whence $\mu = F_\varphi | A$ which completes the proof.

Corollary: Assume G is an affine algebraic group. If the centralizer of G^0 in G is trivial and if $\mathrm{Int}(G)$ is a characteristic subgroup of $\mathrm{Aut}(G)$, then $\mathrm{Aut}(G)$ is an affine algebraically complete group.

Proof: The center of $\mathrm{Aut}(G)$ is then trivial. Let $\psi \in \mathrm{Aut}(G)$. Since $\mathrm{Int}(G)$ is a characteristic subgroup of $\mathrm{Aut}(G)$, the restriction of ψ to $\mathrm{Int}(G)$ is an automorphism of $\mathrm{Int}(G)$. Put $A = B = \mathrm{Aut}(G)$, $\mu = \psi$ in the previous proposition. Then $\psi | \mathrm{Int}(G) = F_\varphi$, where $\varphi \in \mathrm{Aut}(G)$, whence $\psi = F_\varphi$. This is the analog for affine algebraic groups of a well-known fact about abstract groups.

C. Affine algebraic groups with an algebraically complete Borel subgroup

Our main aim in this part is to give a characterization of affine algebraic algebraically complete groups.

Theorem 4.1: Let G be a connected affine algebraic group; then G is algebraically complete if and only if G has a algebraically complete Borel subgroup.

Proof:

Lemma 4.1: Assume G is an affine algebraic group. If a Borel subgroup of G is algebraically complete, then every Borel subgroup of G is. This is clear since Borel subgroups are conjugated (for more details, see Ref. 19).

Suppose now that a Borel subgroup (hence all Borel subgroups(of G is algebraically complete; denote by H the holomorph of G, i.e., $H = G \times \mathrm{Aut}(G)$ (semidirect product).

Since G is connected, it has no center. Then the center of H is trivial, moreover, it follows from Ref. 16 that H is an affine algebraic group and $\forall\, F \in \mathrm{Aut}(G)$, $\exists\, h \in H$, $F = f_h|_G$. From a Steinberg's theorem, every automorpohism F of G fixes a Borel subgroup B; hence $F(B) = hBh^{-1} = B$, the restriction of F to B is an automorphism of B. Then there is a unique $b \in B$ such that $h\beta h^{-1} = b\beta b^{-1}$, $\forall\, \beta \in B$. Therefore, $b^{-1}h$ is an element of $Z_H(B)$, the centralizer of B in H. The restriction to G of the inner automorphism $F_{b^{-1}h}$ of H is an automorphism which fixes every element of B. Then $F_{b^{-1}} | {}_G = 1_G$, whence $hgh^{-1} = bgb^{-1}$, $\forall\, g \in G$ and $F_h | G = F_b$. Then G is algebraically complete.

For the converse, we need the following lemmas.

Lemma 4.2: Nisnevic's theorem[20]: The free product of linear groups having a faithful representation of degree n over some field of characteristic $p \geqslant 0$ has a faithful representation of degree $n+1$ over some field of characteristic p.

Lemma 4.3: Higman, B.H. Neumann, H. Neumann's theorem,[21] see also Kurosh,[15] Vol. 2, p. 53): Let G be a (abstract) group, A and B subgroup of G, Φ an isomorphism of A onto B. There is a group H and $h \in H$ such that:

(i) G is a subgroup of H,

(ii) $\Phi(a) = hah^{-1}$, $\forall\, a \in A$.

Assume now that G is connected and algebraically complete. Then we may identify it with a proper subgroup of $\mathrm{GL}_n(K)$ for some positive integer n. Then there is an element u of $\mathrm{GL}_n(K)$ such that u is not in G. We may assume that u is unipotent, if not, the map $p : \mathrm{GL}_n(K) \to \mathrm{GL}_{n+1}(K)$ defined by

$$p(g) = \begin{pmatrix} g & 0 \\ 0 & 1 \end{pmatrix}, \quad \forall\, g \in G,$$

is a closed immersion of $\mathrm{GL}_n(K)$ into $\mathrm{GL}_{n+1}(K)$. Then we can choose a u as desired, since the characteristic of the ground field is 0 the group (u) generated by u is infinite. Consider now the free product $M = G^*(u)$; G has clearly nontrivial unipotent elements. Let $\omega \in G_u$, with $\omega \neq 1$, and put $v^{-1} = \omega u$; then $v \in M$ and has infinite order. Put $L = G^*(v)$, $U = G^* u^{-1} B u$, and $V = G^* v B v^{-1}$, where B is a Borel subgroup containing ω. Now let F be an automorphism of B; then, from Ref. 21, there is an isomorphism ψ of U onto V such that $\psi(g) = g$, $\forall\, g \in G$ and $\psi(u^{-1}bu) = vF(b)v^{-1}$, $\forall\, b \in B$. Denote by H the free product of M and L with an amalgamated subgroup, by amalgamating U and V in accordance with the isomorphism ψ; then $u^{-1}b\bar{u} = \bar{V}F(b)\bar{V}^{-1}$, $\forall\, b \in B$, where $\bar{x}$ is the coset of $x \in M^* L$. Hence $\bar{u}^{-1}b\bar{u} = \bar{u}^{-1}\omega^{-1}F(b)\omega\bar{u}$, $\forall\, b \in B$. Therefore, $F(b) = \omega b \omega^{-1}$, $\forall\, b \in B$; then $F = F_\omega$ is an inner automorphism of B. Since G and B has the same center, $Z(B) = \{e\}$ which completes the proof.

Corollary 4.1: Let Γ be an affine algebraic group with an algebraically complete Borel subgroup. If Γ is a closed normal subgroup of an affine algebraic group G, then Γ^0 is a direct factor in G. Moreover, $\Gamma = \Gamma^0 \times S$ (direct product), where S is a finite subgroup.

Proof: This follows from Theorem 4.1, Proposition 4.2 and the fact that the connected component of the identify of algebraic group is a characteristic subgroup.

Corollary 4.2: Let G be an affine algebraic group with an algebraically complete Borel subgroup, then:

(a) $\mathrm{Aut}(G)$ is an affine algebraic group,

(b) $\mathrm{Aut}(G)^0 = \mathrm{Int}(G)^0$ is algebraically complete.

Proof: (a) It follows from Theorem 4 that G^0 is algebraically complete, then by Corollary 4.1, $G = G^0 \times S$ where S is a finite subgroup of G, but S is precisely the centralizer of G^0 in G. Then G is a conservative group and $\mathrm{Aut}(G)$ is an affine algebraic group. (Note that, since the characteristic of the ground field is zero, S has only semisimple elements.)

(b) Since G^0 is a characteristic algebraically complete subgroup, we have $\mathrm{Aut}(G)=\mathrm{Aut}(G^0)\times\mathrm{Aut}(S)$ (direct product, see Sec. I, Proposition 1.3 and Corollary 1.2), whence $\mathrm{Aut}(G)=\mathrm{Int}(G)^0\times\mathrm{Aut}(S)$; the map $\chi: G\to\mathrm{Aut}(G)$, defined by $\chi(g)=F_g$, $\forall\, g\in G$, is the morphism of affine algebraic groups, then $\mathrm{Int}(G^0)=\mathrm{Int}(G)^0$ and $\mathrm{Aug}(G)=\mathrm{Int}(G)^0\times\mathrm{Aut}(S)$. Since S is finite, so is $\mathrm{Aut}(S)$; then $\mathrm{Aut}(G)^0=\mathrm{Int}(G)^0$, but $\mathrm{Int}(G)^0=\mathrm{Int}(G^0)$ and $\mathrm{Int}(G^0)$ is isomorphic to G^0 (from Ref. 19), which is algebraically complete.

D. Examples

1. The group $\mathbf{O_{2n+1}(K)}$

Let $n>0$ be an integer and $\mathrm{O}_{2n+1}(K)=\{A\in\mathrm{GL}_{2n+1}(K)\mid t_{AA}=I\}$. $\mathrm{SO}_{2n+1}(K)=\{A\in O_{2n+1}(K)\mid \det(A)=1\}$ is a connected normal subgroup of $\mathrm{O}_{2n+1}(K)$; it has index two in $\mathrm{O}_{2n+1}(K)$ and is algebraically complete. Then $\mathrm{O}_{2n+1}(K)=\mathrm{SO}_{2n+1}(K)Z$, where Z is the centralizer of $\mathrm{SO}_{2n+1}(K)$ in $\mathrm{O}_{2n+1}(K)$. Z is then a subgroup of order two which coincides with the center of $\mathrm{O}_{2n+1}(K)$. Put $Z=\{-I,I\}=Z_2$; we have $\mathrm{O}_{2n+1}(K)=\mathrm{SO}_{2n+1}(K)\times Z_2$ (direct product) (this is known, see for instance Dieudonné[22] or Ref. 23, exposé 5).

2. Two extensions of the group $\mathbb{H}$

(1°) It has been proved in Sec. III that the linear group

$$\mathbb{H}=\left\{\begin{pmatrix}a & b\\ 0 & 1\end{pmatrix}\middle|\, a\in K^*,\ b\in K\right\}$$

is connected, solvable, and algebraically complete. Put

$$\mathbb{U}_2=\left\{\begin{pmatrix}0 & a\\ 0 & 1\end{pmatrix}\middle|\, a\in K\right\},\quad \mathbb{D}_2=\left\{\begin{pmatrix}a & 0\\ 0 & b\end{pmatrix}\middle|\, a,b\in K^*\right\},$$

then $\mathbb{B}=\mathbb{U}_2\times\mathbb{D}_2$ (semidirect product) is a Borel subgroup of $\mathrm{GL}_2(K)$. It is easy to prove that $\mathbb{H}$ is a proper normal subgroup of $\mathbb{B}$, hence $\mathbb{H}$ is a direct factor. Then $\mathbb{B}=\mathbb{H}\times Z_{\mathbb{B}}(\mathbb{H})$, but $Z(\mathbb{B})=Z(Z_{\mathbb{B}}(\mathbb{H}))$ and, since $\mathrm{GL}_2(K)$ is connected, Z (cf29B)$Z(\mathrm{GL}_2(K))=\{\lambda\in I,\lambda\in K^*\}=Z$ is a torus of dimension one. Then $Z_{\mathbb{B}}(\mathbb{H})=Z$ for dimension reasons, whence $\mathbb{B}=\mathbb{H}\times Z$.

(2°) Denote by SL_2 the special linear group of 2×2 matrices over K; put $\Gamma=Z_{\mathrm{SL}_2}(\mathbb{U}_2)$. Γ consists of elements of the form

$$x=\begin{pmatrix}1 & \beta\\ 0 & 1\end{pmatrix}\quad\text{or}\quad x=\begin{pmatrix}-1 & \beta\\ 1 & -1\end{pmatrix},\quad\text{with }\beta\in K.$$

Γ is Abelian and contains $\mathbb{U}_2$; it follows from the structure theorem of nilpotent groups that $\Gamma=\Gamma_u\times\Gamma_s$, where Γ_u (resp. Γ_s) is the unipotent subgroup (resp. the subgroup of semisimple elements) of Γ. Then $\Gamma=\mathbb{U}_2\times\Gamma_s=\{-I,I\}=Z_2$, whence $\Gamma=\mathbb{U}_2\times Z_2$; put

$$S=\left\{\begin{pmatrix}a & 0\\ 0 & 1\end{pmatrix}\middle|\ a\in K^*\right\}.$$

S normalizes Γ in $\mathbb{H}$ and $S\cap\Gamma=\{1\}$. Consider the semidirect product $M=\Gamma\times S=\mathbb{H}$; then $M^0=\Gamma^0\times S$; but $\Gamma^0=\mathbb{U}_2$, whence $M^0=\mathbb{U}_2\times S=\mathbb{H}$. Therefore, $M=\mathbb{H}\times Z_2$ (direct product) and $\mathbb{H}$ is an algebraically complete Borel subgroup of M.

V. ALGEBRAICALLY COMPLETE SEMISIMPLE AFFINE ALGEBRAIC GROUPS

A. Generalities

Proposition 5.1: Let G denote a connected affine algebraically complete group.

(1°) The following properties are equivalent:

(i) G is semisimple,

(ii) G is reductive.

(2°) If G is semisimple, then:

(a) G is an "adjoint" group (i.e., isomorphic to its adjoint $\bar{G}$),

(b) The central universal recovering of G is semisimple (see Ref. 24 for these definitions and examples).

Let G be an affine algebraic group; according to Steinberg,[6] an automorphism F of G is called *semisimple* if there is a algebraic group H containing G and $h\in H_s$ such that $F=F_h\mid G$; F is called *quasisemisimple* if its fixes a Borel subgroup (of G) and a maximal torus thereof.

Proposition 5.2: Let G be an affine algebraically complete group; an automorphism F of G is semisimple if and only if there is $x\in G_s$ such that $F=F_x$.

Proof: Assume $F\in\mathrm{Aut}(G)$ is semisimple. Then there is an algebraic group H containing G and $h\in H_s$ such that $F=F_h\mid G$. Since G is algebraically complete, there is an unique $x\in G$ such that $F=F_x$. But $hGh^{-1}=G$ implies that $h\in N_H(G)$: The normalizer of G in H. Now $N_H(G)=G\times Z$ (direct product), where Z is the centralizer of G in $N_H(G)$, but Z is precisely the centralizer of G in H. Then $h=\gamma\zeta$, where $\gamma\in G$, $\zeta\in Z$ commute. Since h is semisimple, so is γ and ζ; but $\forall\, g\in G$, $hgh^{-1}=xgx^{-1}$, whence $x^{-1}h\in Z$ and $x^{-1}\gamma\in Z$; then $x^{-1}\gamma\in Z\cap G=(1)$ implies $x=\gamma$ is semisimple; the converse is obvious.

Corollary: If G is connected and $\gamma\in$G as above, then γ is an element of a maximal torus T of some Borel subgroup B. Then the isomorphism $F=F_\gamma$ fixes B and T (i.e., F is a quass: quasisemisimple).

Theorem (Steinberg[6]): Every semisimple automorphism is quasisemisimple.

Proposition 5.3: Let G be a connected affine algebraically complete semisimple group; then every quasisemisimple automorphism of G is semisimple.

The proof is based on the fact that, if G is semisimple and connected, then for a Borel subgroup B of G containing a maximal torus T, we have $B\cap N_G(T)=T$.

B. Connected affine algebraically complete groups of semisimple rank 1

Let $\mathrm{GL}_{n+1}(K)$ [resp. $\mathrm{PGL}_{n+1}(K)$] be the general linear (resp. general projective linear) group over K, for some positive integer n. Put $\mathrm{GL}_{n+1}(K)=\mathrm{GL}_{n+1}$ and $\mathrm{PGL}_{n+1}(K)=\mathrm{PGL}_{n+1}$. GL_{n+1} is a connected reductive group of dimension $(n+1)^2$, the center $Z_{n+1}=\{\lambda\mid\lambda\in K^*\}$. Then Z_{n+1} is a

one-dimensional torus. A maximal torus of $\mathbb{GL}_{n+1}$ is a conjugate of D_{n+1}: the group of diagonal matrices of $\mathbb{GL}_{n+1}$ is connected and its dimension is n+1. We have $\mathbb{PGL}_{n+1}=\mathbb{GL}_{n+1}/Z_{n+1}$, then $\mathbb{PGL}_{n+1}$ is connected and its dimension is $(n+1)^2-=n(n+2)$. For $n=1$, put $Z_2=Z$; then $\mathbb{PGL}_2=\mathbb{GL}_2/Z$. We shall prove that $\mathbb{PGL}_2$ is algebraically complete.

Let $j:\mathbb{GL}_2\to\mathbb{PGL}_2$ denote the canonical surjection of $\mathbb{GL}_2$ onto $\mathbb{PGL}_2$.

$$\mathbb{H}=\left\{\begin{pmatrix}a & b\\ 0 & 1\end{pmatrix}\middle|\ a\in K^*,\quad b\in K\right\}$$

is a connected solvable algebraically complete subgroup of $\mathbb{GL}_2$. Then the restriction of j to $\mathbb{H}$ is injective. We can identify $\mathbb{H}$ with its image in $\mathbb{PGL}_2$. A Borel subgroup of $\mathbb{GL}_2$ is a conjugate of $B=\mathbb{U}_2\times\mathbb{D}_2$ and then has dimension 3. Therefore, a Borel subgroup of $\mathbb{PGL}_2$ has dimension 2, hence $\mathbb{H}$ is a Borel subgroup of $\mathbb{PGL}_2$. From Theorem 4, we conclude that $\mathbb{PGL}_2$ is algebraically complete.

1. Semisimple groups of rank 1

Recall that the rank of an affine algebraic group G is the dimension of a Cartan subgroup of G. If G is semisimple, then its rank is the dimension of a maximal torus.

Theorem 5.1: Let G denote a connected affine algebraic group of semisimple rank 1; if G is algebraically complete, then G is isomorphic to $\mathbb{PGL}_2$.

Proof: It is a well-known fact that under these assumptions, there is a surjection $\varphi: G\to\mathbb{PGL}_2$ with kernel I: the intersection of all Borel subgroups of G and $I=Z(G)$, the center of G (see Ref. 2, p. 310); since $Z(G)$ is trivial. φ is bijective so then there is an isomorphism from G onto $\mathbb{PGL}_2$.

Proposition 5.4: Let G be a connected reductive affine algebraically complete group of rank 1. If $F\in\mathrm{Aut}(G)$ fixes a maximal torus, then F is semisimple.

Proof: If $F=F_x\in\mathrm{Aut}(G)$ fixes a maximal torus T, denote by $\mathscr{B}^T$ the set of Borel subgroups containing T. Then $\mathscr{B}^T=\{B,B'\}$, and $B\cap B'=T$. Since $F_x(T)=T$, we have $xBx^{-1}\cap xB'x^{-1}=T$; then F induced a bijection from $\mathscr{B}^T$ onto itself whence either $xBx^{-1}=B$ and $xB'x^{-1}=B'$ or $xBx^{-1}=B'$ and $xB'x^{-1}=B$.

(a) If $xBx^{-1}=B$, then F_x is quasisemisimple hence semisimple (by Proposition 5.3);

(b)If $xBx^{-1}=B'$, we have $xB'x^{-1}=B$, whence $x^2Bx^{-2}=B$, then $x^2\in B\cap N_B(T)=T$; therefore x^2 is semisimple. Let $x=x_ux_s$ be the Jordan decomposition of x ($x_u\in G_u$, $x_s\in G_s$). Then $x^2=x_u^2x_s^2$; since x^2 and x_s^2 are semisimple and commute, we have $x_u^2=1$. Then $x_u=1$ (because the characteristic of the ground field is 0); therefore, x is semisimple and so is F_x.

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The general coupled anharmonic oscillators and the coherent state representation

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We obtain a first order perturbation solution for a system of $2m$, unequal mass, coupled oscillators perturbed by anharmonic terms of homogeneous power $4p$ of the position variables in the coherent state representation.

The problem of anharmonic oscillators is interesting both from theoretical and application aspects. On the theoretical side, efforts are still continuing to find convergent and regular solutions.[1-5] Many problems of physics involving basic interactions of nature, on the other hand, often lead to the differential equations for the anharmonic oscillator systems.

It has been observed recently[2-4] that the use of the coherent state representation in this problem can cure some of the bad features of the conventional perturbation approach. The advantage being that the viscious secular terms are absent in the solution. Also the coherent states are the minimum uncertainty states for which the expectation value of the position operator possesses the classical time dependence in the limit $\hbar \to 0$.

In the present paper we derive a perturbative solution to a quantum mechanical system of $2m$, unequal mass, coupled harmonic oscillators perturbed by anharmonic terms of homogeneous power $4p (p = 1,2,\cdots)$ of the position variables in the coherent state representation. A simple case of this problem has been analyzed quantum mechanically by Banks, Bender, and Wu, and Banks and Bender and in coherent state representation by Dutt and Lakshmanan.[3] The classical solution is achieved in the appropriate limit ($\hbar \to 0$).

Recently, Hioe[6] has considered another aspect of the problem of coupled anharmonic oscillators, namely, the properties of energy levels. He has shown, on the basis of exact numerical analysis in conjunction with Titchmarsh's analytical formulas, that the number of states $N(E)$ with energy less than E for a system of coupled anharmonic oscillators, with anharmonic terms being represented by a polynomial of homogeneous even degree of the coordinates, can be approximated by different polynomials in energy E in harmonic and anharmonic regimes.

The coherent states,[7] which are normalized but overcomplete, for a system of $2m$ harmonic oscillators, are obtained by a superposition of the "$n_i (i = 1,2,\cdots,2m)$ quanta" states $|n_1, n_2, \cdots, n_{2m}\rangle$, corresponding to the energy eigenvalue $\sum_{i=1}^{2m} \hbar\omega_i (n_i + \frac{1}{2})$ as

$$|\alpha_1, \alpha_2, \cdots, \alpha_{2m}\rangle = \exp\left(-\sum_{i=1}^{2m} |\alpha_i|^2/2\right) \times \sum_{\substack{n_1, n_2, \cdots, \\ n_{2m}=0}}^{\infty} \prod_{i=1}^{2m} \frac{\alpha_i^{n_i}}{\sqrt{n_i!}} |n_1, n_2, \cdots, n_{2m}\rangle, \tag{1}$$

where $\alpha_i (i = 1,2,\cdots,2m)$ are $2m$ complex numbers. These coherent states are the eigenstates of the annihilation operator $a_i (i = 1,2,\cdots,2m)$ with the eigenvalue $\alpha_i (i = 1,2,\cdots,2m)$, i.e.,

$$a_i |\alpha_1, \alpha_2, \cdots, \alpha_{2m}\rangle = \alpha_i |\alpha_1, \alpha_2, \cdots, \alpha_{2m}\rangle. \tag{2}$$

One can also verify that

$$\langle \alpha_1, \alpha_2, \cdots, \alpha_{2m} | x_i | \alpha_1, \alpha_2, \cdots, \alpha_{2m}\rangle = 2\lambda_i \sqrt{\frac{\hbar}{2m_i\omega_i}} \cos\omega_i t, \tag{3}$$

where $\alpha_i = -i'\lambda_i \exp(i'\omega_i t) (i' = \sqrt{-1}, i = 1,2,\cdots,2m)$. The classical limit is achieved when $\hbar \to 0$, $\lambda_i \to \infty$ with $2\lambda_i \sqrt{\hbar/2m_i\omega_i} \to A_i$, where α_i is the classical amplitude for the ith oscillator.

The Hamiltonian for the system of $2m$ harmonic oscillators, with anharmonic terms being a homogeneous power, $4p$, of the position variables, is given by

$$H = \sum_{i=1}^{2m} \left(\frac{p_i^2}{2m_i} + \tfrac{1}{2} m_i \omega_i^2 x_i^2\right) + \frac{\alpha}{4p} \left\{ \sum_{i=1}^{2m} a_i x_i^{4p} + \tfrac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{2m} \sum_{s=1}^{2p-1} b_{ij}^s x_i^{2(2p-s)} x_j^{2s} \right\}, \tag{4}$$

where $b_{ij}^s = b_{ji}^s$ and $b_{ij}^s = p_{ij}^{2p-s}$ (i.e., we take the coefficients b_{ij}^s to be symmetrical[5]).

The equation of motion corresponding to the ith oscillator is given by

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$$\frac{d^2x_i}{dt^2}+\omega_i^2x_i+\alpha\frac{a_i}{m_i}x_i^{4p-1}+\alpha\sum_{\substack{j=1\\j\neq i}}^{2m}\sum_{s=1}^{2p-1}2s\frac{b_{ij}^s}{4p}x_j^{2(2p-s)}x_i^{2s-1}=0. \tag{5}$$

Following the lines of Ref. 4, it can be shown that the expectation value of x_i in the coherent state $|\alpha_1,\alpha_2,\cdots,\alpha_{2m}\rangle$ satisfies the classical equation of motion[5] in the limit $\hbar\to 0$.

The eigenvalue and the eigenstate of "$n_i (i=1,2,\cdots,2m)$ quanta" in the presence of weak perturbation (α small but $\neq 0$), using conventional perturbation theory relations, can be obtained as

$$E'_{n_1,n_2,n_{2m}}=\sum_{i=1}^{2m}(n_i+1/2)\hbar\omega_i+\frac{\alpha}{4p}\left\{\sum_{i=1}^{2m}a_iL_{2p}^{n_i}+\sum_{\substack{i,j=1\\i\neq j}}^{2m}\tfrac{1}{2}b_{ij}^sL_s^{n_i}L_{2p-s}^{n_j}\right\},$$

where

$$L_a^{n_k}=\left(\frac{\hbar}{2m_k\omega_k}\right)^a\frac{(2a)!}{a!}\sum_{r=0}^{a}\frac{1}{2^r}C_{a-r}^{n_k}C_r^a \qquad \left(C_r^n=\frac{n!}{(n-r)!r!},\quad k=1,2,\cdots,2m\right) \tag{6}$$

and

$$|n_1,n_2,\cdots,n_{2m}\rangle'=|n_1,n_2,\cdots,n_{2m}\rangle-\frac{\alpha}{8p\hbar}\left\{\sum_{i=1}^{2m}\sum_{q=-2p}^{2p}\left(\frac{a_i}{\omega_i q}\right)M_{2p,q}^{n_i}|n_1,n_2,\cdots,n_i+2q,\cdots,n_{2m}\rangle\right.$$
$$\left.+\sum_{\substack{i,j=1\\i\neq j}}^{2m}\sum_{s=1}^{2p-1}\sum_{\substack{q=-s\\\neq 0}}^{s}\sum_{\substack{q'=-(2p-s)\\\neq 0}}^{2p-s}\frac{b_{ij}^s}{2(\omega_iq+\omega_jq')}M_{s,q}^{n_i}M_{2p-s,q'}^{n_j}\right.$$
$$\times|n_1,n_2,\cdots,n_i+2q,\cdots,n_j+2q',\cdots,n_{2m}\rangle,$$

where

$$M_{a,q}^{nk}=\sum_{r=q}^{a}\left(\frac{\hbar}{2m_k\omega_k}\right)^a\frac{(2a)!(-1)^q\sqrt{n_i!(n_i+2q)!}}{2^{a-r}(a-r)!(r+q)!(r-q)!(n_k+q-r)!}\qquad\begin{pmatrix}k=1,2,\cdots,2m\\a=0,1,\cdots\end{pmatrix}. \tag{7}$$

In deriving the relations (6) and (7) we have exploited the identities

$$(a-a^\dagger)^{2p}=\sum_{r=0}^{p}(-1)^r\frac{(2p)!}{(2p-2r)!r!2^r}:\{(a-a^\dagger)^{2p-2r}\}:,$$
$$(a-a^\dagger)^{2p+1}=\sum_{r=0}^{p}(-1)^r\frac{(2p+1)!}{(2p+1-2r)!r!2^r}:\{(a-a^\dagger)^{2p+1-2r}\}:, \tag{8}$$

where p is a positive integer and : : stands for normal ordering. The perturbed coherent state for the $2m$ oscillators system can be written as

$$|\alpha_1,\alpha_2,\cdots,\alpha_{2m}\rangle'=\exp(-\tfrac{1}{2}\sum_{i=1}^{2m}\lambda_i^2)\sum_{\substack{n_1,n_2,\cdots,\\n_{2m}=0}}^{\infty}\prod_{k=1}^{2m}\frac{(-i'\lambda_k)^{n_k}}{\sqrt{n_k!}}\times\left\{\exp\left(\frac{i'}{\hbar}E'_{n_1,n_2,\cdots,n_{2m}}t\right)|n_1,n_2,\cdots,n_{2m}\rangle'\right\}. \tag{9}$$

The perturbative solution to the equation of motion (5), using the relations (6), (7), and (9), can be obtained as

$$x_i(t)={}'\langle\alpha_1,\alpha_2,\cdots,\alpha_{2m}|x_i|\alpha_1,\alpha_2,\cdots,\alpha_{2m}\rangle'$$

$$\lim\hbar\to 0,\ \lambda_i\to\infty$$

$$2\lambda_i\sqrt{\hbar/2m_i\omega_i}\to A_i\ (i=1,2,\cdots,2m)$$

$$=A_i\cos\psi_it+\alpha\frac{a_i}{2^{4p}m_i\omega_i^2}A_i^{4p-1}\left\{-C_{2p}^{4p-1}\cos\psi_it+\sum_{q=1}^{2p-1}\frac{\cos(2q+1)\psi_it}{q(q+1)}\right\}$$
$$+\alpha\sum_{\substack{j=1\\j\neq i}}^{2m}\sum_{s=1}^{2p-1}\sum_{q'=1}^{2p-s}\sum_{a=-1}^{1}\left[\frac{s}{p}\frac{b_{ij}^s}{2^{4p}m_i\omega_i^2}C_{2p-s+q'}^{2(2p-s)}A_i^{2s-1}A_j^{2(2p-s)}\right.$$
$$\left.\times\left\{-\tfrac{1}{2}C_s^{2s-1}\frac{\cos(2aq'\psi_j+\psi_i)t}{1+aq'\omega_j/\omega_i}+\sum_{\substack{q=1\\\neq 0}}^{s-1}\tfrac{1}{2}C_{s+q}^{2s-1}\frac{\cos(2aq'\psi_j+\overline{2q+1}\,\psi_i)t}{(q+aq'\omega_j/\omega_i)(q+1+aq'\omega_j/\omega_i)}\right\}\right], \tag{10}$$

in which the corrected frequency ψ_i, corresponding to the ith oscillator is given by

$$\psi_i = \{E'_{n_1,n_2,\cdots,n_i,\cdots,n_{2m}} - E'_{n_1,n_2,\cdots,n'_i,\cdots,n_{2m}}\}/\hbar(n_i - n'_i)$$

$$\lim n'_i \to n_i, \hbar \to 0, \quad n_k \to \infty;$$

$$n_k \hbar \to \tfrac{1}{2} m_k \omega_k \omega_k A_k^2 \qquad (k = 1,2,\cdots,2m)$$

$$= \omega_i \left\{ 1 + \frac{\alpha}{m_i \omega_i^2} \left(a_i N_{2p}^i + \sum_{\substack{j=1 \\ j \neq i}}^{2m} \sum_{s=1}^{2p-1} \tfrac{1}{2} b_{ij}^s N_s^i N_{2p-s}^j A_j^2 \right) \right\},$$

where

$$N_a^k = \frac{1}{2^{2a}} C_a^{2a} A_k^{2a-2} \qquad \begin{pmatrix} a = 0,1,2,\cdots; \\ k = 1,2,\cdots,2m \end{pmatrix}. \tag{11}$$

The anharmonicity of the coupled harmonic oscillator system is reflected through the interdependence of amplitudes and frequencies as can be easily seen from the relations (10) and (11). The solution (10) does not have any secular term and shows a resonance character, typical of forced oscillators.

The higher order terms in the perturbation series can be obtained following the above procedure. The calculations are, however, more involved. It is hoped that when more terms become available, the general features of the nonlinearities as well as the characteristics of a coupled system will be more clearly revealed.

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A generalization of the spherical harmonic gradient formula

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The familiar gradient formula is generalized by replacing the gradient operator by an arbitrary solid harmonic of the gradient operator. The result is applied to various multipole expansions of angular momentum eigenstates.

1. INTRODUCTION

The solid harmonic $\mathscr{Y}^k_m(\mathbf{r})\equiv r^k Y^k_m(\hat{r})$ is a homogeneous polynomial of degree k in x,y,z with irreducible transformation properties under R_3 (the three-dimensional rotation group). Let $\mathscr{Y}^k_m(\nabla)$ symbolize the same homogeneous polynomial of $\partial/\partial x, \partial/\partial y, \partial/\partial z$. Since the components of ∇ and $\mathbf{r}$ have the same transformation properties under R_3, $\mathscr{Y}^k_m(\nabla)$ will have the same R_3 transformation properties as $\mathscr{Y}^k_m(\mathbf{r})$ or $Y^k_m(\hat{r})$. Thus if we vector-couple $\mathscr{Y}^k_m(\nabla)$ to a function $f(r)Y^l_m(\hat{r})$,

$$[\mathscr{Y}^k(\nabla)f(r)\,Y^l(\hat{r})\,]^L_M \equiv \sum_{m_1,m_2}(k\ l\ m_1\ m_2\mid L\ M)\ \mathscr{Y}^k_{m_1}(\nabla)f(r)\,Y^l_{m_2}(\hat{r}), \tag{1}$$

the result will be a function of $\mathbf{r}$ with the same R_3 transformation properties as $Y^L_M(\hat{r})$. Then the completeness of the $Y^L_M(\hat{r})$ and their orthogonality properties imply that the angular dependence of (1) is given by $Y^L_M(\hat{r})$, so that we can write

$$[\mathscr{Y}^k(\nabla)f(r)Y^l(\hat{r})\,]^L_M = g^L_{kl}(r)\,Y^L_M(\hat{r}), \tag{2}$$

where the radial function $g^L_{kl}(r)$ is independent of M. The main object of this paper is to find an expression for $g^L_{kl}(r)$ in terms of $f(r)$.

The possible values that L can assume in (2) are $k+l, k+l-2,\ldots,|k-l|$. The restriction to even values of $k+l+L$ is associated with the requirement that both sides of (2) have the same transformation properties under inversion, $\mathbf{r}\to-\mathbf{r}$.

If $k=1$, we have

$$\mathscr{Y}^1_m(\nabla)=\begin{cases}\mp\sqrt{\dfrac{3}{8\pi}}\left(\dfrac{\partial}{\partial x}\pm i\dfrac{\partial}{\partial y}\right), & m=\pm1,\\ \sqrt{\dfrac{3}{4\pi}}\dfrac{\partial}{\partial z}, & m=0.\end{cases}$$

In this case, (2) becomes the well-known gradient formula[1]

$$[\mathscr{Y}^1(\nabla)f(r)Y^l(\hat{r})\,]^L_M = \begin{cases}\left(\dfrac{3}{4\pi}\dfrac{l+1}{2l+3}\right)^{1/2}\left(f'(r)-\dfrac{l}{r}f(r)\right) & Y^{l+1}_M(\hat{r}) \quad \text{if } L=l+1,\\ -\left(\dfrac{3}{4\pi}\dfrac{l}{2l-1}\right)^{1/2}\left(f'(r)+\dfrac{l+1}{r}f(r)\right) & Y^{l-1}_M(\hat{r}) \quad \text{if } L=l-1.\end{cases} \tag{3}$$

In this sense, the expression we will obtain for $g^L_{kl}(r)$ in terms of $f(r)$ can be regarded as a generalization of the gradient formula to cases where $k>1$.

Throughout this paper we will use the Condon–Shortley phase convention for the spherical harmonics, so that $Y^l_m(\hat{z})=\delta_{m,0}((2l+1)/4\pi)^{1/2}$.

2. Derivation of the formula for $g^L_{kl}(r)$.

One way to calculate the right-hand side of (2) would be to express $\mathscr{Y}^k_q(\nabla)$ as a suitably vector-coupled product of k factors $\mathscr{Y}^1_{q'}(\nabla)$, and then to use the gradient formula (3) k times. This would lead to an unwieldy expression, involving a $(k-1)$-fold sum of products of $k-1$ Racah recoupling coefficients. A more fruitful approach takes advantage of the explicit form of the solid harmonics $\mathscr{Y}^n_{\pm n}(\mathbf{r})$,

$$\mathscr{Y}^n_{\pm n}(\mathbf{r})=\frac{(-1)^{(n\pm n)/2}}{2^n n!}\left(\frac{(2n+1)!}{4\pi}\right)^{1/2}(x\pm iy)^n. \tag{4}$$

Thus it is relatively simple to apply $\mathscr{Y}^k_k(\nabla)$ to $f(r)\mathscr{Y}^l_{-l}(\hat{r})$,

$$\begin{aligned}&\mathscr{Y}^k_k(\nabla)f(r)Y^l_{-l}(\hat{r})\\ &=\sum_{L=|k-l|}^{k+l}(k\ l\ k\ -l\mid L\ k-l)\\ &\quad\times[\mathscr{Y}^k(\nabla)f(r)Y^l(\hat{r})\,]^L_{k-l}\\ &=\sum_{L=|k-l|}^{k+l}(k\ l\ k\ -l\mid L\ k-l)\\ &\quad\times g^L_{kl}(r)\,Y^L_{k-l}(\hat{r})\\ &=\frac{(-1)^k}{2^{k+l}\,k!\,l!}\left(\frac{(2k+1)!(2l+1)!}{(4\pi)^2}\right)^{1/2}\\ &\quad\times\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)^k f(r)\frac{(x-iy)^l}{r^l}.\end{aligned} \tag{5}$$

To do the differentiations in (5), we use the identity

$$\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)^k\frac{f(r)}{r^l}(x-iy)^l$$

 0022-2488/78/1912-2558$1.00

$$= \sum_{\nu=0}^{k} \frac{2^{k-\nu}\, k!\, l!}{\nu!(k-\nu)!(l-k+\nu)!} (x+iy)^{\nu} (x-iy)^{l+\nu-k} \times \left(\frac{1}{r}\frac{d}{dr}\right)^{\nu} \frac{f(r)}{r^{l}}. \tag{6}$$

This identity is trivially correct for $k=0$ and all l, and induction on k verifies that it is also true for $k>0$ and all l. According to (4),

$$(x+iy)^{\nu}(x-iy)^{l+\nu-k} = (-1)^{\nu} 2^{l+2\nu-k}\, \nu!(l+\nu-k)! \times \left(\frac{(4\pi)^2}{(2\nu+1)!(2l+2\nu-2k+1)!}\right)^{1/2} \times \mathscr{Y}_{\nu}^{\nu}(\mathbf{r})\, \mathscr{Y}_{-l-\nu+k}^{l+\nu-k}(\mathbf{r}), \tag{7}$$

and the product of the two solid harmonics occurring here can be expressed as

$$\begin{aligned} &\mathscr{Y}_{\nu}^{\nu}(\mathbf{r})\, \mathscr{Y}_{-l-\nu+k}^{l+\nu-k}(\hat{r}) \\ &= \sum_{L=|l-k|}^{l+2\nu-k} (\nu\ l+\nu-k\ \nu\ -l-\nu+k | L\ k-l) \times [\mathscr{Y}^{\nu}(\mathbf{r})\, \mathscr{Y}^{l+\nu-k}(\mathbf{r})]_{k-l}^{L} \\ &= \sum_{L=|l-k|}^{l+2\nu-k} (\nu\ l+\nu-k\ \nu\ -l-\nu+k | L\ k-l) \times \left(\frac{(2\nu+1)(2l+2\nu-2k+1)}{4\pi(2L+1)}\right)^{1/2} \times (\nu\ l+\nu-k\ 0\ 0 | L\ 0)\, r^{l+2\nu-k}\, Y_{k-l}^{L}(\hat{r}). \end{aligned} \tag{8}$$

If we combine (5)–(8), we get

$$\begin{aligned} &(k\, l\, k\ -l | L\ k-l) g_{kl}^{L}(r) \\ &= \left(\frac{(2k+1)!(2l+1)!}{4\pi(2L+1)}\right)^{1/2} \sum_{\nu=0}^{k} \times \frac{(-1)^{k+\nu}(l+\nu-k)!}{2^{k-\nu}(k-\nu)!(l-k+\nu)!} \\ &\times \frac{(\nu\, l+\nu-k\ \nu\ -l-\nu+k | L\ k-L)(\nu\ l+\nu-k\ 0\ 0 | L\ 0)}{((2\nu)!(2l+2\nu-2k)!)^{1/2}} \\ &\times r^{l+2\nu-k} \left(\frac{1}{r}\frac{d}{dr}\right)^{\nu} \frac{f(r)}{r^{l}}. \end{aligned} \tag{9}$$

All the vector-coupling coefficients in (9) have relatively simple explicit expressions,[2]

$$(l_1\, l_2\, l_1\ -l_2 | I\, l_1-l_2) = \left(\frac{(2I+1)(2l_1)!(2l_2)!}{(l_1+l_2-I)!(l_1+l_2+I+1)!}\right)^{1/2}, \tag{10a}$$

$$(l_1\, l_2\, 0\, 0 | I\, 0) = \frac{(-1)^{(l_1+l_2-I)/2}\, [(l_1+l_2+I)/2]!}{((l_1+l_2+I+1)!)^{1/2}} \times \frac{[(2I+1)(l_1+l_2-I)!(l_1-l_2+I)!(-l_1+l_2+I)!]^{1/2}}{[(l_1+l_2-I)/2]!\, [(l_1-l_2+I)/2]!\, [(-l_1+l_2+I)/2]!}. \tag{10b}$$

If these are substituted into (9), and the ν summation index in (9) is replaced by $\mu \equiv \nu + (l-k-L)/2$, we get

$$\begin{aligned} &g_{kl}^{L}(r) \\ &= \frac{(-2)^{(L-k-l)/2}}{[(L+l-k)/2]!\, [(L+k-l)/2]!} \Big((2k+1)(2l+1) \times (k+l-L)!(l+L-k)!(L+k-l)!(k+l+L+1)!/4\pi\Big)^{1/2} \\ &\times \sum_{\mu=0}^{(k+l-L)/2} \frac{(L+\mu)!\, 2^{\mu}\, r^{L+2\mu}}{\mu!(2L+2\mu+1)![(k+l-L)/2-\mu]!} \\ &\times \left(\frac{1}{r}\frac{d}{dr}\right)^{(L+k-l)/2+\mu} \frac{f(r)}{r^{l}}. \end{aligned} \tag{11}$$

This expresses $g_{kl}^{L}(r)$ of (2) in terms of $f(r)$ and its derivatives. Equation (11) is the main result of this paper.

It is also possible to relate $g_{kl}^{L}(r)$ to $f(r)$ via an integral relation. We express $f(r)Y_m^l(\hat{r})$ in terms of its Fourier transform,

$$f(r)Y_m^l(\hat{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\mathbf{q}\cdot\mathbf{r}} F(q) Y_m^l(\hat{q}) d^3q, \tag{12}$$

where $f(r)$ and $F(q)$ are related by

$$f(r) = i^{l} \left(\frac{2}{\pi}\right)^{1/2} \int_0^{\infty} j_l(qr) F(q) q^2\, dq, \tag{13a}$$

$$F(q) = i^{-l} \left(\frac{2}{\pi}\right)^{1/2} \int_0^{\infty} j_l(qr') f(r') r'^2\, dr'. \tag{13b}$$

Here j_l denotes the spherical Bessel function. Since

$$\frac{\partial}{\partial x} e^{i\mathbf{q}\cdot\mathbf{r}} = i q_x e^{i\mathbf{q}\cdot\mathbf{r}}, \quad \text{etc.},$$

it follows that

$$\mathscr{Y}_n^k(\nabla) e^{i\mathbf{q}\cdot\mathbf{r}} = i^k \mathscr{Y}_n^k(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}.$$

Application of $\mathscr{Y}_n^k(\nabla)$ to the right-hand side of (12) then yields

$$g_{kl}^{L}(r) = \int_0^{\infty} K(r,r') f(r') r'^2\, dr', \tag{14a}$$

$$K(r,r')=i^{k+L-l}\frac{2}{\pi}\left(\frac{(2k+1)(2l+1)}{4\pi(2L+1)}\right)^{1/2}$$
$$\times(k\,l\,0\,0\,|\,L\,0)$$
$$\times\int_0^\infty j_L(qr)j_l(qr')\,q^{k+2}\,dq. \tag{14b}$$

In particular, if $f(r)$ is itself a spherical Bessel function $j_l(\kappa r)$, the r' integration in (14a) can be done immediately,

$$\int_0^\infty j_l(qr')j_l(\kappa r')r'^2\,dr'=\frac{\pi}{2}\frac{\delta(q-\kappa)}{q\kappa},$$

which leads to

$$g_{kl}^L(r)=i^{k+L-l}\left(\frac{(2k+1)(2l+1)}{4\pi(2L+1)}\right)^{1/2}$$
$$\times(k\,l\,0\,0\,|\,L\,0)\kappa^k j_L(\kappa r) \tag{15}$$
$$[f(r)\rightleftharpoons j_L(\kappa r)\,].$$

This equation can be shown to be consistent with the more general formula (11), if use is made of the recursion relations of the $j_l(\kappa r)$. Since the spherical Neumann functions $n_l(\kappa r)$ and spherical Hankel functions $h_l^{(1)}$ and $h_l^{(2)}(\kappa r)$ obey the same recursion relations as the $j_l(\kappa r)$, they will also obey (15) with $j_L(\kappa r)$ on the right replaced by $n_L(\kappa r)$, $h_L^{(1)}(\kappa r)$, and $h_L^{(2)}(\kappa r)$, respectively.

3. APPLICATION TO TAYLOR EXPANSIONS

The Taylor expansion of a function ψ about the point $\mathbf{r}$ can be written

$$\psi(\mathbf{r}+\mathbf{s})=\sum_n\frac{(\mathbf{s}\cdot\nabla)^n}{n!}\psi(\mathbf{r}). \tag{16}$$

To convert this into a multipole expansion, we note that, for any two vectors $\mathbf{a}$ and $\mathbf{b}$,

$$(\mathbf{a}\cdot\mathbf{b})^n=a^n b^n\,(\cos\theta)^n$$
$$=a^n b^n\sum_{k=n,n-2,n-4,\cdots}\frac{(2k+1)n!}{2^{(n-k)/2}[(n-k)/2]!(k+n+1)!!}$$
$$\times P_k(\cos\theta). \tag{17}$$

The spherical harmonic addition theorem can be written

$$P_k(\cos\theta)=(-1)^k\frac{4\pi}{(2k+1)^{1/2}}[Y^k(\hat a)\,Y^k(\hat b)]_0^0.$$

If this is substituted into (17), we get

$$(\mathbf{a}\cdot\mathbf{b})^n=4\pi n!\sum_k\frac{(-1)^k(2k+1)^{1/2}(a^2b^2)^{(n-k)/2}}{2^{(n-k)/2}[(n-k)/2]!(k+n+1)!!}$$
$$\times[\mathscr{Y}^k(\mathbf{a})\,\mathscr{Y}^k(\mathbf{b})\,]_0^0,$$

which, when applied to (14), yields

$$\psi(\mathbf{r}+\mathbf{s})=4n\sum_{k=0}^\infty(-1)^k(2k+1)^{1/2}$$
$$\times\left(\sum_{\mu=0}^\infty\frac{s^{2\mu}(\nabla^2)^\mu}{2^\mu\mu!(2k+2\mu+1)!!}\right)$$
$$\times[\mathscr{Y}^k(\mathbf{s})\,\mathscr{Y}^k(\nabla)\,]_0^0\psi(\mathbf{r}). \tag{18}$$

Now suppose that $\psi(\mathbf{r})$ transforms under rotations like $Y_m^l(\hat r)$. Thus

$$\psi(\mathbf{r})\equiv\psi_m^l(\mathbf{r})=f(r)\;Y_m^l(\hat r), \tag{19}$$

and we have

$$[\mathscr{Y}^k(\mathbf{s})\,\mathscr{Y}^k(\nabla)\,]_0^0 f(r)\;Y_m^l(\hat r)$$
$$=\sum_L U(kk\,ll;0L)$$
$$\times[\mathscr{Y}^k(\hat s)\,[\mathscr{Y}^k(\nabla)f(r)Y^l(\hat r)\,]^L\,]_m^l$$
$$=\sum_L(-1)^{k+l-L}\left(\frac{2L+1}{(2k+1)(2l+1)}\right)^{1/2}$$
$$\times g_{kl}^L(r)\;Y_m^l(\hat r). \tag{20}$$

We have used here the explicit expression for the Racah coefficient $U(k\,k\,l\,l;0L)$. The function $g_{kl}^L(r)$ in (20) is related to $f(r)$ in (19) via (2) and (11). The phase factor in the L-sum in (20) can be omitted, since we know that the only allowed L-values make $k+l-L$ even. The Laplacian operator ∇^2 applied to the r-dependent part of (20) gives

$$\nabla^2 g_{kl}^L(r)\;Y_M^L(\hat r)$$
$$=\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{L(L+1)}{r^2}\right)g_{kl}^L(r)\;Y_M^L(\hat f).$$

Finally, we obtain the general expression

$$\psi_m^l(\mathbf{r}+\mathbf{s})=4\pi\sum_{\substack{k,L\\(k+l+L\ \text{even})}}(-1)^k\left(\frac{2L+1}{2l+1}\right)^{1/2}$$
$$\times\left\{\sum_{\mu=0}^\infty s^{2\mu+k}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{L(L+1)}{r^2}\right)^\mu\right.$$
$$\left.\times[2^\mu\mu!/(2k+2\mu+1)!!\,]\right\}^{-1}g_{kl}^L(r)$$
$$\times[Y^k(\hat s)\,Y^L(\hat r)\,]_m^l, \tag{21a}$$

or equivalently,

$$\int [Y^k(\hat{s})\, Y^L(\hat{r})\,]^{*l}_m \psi^{\,l}_m(\mathbf{r}+\mathbf{s})\, d\hat{r}\, d\hat{s}$$

$$=(-1)^k 4\pi \left(\frac{2L+1}{2l+1}\right)^{1/2}$$

$$\times \sum_{\mu=0}^{\infty} \Big[s^{2\mu+k} \left(\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} - L\frac{(L+1)}{r^2}\right)^{\mu} /$$

$$2^{\mu}\mu!(2k+2\mu+1)!!\,]\, g^{L}_{kl}(r). \tag{21b}$$

As an example of the use of (21), we calculate the overlap between wavefunctions $\psi^{\,l_1}_{m_1}$ and $\psi^{\,l_2}_{m_2}$ calculated in nearby spherically symmetric potential wells. Let one well be centered at the origin, and the other centered at a point shifted from the origin by vector $\mathbf{s}$. The corresponding wavefunctions are

$$\psi^{\,l_1}_{m_1}(\mathbf{r}) = u_{l_1}(r)\, Y^{l_1}_{m_1}(\hat{r}), \tag{22a}$$

$$\psi^{\,l_2}_{m_2}(\mathbf{r}-\mathbf{s}) = u_{l_2}(\,|\vec{r}-\vec{s}\,|\,)\, Y^{l_2}_{m_2}(\mathbf{r}-\mathbf{s}). \tag{22b}$$

Using (21a), we find that

$$\int \psi^{*l_1}_{m_1}(\mathbf{r})\, \psi^{\,l_2}_{m_2}(\mathbf{r}-\mathbf{s}) d^3r$$

$$=4\pi \sum_{\substack{k \\ (k+l_1+l_2 \text{ even})}} \mathscr{Y}^k_{m_2-m_1}(\mathbf{s})\, (k\, l_1\, m_2-m_1\, m_1 \,|\, l\, m_2)$$

$$\times \left(\frac{2l_1+1}{2l_2+1}\right)^{1/2} \int_0^{\infty} u^{*}_{l_1}(r) \sum_{\mu=0}^{\infty} \Big[s^{2\mu} \left(\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr}\right.$$

$$\left. - \frac{l_1(l_1+1)}{r^2}\right)^{\mu} / 2^{\mu}\mu!(2k+2\mu+1)!! \Big] g^{\,l_1}_{k,l_2}\, r^2\, dr. \tag{23a}$$

For a sufficiently small shift $\mathbf{s}$, the dominant term for each k will have $\mu=0$,

$$\int \psi^{*l_1}_{m_1}(\mathbf{r})\, \psi^{\,l_2}_{m_2}(\mathbf{r}-\mathbf{s}) d^3r \underset{s\to 0}{\longrightarrow} 4\pi \sum_k \mathscr{Y}^k_{m_2-m_1}(\mathbf{s})$$

$$\times \frac{(k\, l_1\, m_2-m_1\, m_1 \,|\, l_2\, m_2)}{(2k+1)!!} \left(\frac{2l_1+1}{2k+1}\right)^{1/2}$$

$$\times \int_0^{\infty} u^{*}_{l_1}(r)\, g^{\,l_1}_{kl_2}(r) r^2\, dr\,. \tag{23b}$$

The function $g^{\,l_1}_{kl_2}(r)$ in (23a) and (23b) is obtained by replacing $f(r)$ or the right-hand side of (11) by $u_{l_2}(r)$ from (22b).

Another example of the use of (21) is in the calculation of the interaction energy E between two separated density distributions $\rho_1(\mathbf{r}_1)$ and $\rho_2(\mathbf{r}_2)$ due to a central potential $V(|\mathbf{r}_1-\mathbf{r}_2|)$,

$$E(\mathbf{r}) = \int d^3r_1\, d^3r_2 \rho_1(\mathbf{r}_1)\rho_2(\mathbf{r}_2) V(|\mathbf{r}-\mathbf{r}_1+\mathbf{r}_2|)\,. \tag{24}$$

We perform a Slater expansion on V

$$V(|\mathbf{r}-\mathbf{t}\,|) = \sum_l f_l(r,t) P_l(\hat{r}\cdot\hat{t})$$

$$= 4\pi \sum_l \frac{(-1)^l}{(2l+1)^{1/2}} f_l(r,t)$$

$$\times [Y^l(\hat{r})\, Y^l(\hat{t})\,]^0_0. \tag{25}$$

We substitute this expansion in (24), with $\mathbf{t}=\mathbf{r}_1-\mathbf{r}_2$, and then use (21a) to separate the $\mathbf{r}_1,\mathbf{r}_2$ dependence. The result is the following multipole expansion of $E(r)$

$$E(\mathbf{r}) = (4\pi)^2 \sum_{\substack{l \\ l_1,l_2}} \frac{(2l_2+1)^{1/2}}{2l+1}$$

$$\times \sum_{\mu=0}^{\infty} \frac{\{[q^{\mu,l_1} Q^{\mu l_1 l l_2}(r)\,]^l Y^l(\hat{r})\,\}^0_0}{2^{\mu}\mu!(2l_1+2\mu+1)!!}. \tag{26a}$$

Here $q^{\mu,l_1}_{m_1}$ and $Q^{\mu l_1 l l_2}_{m_2}(r)$ are defined by

$$q^{\mu,l_1}_{m_1} \equiv \int r_1^{2\mu+l_1} Y^{l_1}_{m_1}(\hat{r}_1)\rho_1(\mathbf{r}_1) d^3r_1, \tag{26b}$$

$$Q^{\mu l_1 l l_2}_{m_2}(r) \equiv \int \left[\frac{1}{r_2^2}\frac{d}{dr_2} r_2^2 \frac{d}{dr_2} - \frac{l_2(l_2+1)}{r_2^2}\right]^{\mu}$$

$$\times g^{\,l_2}_{l_1,l}(r,r_2)\, Y^{l_2}_{m_2}(\hat{r}_2)\rho_2(\mathbf{r}_2) d^3r_2, \tag{26c}$$

with $g^{\,l_2}_{l_1,l}(r,r_2)$ calculated from $f_l(r,r_2)$ by means of (11). In the special case in which V is a Coulomb interaction, $f_l(r,t)$ in (25) is t^l/r^{l+1}. Then $g^{\,l_2}_{l_1,l}(r,r_2)$ is nonzero only if $l=l_1+l_2$, the μ sums in (11) and (26a) consists only of the $\mu=0$ terms, and the sum in (26a) simplifies to

$$E(\mathbf{r}) = (4\pi)^{3/2} \sum_l \frac{1}{r^{l+1}} \sum_{\substack{l_1,l_2 \\ (l_1+l_2=l)}} (-1)^{l_1}$$

$$\times \left(\frac{(2l)!}{(2l_1+1)!(2l_2+1)!}\right)^{1/2}$$

$$\times \{[q^{0,l_1}(1)\, q^{0,l_2}(2)\,]^l Y^l(\hat{r})\,\}^0_0. \tag{27}$$

An expansion of the type (21a) was given by Sawaguri and Tobocman.[3] The r,s dependence of the $[Y^k(\hat{s})\, Y^L(\hat{r})\,]^l_m$ term in their expansion is expressed in

terms of a sum of products of what they call "modified" harmonic-oscillator functions," $\mathcal{F}^{k}_{n_1}(\alpha_1,\beta_1 s)$ $\mathcal{F}^{L}_{n_2}(2,\beta_2 r)$. The scale parameters $\alpha_1, \alpha_2, \beta_1$, and β_2 are chosen to make the n_1, n_2 expansion coverge as rapidly as possible. The r, s dependence of our expansion (21a) involves power of s and the original function $f(r)$ and its derivatives. It can be expected to converge best in situations in which s is small compared to the distance over which $f(r)$ changes by an appreciable fraction of itself.

A simple application of (21a) occurs when $f(r)=j_l(\kappa r)$ so that $g^{L}_{kl}(r)$ in (21a) is given by (15). If we use the fact that

$$\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{L(L+1)}{r^2}\right)j_L(\kappa r)=-\kappa^2 j_L(\kappa r),$$

the μ-sum in (21a) can be expressed as

$$\sum_{\mu=0}^{\infty}\frac{(\kappa s)^{k+2\mu}(-1)^{\mu}}{2^{\mu}\mu!(2k+2\mu+1)!!}=j_k(\kappa s).$$

Thus we have

$$j_l(\kappa|\mathbf{r}+\mathbf{s}|)\,Y^{l}_{m}(\mathbf{r}+\mathbf{s})\hat{}=\sum_{k,L}i^{L-k-l}\,(4\pi(2k+1)\,)^{1/2}\times(k\,l\,0\,0|L\,0)\;\;j_k(\kappa s)j_L(\kappa r)\times[\,Y^{k}(\hat{s})\,Y^{L}(\hat{r})\,]^{l}_{m}.$$

Analogous equations can be derived for $n_l(\kappa r)$ and $h^{(1)}_{l}(\kappa r)$. Expansion relations of this form for multipole fields have been given by Danos and Maximon.[4]

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Analysis of the neutron slowing down equation

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The infinite series solution of the elementary neutron slowing down equation is studied using the theory of entire functions of exponential type and nonharmonic Fourier series. It is shown from Muntz–Szasz and Paley–Wiener theorems, that the set of exponentials $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$, where $\{\lambda_n\}_{n=-\infty}^{\infty}$ are the roots of the transcendental equation in slowing down theory, is complete and forms a basis in a lethargy interval ϵ. This distinctive role of the maximum lethargy change per collision is due to the Fredholm character of the slowing down operator which need not be quasinilpotent. The discontinuities in the derivatives of the collision density are examined by treating the slowing down equation in its differential-difference form. The solution (Hilbert) space is the union of a countable number of subspaces $L_2(-\epsilon/2, \epsilon/2)$ over each of which the exponential functions are complete.

1. INTRODUCTION

A complete solution of the neutron slowing down equation in an infinite homogeneous medium with isotropic elastic scattering and constant cross sections has been obtained as an infinite sum of exponentials with the exponents expressed in terms of the roots of a certain transcendental equation.[1] This solution is valid for all magnitudes of absorption and all moderator masses, and gives accurate results, as numerical calculations performed in Ref. 1 show, with a reasonably small number of terms of the infinite exponential sum. A series such as that encountered in the solution of the infinite medium slowing down equation represents what is known as a nonharmonic Fourier series,[2] which is essentially a series given in terms of a countably infinite linearly independent set $\{g_n(u)\}_{n=-\infty}^{\infty}$ in a Hilbert space H. This set is neither orthonormal nor even orthogonal, and the study of a series in terms of them involves problems of the closure of the set together with the related though nontrivial question of being able to uniquely associate with every linear combination of the $\{g_n(u)\}_{n=-\infty}^{\infty}$ a vector in its closed linear span, $V(G)[g=\{g_n(u): -\infty \leqslant n \leqslant \infty\}]$. Of course, the first problem implies the second if G is orthonormal; in the present case however, where G is merely linearly independent, they must be investigated separately.[3] The object of the present paper is to consider the series solution of the neutron slowing down equation from the viewpoint of a nonharmonic Fourier series in a suitably constructed linear manifold $L_2(a,b)$ of the Hilbert space H.

The plan of this paper is as follows. In Sec. 2, the problem and its solution is briefly discussed, and in Sec. 3, the linear manifold $L_2(a,b)$ with the appropriate a and b, are constructed. Section 4 contains a discussion of the closure of the set of exponential functions and also shows that any arbitrary function in $L_2(a,b)$ can be suitably constructed in terms of this basis set. In the next section, we study the question of the discontinuities in the solution by considering the slowing down equation in its differential difference form. This analysis follows standard procedures.[4] Finally, we end the paper with some comments and discussions.

2. THE PROBLEM AND ITS SOLUTION

We are concerned with the representation of the complete solution of the elementary slowing down equation

$$\psi(u)=S(u)+\lambda\int_{u-\epsilon}^{u} du'\, e^{u'-u}s(u')\psi(u'), \quad u>\epsilon. \quad (1)$$

Here,

$\psi(u)$ is the collision density of neutrons in the medium,

$S(u)$ is a source of neutrons independent of ψ,

$s(u)=\sigma_s(u)/\sigma_t(u)$ is the ratio of scattering to total cross sections of the moderator of mass A, and

$$\lambda=(1-\alpha)^{-1}, \quad \epsilon=-\ln\alpha, \quad \alpha=\left(\frac{A-1}{A+1}\right)^2.$$

Equation (1) is the simplest equation for the slowing of neutrons in a moderating, nonmultiplying medium and can be considered as the counterpart of the one-speed equation in a nonmoderating purely diffusing medium. While the solution of this latter equation has been studied extensively in the literature,[5,6] consideration of Eq. (1) has been confined mostly to qualitative discussions on the nature of its solutions.[5,7] Actual calculation of the neutron flux involves, as in the one-speed case, the roots of a transcendental equation. A general prescription for computing all these roots and thereby obtaining the solution is now available.[1,8] This solution is in the form of a nonharmonic Fourier series, and, as pointed out in the Introduction, gives good numerical results. In this paper we establish a mathematical foundation for such a representation of the collision density.

For the sake of completeness, we give below a short sketch of the solution of (1). This discussion is based on Ref.

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1 to which the interested reader is directed for further details. The solution to the slowing down equation with a delta source $\delta(u)$ and cross sections that are constant in energy can be written as the infinite series,

$$\psi(u)=\sum_{n=0}^{\infty} a(\lambda_n^*)\exp(-\lambda_n^* u), \quad u>\epsilon, \tag{2}$$

where λ_n^* are the roots of

$$\lambda^*=1-\lambda s+\lambda\alpha s\exp(\lambda^*\epsilon) \tag{3}$$

and

$$a(\lambda_n^*)=\frac{1-\lambda_n^*}{1-\lambda\alpha\epsilon s+\exp(\lambda_n^*\epsilon)}. \tag{4}$$

Equation (3) has only one real root and an infinity of complex roots. The real root can be obtained by iteration from the equation[8]

$$\xi^*=1-\alpha\left(\frac{\xi^*}{a}-1\right)\frac{\exp(a\epsilon/\xi^*)-1}{1-\alpha\exp(a\epsilon/\xi^*)}, \tag{5}$$

where $a=1-s$ and $\xi^*=a/\lambda_0^*$, while the complex roots are evaluated as follows. Rewrite (3) as

$$z=ce^z, \tag{6}$$

where

$$z=\epsilon(\lambda^*-b_0), \quad b_0=1-\lambda s, \quad c=\lambda\alpha\epsilon s\exp(b_0\epsilon).$$

If the constant c lies between zero and e^{-1}, which is true in our case, then the roots of (6) in the upper half plane lie one in each strip

$$2n\pi<y<(2n+1)\pi, \quad n=1,2,\cdots, \quad z=x+iy,$$

at the only intersection of the branches of the curves

$$y=(c^2e^{2x}-x^2)^{1/2}$$

and

$$x=y\cot y.$$

Separating (6) into real and imaginary parts, we have

$$x=ce^x\cos y, \tag{7}$$

$$y=ce^x\sin y, \tag{8}$$

and from (7), the limits on y are sharpened as

$$2n\pi<y_n<2n\pi+\frac{\pi}{2}, \quad n=1,2,3,\cdots. \tag{9}$$

For practical evaluation of the x_n and y_n equations (7) and (8) are then cast in a form suitable for successive iteration of these quantities.[1] Finally, the desired parameters $\mathrm{Re}\lambda_n^*$ and $\mathrm{Im}\lambda_n^*$ are related to the x_n and y_n by

$$\mathrm{Re}\lambda_n^*=\frac{x_n}{\epsilon}+b_0, \tag{10}$$

$$\mathrm{Im}\lambda_n^*=\frac{y_n}{\epsilon}. \tag{11}$$

For large n, x_n and y_n can be approximated as

$$y_n=2n\pi+\frac{\pi}{2}, \tag{12}$$

$$x_n=\ln\left(\frac{y_n}{c}\right). \tag{13}$$

Having thus obtained all the roots λ_n^*, the neutron collision density for $u>\epsilon$ can be obtained from Eqs. (2) and (4).

It should be clearly noted that the above analysis is valid only if $u>\epsilon$. To study the nature of the solution when $0\leqslant u\leqslant\epsilon$, it is best to cast the slowing down equation in its differential-difference form,[4]

$$\psi'(u)+b_0\psi(u)+b_1\psi(u-\epsilon)=0, \quad u>\epsilon, \tag{14}$$

where $b_0=1-\lambda s$, $b_1=\lambda\alpha s$. As u cannot be negative we must have

$$\psi'(u)+b_0\psi(u)=0, \quad 0\leqslant u\leqslant\epsilon, \tag{15}$$

with the initial condition $\psi(0)=\lambda s$. The main point to emphasize here is that $\psi(u)$ satisfies different equations in $u<\epsilon$ (an ordinary first-order differential equation) and for $u>\epsilon$ (a differential-difference equation), hence the solutions in these two regions will be different. In particular, the two solutions need not be equal at $u=\epsilon$ unless some additional conditions are satisfied. This simple discussion brings out a basic point in the nature of the solution, viz., it satisfies different equations in two different u regions, and this is responsible for a discontinuity unless some additional restrictions are imposed on the solution. These points will be taken up in greater detail in Sec. 5, where the discontinuities in the derivatives of $\psi(u)$ will be studied.

A. Mathematical preliminaries

Solution (2) to the slowing down equation (1) is expressed in terms of the linearly independent set $\{g_n(u)\}_{n=-\infty}^{\infty}$ where $g_n(u)=\exp(-\lambda_n^* u)$. The index n takes values appropriate to the roots of the transcendental equation (6). Since the complex roots of (6) occur in conjugate pairs, the index can be made to take all integral values in $(-\infty,\infty)$ as follows.

If $\lambda_n^*=\theta_n\pm i\rho_n$, then using

$\lambda_n^*=\theta_n+i\rho_n, \quad n<0,$

$\lambda_n^*=\theta_0, \quad n=0, \quad \lambda_n^*=\theta_n-i\rho_n, \quad n>0,$

the set G becomes

$$\{\exp[i(-\rho_n+i\theta_n)u]\}_{n=-\infty}^{-1}, \quad \exp(-\theta_0 u),$$

$$\{\exp[i(\rho_n+i\theta_n)u]\}_{n=1}^{\infty}.$$

We will thus examine solution (2) in terms of the linearly independent set $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ where the substitution $\lambda_n=-i\lambda_n^*$ has been made.

The basic theory of series of the type $\Sigma_{n=-\infty}^{\infty} a_n\exp(i\lambda_n u)$ has been given in two different approaches by Paley and Wiener[2] and Muntz and Szasz.[9] While the former have been concerned with conditions under which the linearly independent set $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ is

not only closed but also forms a basis in the linear manifold $L_2(a,b)$, Muntz–Szasz theorem examines when $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ merely spans $L_2(a,b)$. Both these theorems are in the form of conditions on the $\{\lambda_n\}_{n=-\infty}^{\infty}$. The Paley–Wiener theorem is, however, more comprehensive because it lays down conditions under which a linearly independent set behaves like an orthonormal set in as far as its behavior with respect to the representation of an arbitrary function in its closed linear span is concerned. This condition therefore implies the Muntz–Szasz condition. The converse, however is not necessarily true. Thus the Paley–Wiener theorem not only tells us when $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ spans the particular subspace $L_2(a,b)$ but also ensures that every linear combination of this set converges in the subspace. Because the set is not orthonormal (or orthogonal), the Muntz theorem on the closure of a set of linearly independent functions does not necessarily imply that every sequence $S_N=\Sigma_{-N}^{N}+a_n\exp(i\lambda_n u)$ is Cauchy in $L_2(a,b)$. As an example of how this situation may arise, consider the following example from Naylor and Sell.[3] Construct the linearly independent set $\{x_n\}_{n=1}^{\infty}$

$$x_n=\left(\cos\frac{1}{n}\right)y+\left(\sin\frac{1}{n}\right)z_n,\quad n=1,2,3,\cdots,$$

from an orthonormal set $\{y,z_1,z_2,z_3,\cdots\}$ in a Hilbert space H. Then it is not true that every $y\in V(A)$ where $V(A)$ is the closed linear subspace of H spanned by $A=\{x_n\}_{n=1}^{\infty}$ [i.e., $V(A)$ is the set of all *finite* linear combinations of the $\{x_n\}$], can be represented in the form

$$y=\alpha_1x_1+\alpha_2x_2+\cdots.$$

The condition under which it can be so done is the basic content of the Paley–Wiener Theorem. We shall examine below both these conditions for the neutron slowing down equation and demonstrate the validity of our method of obtaining the neutron flux.

3. THE SUBSPACE $L_2(a,b)$

In this section we construct the linear subspace $L_2(a,b)$ of the Hilbert space H appropriate for the solution of the slowing down equation and show in the next section that it is the union of a countable number of closed linear manifolds spanned by the set G, and that any vector in these manifolds can be suitably approximated by a (finite) linear combination of the $\{g_n(u)\}_{n=-\infty}^{\infty}$.

Consider the integral equation (1) having the integral operator

$$K(u,u')=\lambda\int_{u-\epsilon}^{u}du s(u')\,e^{u'-u}$$

which is generated by the kernel

$$k(u,u')=s(u')e^{u'-u},\quad u,u'\in(\epsilon,u_m),$$

where u_m is some maximum final lethargy. Note that $\lambda=(1-\alpha)^{-1}$ is a fixed constant and is not an eigenvalue parameter of the integral equation. In the interval (ϵ,u_m) the kernel $k(u,u')$ is zero for $u'>u$ (no upscattering of neutrons) as also for $u'<u-\epsilon$ (neutrons can gain no more than fixed lethargy in each collision). The kernel generates what may therefore be considered a two-sided Volterra operator with the Fredholm property of a constant interval of integration, ϵ. Thus the integral operator K can be expected to possess a combination of the properties of the Fredholm and Voltera operators. It will be shown in the following that this is true.

In the space $\mathbb{L}_2((\epsilon,u_m)\times(\epsilon,u_m))$ the kernel $k(u,u')$ has the norm

$$|\|k(u,u')\\|=\left(\int_{\epsilon}^{u_m}du\int_{\epsilon}^{u_m}du'\,\lambda^2s^2(u')\,e^{2(u'-u)}\right)^{1/2}<\infty,$$

and according to standard properties of integral equations

$$\|K\|=|\|k\||,$$

since it can be easily shown that

$$\|K\psi\|\leqslant|\|k\||\|\psi\|,$$

where

$$\|\psi\|=\left(\int_{\epsilon}^{u_m}du\,|\psi(u)|^2\right)^{1/2}.$$

The physical quantity $\psi(u)$ is, of course, real valued; the expressions (2) and (3) lead to[1]

$$\psi(u)=\frac{1-\theta_0}{1-\lambda\alpha\epsilon s\,\exp(\theta_0\epsilon)}\exp(-\theta_0u)$$

$$+2\sum_{n=1}^{\infty}\frac{\exp(-\theta_nu)}{\mu_n^2+\tau_n^2}$$

$$\times[\beta_n\cos\rho_nu+\eta_n\sin\rho_nu],$$

where,

$$\mu_n=1-\lambda\alpha\epsilon s\exp(\theta_n\epsilon)\cos\rho_n\epsilon,$$

$$\tau_n=\lambda\alpha s\epsilon\exp(\theta_n\epsilon)\sin\rho_n\epsilon,$$

$$\beta_n=\delta_n\mu_n+\rho_n\tau_n,$$

$$\eta_n=\delta_n\tau_n-\rho_n\mu_n,\quad\text{and }\delta_n=1-\theta_n.$$

The operator $K:L_2(\epsilon,u_m)\to L_2(\epsilon,u_m)$ is obviously compact, hence it has at most a pure point spectrum. For an arbitrary source $S(u)$, the solution of the integral equation involves an inversion of the operator $(I-K)$; hence if the spectral radius of K is less than 1, the inversion, and hence the solution (2) is justified. We now prove that this is indeed the case.

The proof is standard and straightforward. Let $r_0(K)$ denote the spectral radius of K, i.e.,

$$r_\sigma(K)=\lim_{n\to\infty}\|K^n\|^{1/n}.$$

Now[8]

$$K^nS=\int_{u-\epsilon}^{u}du_1\lambda s(u_1)\,e^{u_1-u}$$

$$\times\int_{u_1-\epsilon}^{u_1}du_2\lambda s(u_2)\,e^{u_2-u_1}$$

$$\times\cdots\int_{u_{n-1}-\epsilon}^{u_n-1}du_n\lambda s(u_n)\,e^{u_n-u_{n-1}}S(u_n)$$

$$=(-1)^{n-1}\frac{1}{(n-1)!}\int_{u-\epsilon}^{u} du_1 e^{u_1-u}s(u_1)$$
$$\times\left[\int_u^{u_1} du_2\, s(u_2)\right]^{n-1} s(u_1)+\Psi_n(u).$$

Hence

$$\|K^n S\| \leqslant \|\Psi_n(u)\| + \frac{1}{(n-1)!}$$
$$\times\left|\left|\int_{u-\epsilon}^{u} du_1 e^{u_1-u}s(u_1)\right.\right.$$
$$\left.\left.\times\left[\int_u^{u_1} du_2 s(u_2)\right]^{n-1} S(u_1)\right|\right|$$
$$\leqslant \|\Psi_n(u)\| + \frac{1}{(n-1)!}$$
$$\times\left\{\int_{\epsilon}^{u_m} du\left|\int_{u-\epsilon}^{u} du_1 e^{u_1-u}s(u_1)\right.\right.$$
$$\left.\left.\times\left[\int_u^{u_1} du_2 s(u_2)\right]^{n-1} S(u_1)\right|^2\right\}^{1/2}$$

and

$$\|K^n\| \leqslant \frac{\|\Psi_n(u)\|}{\|S(u)\|} + \frac{1}{(n-1)!}\frac{\|J_{n-1}(u)\|}{\|S(u)\|},$$

where $J_{n-1}(u)$ is the integral term on the right-hand side of the above inequality.

Thus

$$r_\sigma(K) \leqslant \lim_{n\to\infty} \|\Psi_n(u)\|^{1/n}.$$

Since $\lim_{n\to\infty}\Psi_n(u)=0$ for the series $\Sigma_n^\infty \Psi_n(u)$ to converge, $r_\sigma(K)$ need not necessarily be zero. Thus there may be a discrete point spectrum of the slowing down equation of the form

$$\mu_n\psi_n - K\psi_n = 0.$$

We shall now obtain an upper limit for the spectral radius and show that it is less than 1.

Since

$$r_\sigma(K) < \lim_{n\to\infty} \|K^n\|_\infty^{1/n}, \tag{16}$$

where $\|\cdots\|_\infty$ is the supremum norm, we obtain as an upper bound to the spectral radius in $L_2(\epsilon,u_m)$, on evaluation of (16),

$$r_\sigma(K) < s_m$$
$$\leqslant 1.$$

The inversion process is thus valid and the Neuman series representation is justified. This points, however, to the care that must be exercised in solving the slowing down equation in possible cases where $\mu < 1$.

4. COMPLETENESS OF $\{\exp(i\lambda_n(u))\}_{n=-\infty}^{\infty}$

We now examine the completeness, or what is the same in L_2, *closure, of the set of exponentials* $\{exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ in $L_2(e,u_m)$. It will turn out that the set is closed over every interval of length ϵ, starting from $u=\epsilon$. Thus the linear space is a union of a countable number of subspaces. The arguments in providing the completeness of the exponential set is based on the fact that the λ_n are (essentially) the zeros of an entire function of exponential type ϵ,

$$f(z)=z-1+\lambda s-\lambda\alpha s\exp(z\epsilon). \tag{17}$$

We know from our previous discussions that the $\{\lambda_n\}$ converge to infinity; hence there exists[10] an integer $\chi\geqslant 0$ such that

$$\frac{1}{|\lambda_0|^\chi} + 2\sum_{n=1}^{\infty}\frac{1}{|\lambda_n|^\chi} = \infty$$

while

$$\frac{1}{|\lambda_0|^{\chi+1}} + 2\sum_{n=1}^{\infty}\frac{1}{|\lambda_n|^{\chi+1}} < \infty \tag{18}$$

and $f(z)$ can be represented as the infinite product

$$f(z)=e^{g(z)}\prod_{n=-\infty}^{\infty}\left(1-\frac{z}{\lambda_n}\right)$$
$$\times\exp\left(\frac{z}{\lambda_n}+\frac{z^2}{2\lambda_n^2}+\cdots+\frac{z^\chi}{\chi\lambda_n^\chi}\right),$$

where $g(z)$ is an entire function.

Another representation of functions of exponential type σ is of significance. This is a result due to Paley and Wiener (Ref. 2, p. 12) which states that an entire function $f(z)$ of exponential type σ bounded on the real axis according to

$$\int_{-\infty}^{\infty}|f(x)|^2\,dx < \infty$$

can be expressed as

$$f(z)=\int_{-\sigma}^{\sigma} h(u)e^{izu}\,du, \tag{19}$$

for some $h(u)\in L_2(-\sigma,\sigma)$.

Since the function in Eq. (17) is an entire function of exponential type ϵ, it follows that it must have a Paley–Wiener representation of the form (19), and also, obviously,

$$f(\lambda_n)=\int_{-\epsilon}^{\epsilon} h(u)e^{i\lambda_n u}\,du=0 \tag{20}$$

for all n when $h(u)\neq 0$. Not all arbitrary $\{\lambda_n\}$ will possess this property, viz. that $f\{\lambda_n\}=0$ but $f(z)=0$. A sequence admitting such a representation of an entire function has been called by Luxemberg Ω-admissible.[11] From the definition of the closedness of a set of functions, Eq. (20) implies that $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ cannot be closed over an interval of length 2ϵ. To study if it is closed over any other interval, define, after Luxemberg,[11] a quantity $L(\lambda)$ depending on the $\{\lambda_n\}$, as

$L(\lambda)=\inf\{l_f: f(z)$ is an entire function of exponential type bounded on the real axis and $f(\lambda_n)=0$ for all $n\}$.

Here l_f is the length of the indicator diagram $h_f(\theta)$ of the

function $f(z)$. $L(\lambda)$ is the minimum of the lengths of the indicator diagrams of all those functions that have the above representation in terms of the Ω-admissible sequence $\{\lambda_n\}$. Because $h_f(\theta)$ satisfies the inequality[10]

$$-\sigma \leqslant h_f(\theta) \leqslant \sigma,$$

$L(\lambda)$ restricts the functions $f(z)$ that can be represented in the form (19) and (20) in terms of the chosen $\{\lambda_n\}$ by placing a lower bound on the type of the function. The connection between $L(\lambda)$ and Eq. (18) is contained in the result,[8,10] that if $\chi=0$, then $L(\lambda)=0$. This means that if $\Sigma(1/\lambda_n)$ converges, then $\{\lambda_n\}$ is Ω-admissible in all intervals $(-\sigma,\sigma)$ and hence $\{e^{i\lambda_n u}\}_{n=-\infty}^{\infty}$ cannot be closed in any of the spaces $L_2(-\sigma,\sigma)$, $\sigma>0$. Conversely, it can also be shown[11] that if $L(\lambda)>0$, then $\{e^{i\lambda_n u}\}$ is closed over any interval of length less than $L(\lambda)$ [and obviously, from the above discussions, it is not closed in an interval equal to or greater than $L(\lambda)$]. Thus the necessary and sufficient condition for the closure of a set of exponentials over an interval [equal to $L(\lambda)$] is that $\Sigma(1/\lambda_n)$ diverges. Note that though the sum is independent of the interval, the quantity L is a function of $\{\lambda_n\}$. This criterion for closure is the Muntz–Szasz condition. The most important fact to note in the above analysis is that the interval is an upper limit of the regions over which a set of functions can be complete, because for any greater interval representations (19) and (20) must hold. Stated otherwise, this means that if the sequence were not complete in this interval, by the very definition of $L(\lambda)$, the interval would have been included in it. In our case $f(z)$ is of type ϵ (>0 for finite moderator mass A), hence by the above arguments,

$$\frac{1}{|\lambda_0|}+2\sum_{1}^{\infty}\frac{1}{|\lambda_n|} \tag{21}$$

cannot converge and $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ must be close in some interval of length less than 2ϵ. We do not know the precise value of $L(\lambda)$, and therefore the precise closure interval. All that the fact $f(z)$ is of type ϵ and satisfies (20) signifies is that $L(\lambda)\leqslant 2\epsilon$.[12]

The divergence of (21) can also be proved simply as follows:

$$\epsilon|\lambda_n| \leqslant \left(2n\pi+\frac{\pi}{2}\right)+\frac{1}{c}\left(2n\pi+\frac{\pi}{2}\right)+b_0\epsilon$$

$$\leqslant \frac{2}{c}\left(2n\pi+\frac{\pi}{2}\right)+b_0\epsilon,$$

i.e.,

$$\frac{c\epsilon}{2}|\lambda_n| \leqslant 2n\pi+\frac{\pi}{2}+\frac{cb_0}{2\epsilon}$$

and

$$\sum\frac{1}{|\lambda_n|} \geqslant \sum\frac{1}{n+a},$$

where a is a positive finite constant. Hence $\Sigma(1/\lambda_n)$ diverges and $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ spans some interval of length less than 2ϵ. Muntz's theorem, without a lower bound for $L(\lambda)$, has not given us the exact interval over which these exponentials are complete, and of course does not automatically guarantee the possibility of expressing any arbitrary function in the interval by a linear combination of these exponentials. To know when this will be possible, and to obtain the exact completeness interval, we will further sharpen our result by the application of Paley and Wiener's theorem. Consider the complete orthonormal set in an interval less than 2ϵ, ϵ say, i.e., the set

$$\left\{\frac{1}{\sqrt{\epsilon}}\exp\left(i\frac{2\pi}{\epsilon}nu\right)\right\}_{n=-\infty}^{\infty} \quad \text{in} \quad L_2\left(-\frac{\epsilon}{2},\frac{\epsilon}{2}\right),$$

in which it is also a basis. Now for a nonorthogonal set, Paley and Wiener's theorem states[13] that if $\{\lambda_n\}_{n=-\infty}^{\infty}$ is real and if

$$\left|\lambda_n-\frac{2\pi}{\epsilon}n\right| \leqslant L, \tag{22}$$

then the sequence $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ is closed in $L_2(-\epsilon/2,\epsilon/2)$ and possesses a unique biorthogonal set $\{h_n(u)\}_{n=-\infty}^{\infty}$ such that the series

$$\sum_{n=-\infty}^{\infty}\left(\frac{e^{i(\pi/\epsilon)nu}}{2\epsilon}\int_{-\epsilon/2}^{\epsilon/2}f(x)e^{-i(\pi/\epsilon)nx}\,dx - e^{i\lambda_n u}\int_{-\epsilon/2}^{\epsilon/2}f(x)h_n(x)\,dx\right)$$

converges uniformly to zero over any interval $(-\epsilon/2+\delta\leqslant u\leqslant\epsilon/2-\delta)$ for every $\delta>0$, and over any such interval the summability properties of

$$\sum_{n=-\infty}^{\infty}e^{i\lambda_n u}\int_{-\epsilon/2}^{\epsilon/2}f(x)h_n(x)\,dx$$

are uniformly the same as those of the Fourier series of $f(u)$ provided L has a fixed upper bound depending on the interval of completeness.

In $L_2(-\pi,\pi)$, inequality (22) takes the form

$$|\lambda_n-n| \leqslant L.$$

Estimates of L for this case have been given by Paley and Wiener, Duffin and Eachus, and Kadec, as

$$L<\frac{1}{\pi^2}=0.10, \quad \text{Paley–Wiener}^2$$

$$L<\frac{\ln 2}{\pi}=0.22, \quad \text{Duffin–Eachus}^{14}$$

$$L<0.25, \quad \text{Kadec}^{15}$$

and it has been shown by Levinson[13] that $L<0.25$ is the best possible estimate in the sense that the set $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ with

$$\lambda_n=n-\tfrac{1}{4}, \quad n>0,$$

$$\lambda_n=0, \quad n=0,$$

$$\lambda_n=n+\tfrac{1}{4}, \quad n<0,$$

is closed in $L_2(-\pi,\pi)$ but does not satisfy the conclusion in the second part of Paley and Wiener's theorem. It is to be

noted that Muntz's convergence criterion will be met for all finite values of L, but unless L is suitably restricted by a Paley–Wiener condition of the type (22), $\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ will fail to be a basis in the chosen space. In $L_2(-\epsilon/2,\epsilon/2)$ it is easy to verify that the Duffin–Eachus condition becomes

$$L < \frac{2\ln 2}{\epsilon}$$

and hence the best possible estimate of L, corresponding to that of Kadec is

$$L < \frac{\pi/2}{\epsilon}.$$

If the $\{\lambda_n\}$ are complex, the analysis becomes much more complicated and can be found in Ref. 16. Basic to the existence of a condition of the type (22) is the uniform boundedness of the imaginary parts of λ_n, and it apparently has not been possible to remove this restriction. This, however, does not appear to be a particularly insurmountable problem when one recalls some of the basic definitions. Thus even though the set $\{g_n\}$ is countably infinite, its linear span is the collection of all *finite* linear combinations. Hence, in the application of the Paley–Wiener theorem, we need consider only finite linear combinations of the exponential functions and if the imaginary parts of λ_n increase monotonically, then, for all finite n, $\mathrm{Im}\lambda_n$ is finite, and the restriction given in Ref. 16 can be applied. These arguments are formalized in the following theorem.[3]

Let $\{g_n\}$ be a countable linearly independent set in a Hilbert space H. Further assume that there are $D>0$ and $\delta>0$ such that

$$\delta^2 \sum_{n=1}^{N} |\beta_n|^2 \leqslant \left\| \sum_{n=1}^{N} \beta_n g_n \right\|^2 \leqslant D^2 \sum_{n=1}^{N} |\beta_n|^2,$$

for all $\beta_1,\beta_2,\ldots,\beta_N$, $N=1,2,3,\cdots$. Then each $y\in\overline{V(G)}$ where $V(G)$ is closed linear subspace of H spanned by the $\{g_n\}$, can be expressed uniquely in the form

$$y=\alpha_1 g_1+\alpha_2 g_2+\cdots,$$

where the α_i are scalars. It is to be observed that the Paley–Wiener theorem quoted in the form above is a direct consequence of the above result. (For the original statement of the theorem, see Ref. 2, Chapter VII.) In our case $\mathrm{Im}\lambda_n\equiv\theta_n$ is finite for finite n, and condition (22) takes the form,[16]

$$\left|\mathrm{Re}\lambda_n - \frac{2\pi}{\epsilon}n\right| \leqslant L < \frac{\pi/2}{\epsilon}. \tag{23}$$

Therefore,

$$\left|\mathrm{Re}\lambda_n - \frac{2\pi}{\epsilon}n\right| = \left|\rho_n - \frac{2\pi n}{\epsilon}\right|$$

$$= \left|\frac{2\pi n}{\epsilon} + \frac{c_n}{\epsilon} - \frac{2\pi n}{\epsilon}\right|.$$

Since $c_n\uparrow\pi/2$ as $n\to\infty$ [cf., for example, (12)], we have

$$\left|\mathrm{Re}\lambda_n - \frac{2\pi}{\epsilon}n\right| < \frac{\pi/2}{\epsilon},$$

and inequality (23) is verified. This means that in an interval of length ϵ, the solution of the slowing down equation can be uniformly approximated by a finite linear combination of the exponentials. We also wish to point out that the distinctive role that the interval ϵ plays is due to the Fredholm character of the slowing down equation in its having a constant interval of integration, ϵ. Notice how the finiteness of the series is essential for the validity of the strict inequality in (23), because $c_n\uparrow\pi/2$ as $n\to\infty$. The exponentials $\{\exp(i\lambda_n u)\}_{n=-\infty}^{\infty}$ thus forms a basis in $L_2(-\epsilon/2,\epsilon/2)$ and the series solution is justified. It should be noted that the interval was considered as $(-\epsilon/2,\epsilon/2)$ merely because it is of the form used in Paley–Wiener's theorem, thus enabling a direct comparison with the condition (22) in its standard form.

5. THE DERIVATIVES $\psi^{(n)}(u)$

A differential-difference equation of the form (14) has the remarkable property of possessing discontinuities in the derivatives of its solution at the points $n\epsilon$. A lucid description of such equations is given, on the basis of classical analysis, in Bellman and Cooke,[4] and the interested reader should consult this work, particularly Chapter 3. We give below an account of the discontinuities, and follow Bellman and Cooke[4] in our approach.

The slowing down equation can be written as

$$\psi'(u)+b_0\psi(u)+b_1\psi(u-\epsilon)=0, \quad u>\epsilon, \tag{14}$$

$$\psi'(u)+b_0\psi(u)=0, \quad u\leqslant\epsilon, \tag{15}$$

where $b_0=1-\lambda s$, $b_1=\lambda\alpha s$. As explained in Sec. 2 the discontinuity at $u=\epsilon$ is because $\psi(u)$ satisfies the different equations (14) and (15) in different regions, and the solutions need not match at $u=\epsilon$ unless some additional conditions are met. From (14) it is also clear that because $\psi(u)$ is discontinuous at $u=\epsilon$, $\psi'(u)$ cannot be continuous at $u=2\epsilon$. The discontinuity in $\psi(u)$ at $u=\epsilon$ is propagated forward to $u=2\epsilon$ as a discontinuity in $\psi'=(u)$. To find out more about the behavior of $\psi'(u)$, differentiate (14). Then $\psi'(u)$ satisfies the equation

$$(\psi'(u))'+b_0(\psi'(u))-b_1[b_0\psi(u-\epsilon)+b_1\psi(u(2\epsilon)]=0. \tag{24}$$

Again, since u cannot be negative, this equation will be valid for $u>2\epsilon$ only, and $\psi'(u)$ can be represented in this region by a sum of exponentials just as $\psi(u)$ can be so expressed for $u>\epsilon$. Thus $\psi(u)$ is of class C^0 on (ϵ,u_m) and of class C^1 on $(2\epsilon,u_m)$. [That $\psi(u)$ is continuous for $u>\epsilon$ and $\psi'(u)$ for $u>2\epsilon$, can be seen simply.]

The condition under which $\psi(u)$ will be continuous at $u=\epsilon$ can be found as follows. From (15)

$$\psi(\epsilon_+)=-\frac{1}{b_0}[\psi'(\epsilon_+)+b_1\psi(0_+)\ ],$$

and from (14)

$$\psi(\epsilon_-)=-\frac{1}{b_0}\psi'(\epsilon_-).$$

If $\psi(\epsilon_+)=\psi(\epsilon_-)$, then

$$\psi'(\epsilon_+)=\psi'(\epsilon_-)-b_1\psi(0_+). \tag{25}$$

Thus there will be no discontinuity in $\psi(u)$ at $u=\epsilon$, if the above additional condition is satisfied. One way to meet the condition is to choose $b_1=0$, when equations (14) and (15) become identical and $\psi'(\epsilon_+)=\psi'(\epsilon_-)$ is automatically valid. If $b_1\neq 0$, but is a given fixed constant ($b_1=\lambda\alpha s$), (25) cannot be satisfied for it is impossible to specify both the value of a function and its derivative at the initial point for the solution of a first order inhomogeneous differential equation which is what (14) is, once $\psi(u)$ is obtained from (15). Hence there will be a discontinuity in $\psi(u)$ at $u=\epsilon$. Following a similar procedure for $\psi'(u)$ at $u=2\epsilon$, we get

$$\psi'(2\epsilon_-)=-[b_0\psi(2\epsilon_-)+b_1\psi(\epsilon_-)],$$

$$b_0\psi'(2\epsilon_+)=-[\psi''(2\epsilon_+)-b_1(b_0\psi(\epsilon_+)+b_1\psi(0_+))].$$

If $\psi'(2\epsilon_-)=\psi'(2\epsilon_+)$, then

$$\psi''(2\epsilon_+)=b_0^2\psi(2\epsilon_-)+b_0b_1\ [\psi(\epsilon_+)+\psi(\epsilon_-)\ ]+b_1^2\psi(0_+). \tag{26}$$

Again, it is not possible to specify both $\psi'(u)$ and, from (26), $\psi''(u)$ at $u=2\epsilon$ in the solution of $\psi'(u)$; hence a discontinuity at $u=2\epsilon$ in $\psi'(u)$ exists. This process can be continued for each $\psi^{(n)}(u)$, which will show that $\psi^{(n)}(u)$ satisfies two different differential difference equations, one to the left and the other to the right of $(n+1)\epsilon$, and equality of $\psi^{(n)}(u)$ at these points would mean the specification of both $\psi^{(n)}(u)$ and $\psi^{(n+1)}(u)$ at $(n+1)\epsilon$. This being impossible, the discontinuities cannot be eliminated. In the regions $u<(n+1)\epsilon$ and $u>(n+1)\epsilon$, the differential-difference equations will have their respective exponential solutions, and these solutions cannot be matched at the points $(n+1)\epsilon$.

6. CONCLUSIONS AND DISCUSSIONS

In this paper we have used the theory of entire functions of exponential type to analyze the elementary neutron slowing down equation. This approach, it is felt, is more versatile and is more easily adapted for the analysis of problems of greater complexity than the classical Laplace transform–residue integration technique.[4] In such a problem, for example the slowing down of neutrons in a mixture,[8] once the transcendental equation corresponding to (3) has been obtained, the analysis of Sec. 4 can be applied almost straightforwardly. As discussed previously,[8] the transcendental equation in such a case consists of a sum of exponentials, and hence the type of $f(z)$ will be the maximum value of ϵ corresponding to the lightest element in the mixture.

The main burden of the discussion in Sec. 4 revolved around the correct interpretation, and hence the distinction, between the theorems of Paley–Wiener and Muntz–Szasz. To the best of the knowledge of the authors, the distinction as presented here is not available in the literature, and papers dealing with one of these theorems almost always exclude a discussion of the other. The Muntz–Szasz condition, interpreted in the light of the theory of entire functions,[11] leads to an upper bound of the interval over which a sequence of exponentials can possibly be closed. In the case of the neutron slowing down equation, we obtained this upper limit from the Paley–Wiener theorem, which in addition ensured that the sequence is a basis in the Hilbert space.

To study the discontinuities in the derivatives of the collision density $\psi(u)$, the simplest approach seems to be based on the theory of differential–difference equation. Since the $\psi^{(n)}(u)$ satisfy different such equations for $u<(n+1)\epsilon$ and $u>(n+1)\epsilon$, the point $u=(n+1)\epsilon$ is a point of discontinuity unless the derivative $\psi^{(n+1)}((n+1)\epsilon_+)$ is also specified. Since it is not possible to do so, the discontinuities at these points remain. Also, the discontinuity at a forward point is due to the propagation of the discontinuity at the preceeding point. It may be pointed out as a passing remark, that $\psi(u)$ might have been continuous at $u=\epsilon$ if it were possible to choose the function in $u\leqslant\epsilon$ arbitrarily.[4] This, however, cannot be as $\psi(u)$ must satisfy Eq. (15).

In conclusion, we wish to remark that the arguments used in truncating the infinite series in Sec. 4 will hardly satisfy the purist. In lieu of any other alternative, however, we found it sufficient for our purpose. A detailed investigation of this point, i.e., relaxation of the condition of uniform boundedness of $\mathrm{Im}(\lambda_n)$, nevertheless appears to be in order.

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On the structure of divergence-free tensors

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Contravariant rank two tensors which are divergence-free on one index and which are constructed from the metric tensor, an auxiliary collection of arbitrary tensor fields, and the first and second partial derivatives of these quantities are classified. The results generalize existing mathematical arguments in support of the Einstein field equations.

1. INTRODUCTION

In gravitational field theories such as general relativity, contravariant rank two tensors A^{rs} which are divergence-free play a significant and well-known role. In this paper we shall classify those tensors which are locally of the form

$$A^{rs}=A^{rs}(g_{ij};g_{ij,h};g_{ij,hk};\rho_Q;\rho_{Q,h};\rho_{Q,hk}), \tag{1.1}$$

and which satisfy

$$A^{rs}{}_{|s}=0. \tag{1.2}$$

Here g_{ij} represents the components of a nondegenerate symmetric tensor defined on an n-dimensional orientable manifold M while ρ_Q symbolically denotes a collection of tensor fields of arbitrary rank and weight which are independent of g_{ij}. Covariant differentiation, as denoted in (1.2) by a vertical bar, is defined in terms of the Christoffel symbols Γ^h_{ij}. It should be emphasized that in classifying A^{rs} we do *not* assume it to be symmetric, divergence-free with respect to the index r or a polynomial in any of its variables. Nevertheless, as the following theorem indicates, a rather precise characterization of A^{rs} is obtained.

Theorem: If A^{rs} is a tensorial concomitant of the type (1.1) and satisfies (1.2), then

$$A^{rs}=B^{rs}+C^{rs}, \tag{1.3}$$

where B^{rs} is a symmetric divergence-free tensor of the type[1]

$$B^{rs}=B^{rs}(g_{ij};g_{ij,h};g_{ij,hk}), \tag{1.4}$$

and C^{rs} is a skew-symmetric divergence-free tensor of the type (1.1). Moreover, C^{rs} decomposes into the form

$$C^{rs}=D^{rs}+E^{rst}{}_{|t}, \tag{1.5}$$

where D^{rs} is a skew-symmetric divergence-free tensor of the type (1.4) and E^{rst} is an appropriate totally skew-symmetric tensor.

As immediate consequences of this theorem we have the following three corollaries.

Corollary 1: If A^{rs} is a tensorial concomitant of the type (1.1), then $A^{rs}{}_{|s}=0$ if, and only if $A^{rs}{}_{|r}=0$.

Corollary 2: If A^{rs} is a symmetric divergence-free concomitant of the type (1.1), than A^{rs} is independent of the fields ρ_Q and their derivatives.

Corollary 3: In a space of four dimensions, the most general divergence-free tensor of the type (1.1) is

$$A^{rs}=aG^{rs}+bg^{rs}+E^{rst}{}_{|t}, \tag{1.6}$$

where G^{rs} is the Einstein tensor, g^{rs} the inverse of g_{rs} and a and b are constants. If, in addition, A^{rs} is independent of $\rho_{Q,hk}$, then E^{rst} is explicitly given by

$$E^{rst}=\epsilon^{rstu}(V^Q\rho_{Q|u}+W_u),$$

where V^Q and W_u are arbitrary concomitants of g_{ij} and ρ_Q.

If the underlying manifold M is a spacetime, then we may replace the tensor g_{ij} by the generalized Pauli spin-matrices and assume that the fields defining ρ_Q are spin-tensorial in nature. Provided A^{rs} is now treated as a scalar under spinor (i.e., tetrad) transformations, the previous results can be reproduced verbatim and Eqs. (1.3)–(1.6) remain valid. The proof of these results depend upon several technical innovations and involves numerous lengthy calculations. Consequently in the next section we shall briefly describe the proof by outlining the main steps.[2]

These results lead us to a generalization of that derivation of general relativity in which the gravitational field equations are assumed to be of the form

$$V^{rs}=T^{rs}. \tag{1.7}$$

Here T^{rs} is the energy-momentum tensor for the external, i.e., nongravitational, source fields and V^{rs} is a tensor which is usually constructed from only those fields which characterize the gravitational field. To ensure that (1.7) implies

$$T^{rs}{}_{|s}=0$$

it is customary to restrict V^{rs} by the identity

$$V^{rs}{}_{|s}=0.$$

If, for example, V^{rs} is assumed to be a tensorial concomitant of the type

$$V^{rs}=V^{rs}(g_{ij};g_{ij,h};g_{ij,hk}), \tag{1.8}$$

then it is known[3] that V^{rs} is a linear combination of G^{rs} and g^{rs} in which case (1.7) gives rise to the usual Einstein field equations with cosmological term,

 0022-2488/78/1912-2570$1.00

$$aG^{rs}+bg^{rs}=T^{rs}. \tag{1.9}$$

Consequently if for some reason one wishes to modify the Einstein field equations then, as emphasized by Ehlers,[4] the assumption (1.8) would have to be changed. One possible alternative to (1.8) would be to assume that V^{rs} is of the type (1.1), where the fields ρ_Q represent either the external source fields or auxiliary gravitational variables. However, the above results clearly indicate that even under these very general circumstances, *the Einstein field equations must inevitably be retained.* Furthermore, our analysis shows that any attempt to modify T^{rs} by adding to it a symmetric divergence-free tensor of the type (1.1) cannot lead to different gravitational field equations.[5]

Finally, we would like to point out that a considerable effort has been made in recent years[6-14] to classify tensors S^{rs} of the type (1.1) which satisfy certain identities arising either from properties enjoyed by the energy–momentum tensors of general relativity or from the conservation laws derived from invariant variational principles. All of these identities may be expressed in the form

$$S^{rs}{}_{|s}=U^r, \tag{1.10}$$

where U^r is a vector which is constructed in a prescribed fashion. Since (1.10) is linear in S^{rs}, it follows that U^r uniquely determines S^{rs} up to a divergence-free tensor of the type (1.1). Therefore, in view of our present work, *a knowledge of U^r suffices to characterize S^{rs}*. Accordingly, it is anticipated that the results of this paper will simplify the existing solutions to classification problems of this kind and perhaps lead to new results in this area.

2. THE PROOF OF THE THEOREM

We denote the infinitesimal generators for the coordinate transformations of the tensor fields by[15] $F_i{}^j{}_Q{}^R$. Consequently, the covariant derivative of ρ_Q assumes the form

$$\rho_{Q|h}=\rho_{Q,h}-\Gamma^R_{Qh}\rho_R,$$

where $\Gamma^R_{Qh}=F_i{}^j{}_Q{}^R\Gamma^i_{jh}$, in which case

$$\rho_{Q|hk}-\rho_{Q|kh}=-R_Q{}^R{}_{hk}\rho_R,$$

where $R_Q{}^R{}_{hk}=F_i{}^j{}_Q{}^R R_j{}^i{}_{hk}$. If ξ_Q denotes another collection of tensor fields of the same type as ρ_Q, then the *principle form of the tensorial concomitant*

$$T^U=T^U(g_{ij};\ldots;g_{ij,i_1\ldots i_m};\rho_Q;\ldots;\rho_{Q,i_1\ldots i_m})$$

with respect to ξ_Q is the tensor[16,17]

$$P^U(\xi)=\sum_{l=0}^{m}(\partial^{Qi_1\cdots i_l}T^U)\xi_{Q,i_1\cdots i_l}, \tag{2.1}$$

where

$$\partial^{Qi_1\cdots i_l}T^U=\frac{\partial T^U}{\partial\rho_{Q,i_1\cdots i_l}}.$$

Since $\xi_{Q,i_1\cdots i_l}$ can be expressed as a unique linear combination of the symmetrized covariant derivatives $\xi_Q,\xi_{Qi_1},\ldots,\xi_{Q|(i_1\cdots i_l)}$,

$$P^U(\xi)=\sum_{l=0}^{n}T^{U;Qi_1\cdots i_l}\xi_{Qi_1\cdots i_l} \tag{2.2}$$

where $T^{U;Qi_1\cdots i_l}$ is the tensorial derivative[18] of T^U with respect to $\rho_{Qi_1\cdots i_l}$. It is not difficult to show[19] that for $m=2$,

$$T^{U;Qhk}=\partial^{Qhk}T^U$$

$$T^{U;\,Qhk}=\partial^{Qh}T^U+2\Gamma^Q_{Sk}\partial^{Shk}T^U+\Gamma^h_{lk}\partial^{Qlk}T^U$$

and

$$T^{U;Q}=\partial^Q T^U+\Gamma^Q_{Sh}(\partial^{Sh}T^U+\Gamma^S_{Tk}\partial^{Thk}T^U)+\Gamma^Q_{Sh,k}\partial^{Shk}T^U.$$

The transformation properties of T^U lead to certain differential *invariance identities*, one of these being (again for $m=2$),

$$2T^{U;l(j,hk)}g_{li}+T^{U;Q(hk}F_i{}^{j)R}_{Q}\rho_R=0, \tag{2.3}$$

where

$$T^{U;lj,hk}=\frac{\partial T^U}{\partial g_{lj,hk}}.$$

The following lemma will be used to show that if A^{rs} is a divergence-free concomitant of the type (1.1), then it is a polynomial in the second derivatives of both g_{ij} and ρ_Q.

Lemma 2.1: Let S denote a set with n elements and for integers $p,q\geqslant 1$ let

$$f=f(s_1,\ldots,s_p,t_1,u_1,\ldots,t_q,u_q):S^{p+2q}\to\mathbb{R}$$

be any function with the following three properties:

(i) it is totally skew-symmetric in the arguments $s_1,s_2,\ldots,s_p$, e.g.,

$$f(s_1,s_2,\ldots s_p,t_1,\ldots,u_q)=-f(s_2,s_1,\ldots s_p,t_1,\ldots,u_q);$$

(ii) it is a symmetric in the arguments t_lu_l for each $l=1,2,\ldots,q$, e.g.,

$$f(s_1,\ldots s_p,t_1,u_1,\ldots,u_q)=f(s_1,\ldots s_p,u_1,t_1,\ldots,u_q);$$

and

(iii) it satisfies the cyclic identity with respect to the arguments $s_kt_lu_l$ for each $k=1,\ldots,p$ and $l=1,\ldots,q$ e.g.,

$$f(s_1,\ldots s_p,t_1,u_1,\ldots,u_q)+f(u_1,\ldots s_p,s_1,t_1,\ldots,u_q)+f(t_1,\ldots,s_p,u_1,s_1,\ldots,u_q)=0.$$

Then f vanishes identically whenever $p+q>n$.

Proof: We introduce subsets A and $B_{\sigma,l}$ of S^{p+2q} with the definitions

$$A=\{(s_1,\ldots,s_p,t_1,u_1,\ldots,t_q,u_q)\,|$$

each $\sigma\in S$ occurs at least twice amongst the components $s_1,\ldots,s_p,t_1,u_1,\ldots,t_q,u_q\}$

for each $\sigma\in S$ and $l=1,2,\ldots,q$,

$$B_{\sigma,l}=\{(s_1,\ldots,s_p,t_1,u_1,\ldots,t_q,u_q)\,|\,\sigma\notin\{t_j,u_j\}\ \text{for all}\ j\neq l\}.$$

The union of all the sets A and $B_{\sigma,l}$ equals S^{p+2q} and so it suffices to prove that the restrictions of f to A and to $B_{\sigma,l}$ vanish. The former may be established using arguments devised by Lovelock[20] while the latter follows by induction on n.

In the next lemma n' equals n or $n+1$ according to whether n is even or odd.

Lemma 2.2: Let $T^{rs,i_1j_1,i_2j_2\cdots i_pj_p}$ be a tensorial concomitant of g_{ab} which enjoys the following symmetry properties:

(i) it is symmetric in the indices i_lj_l for all $l=1,2,\ldots,p$; and

(ii) it satisfies the cyclic identity with respect to the indices si_lj_l for all $l=1,2,\ldots,p$.

Then, provided $n>2$ and $1\leqslant p\leqslant n'-2$, $T^{rs,i_1j_1,\ldots,i_pj_p}$ satisfies the cyclic identity with respect to the indices ri_lj_l for all $l=1,2,\ldots,p$. If $p<n'-2$, then $T^{rs,i_1j_1\cdots i_pj_p}$ is also symmetric in the indices rs.

Proof: We shall establish this lemma by induction on p. For $p=1$ and $n>2$, the result follows from the explicit construction of the most general tensorial concomitant which satisfies (i) and (ii).[21] Let us now suppose that the lemma is true for $p=q-1$, where $2\leqslant q\leqslant n'-2$, and proceed to establish its validity when $p=q$. On multiplying the invariance identity

$$g^{tr}T^{us,i_1j_1\cdots i_qj_q}+g^{ts}T^{ru,i_1j_1\cdots i_qj_q}+\sum_{l=1}^{q}[g^{ti_l}T^{rs,i_1j_1\cdots uj_l\cdots i_qi_q}+g^{tj_l}T^{rs,i_1j_1\cdots i_lu\cdots i_qj_q}]$$

$$=g^{ur}T^{ts,i_1j_1\cdots i_qj_q}+g^{us}T^{rt,i_1j_1\cdots i_qj_q}+\sum_{l=1}^{q}[g^{ui_l}T^{rs,i_1j_1\cdots tj_l\cdots i_qj_q}+g^{uj_l}T^{rs,i_1j_1\cdots i_lt\cdots i_qj_q}]$$

by g_{ts}, on replacing u by s, and by repeatedly invoking properties (i) and (ii), it is found that

$$T^{sr,i_1j_1\cdots i_qj_q}+(n-q-1)\,T^{rs,i_1j_1\cdots i_qj_q}=g^{rs}U^{i_1j_1\cdots i_qj_q}-\tfrac{1}{2}\sum_{l=1}^{q}\Big[g^{si_l}V^{rj_l,i_1j_1\cdots(i_lj_l)\hat{}\cdots i_qj_q}_{(l)}+g^{sj_l}V^{ri_l,i_1j_1\cdots(i_lj_l)\hat{}\cdots i_qj_q}_{(l)}\Big] \tag{2.4}$$

where

$$U^{i_1j_1\cdots i_qj_q}=T^{ts,i_1j_1\cdots i_qj_q}g_{ts},$$

$$V^{rs,i_1j_1\cdots(i_lj_l)\hat{}\cdots i_qj_q}_{(l)}=T^{rs,i_1j_1\cdots i_{l-1}j_{l-1}abi_{l+1}j_{l+1}\cdots i_qj_q}g_{ab},$$

and the circumflex ( )$\hat{}$ enclosing a pair of indices indicates that those indices are to be deleted.

Since the induction hypothesis is applicable to $V^{rs,i_1j_1\cdots i_qj_q}_{(l)}$ each $V^{rs,i_1j_1\cdots i_qj_q}_{(l)}$ is symmetric in the indices rs. It now follows that each of these tensors is also symmetric under interchange of the pairs of indices rs and i_hj_h for all $h=1,2,\ldots,q-1$. By multiplying (2.4) by g_{rs} we therefore obtain the relation

$$U^{i_1j_1\cdots i_qj_q}=\frac{1}{q}\sum_{l=1}^{q}V^{i_1j_1,i_2j_2\cdots i_qj_q}_{(l)},$$

which implies that $U^{i_1j_1\cdots i_qj_q}$ enjoys all the symmetry properties of $V^{i_1j_1,i_2j_2\cdots i_qj_q}_{(l)}$. Consequently if we successively cycle on the indices $ri_{2l-1}j_{2l-1}$ and $si_{2l}j_{2l}$ in (2.4) we find, after a simple analysis of the resulting equation, that

$$U^{i_1j_1i_2j_2\cdots i_qj_q}=V^{i_1j_1i_2j_2\cdots i_qj_q}_{(l)}$$

for each $l=1,2,\ldots,q$. In view of this result and the various symmetry properties of $U^{i_1j_1\cdots i_qj_q}$, (2.4) simplifies to

$$T^{sr,i_1j_1\cdots i_qj_q}+(n-q-1)\,T^{rs,i_1j_1\cdots i_qj_q}=g^{rs}U^{i_1j_1\cdots i_qj_q}-\tfrac{1}{2}\sum_{l=1}^{q}[g^{si_l}U^{i_1j_1\cdots rj_l\cdots i_qj_q}+g^{sj_l}U^{i_1j_1\cdots i_lr\cdots i_qj_q}].$$

On account of the invariance identity for $U^{i_1j_1\cdots i_qj_q}$, the left-hand side of this equation is symmetric in rs and satisfies the cyclic identity on si_lj_l. Since the same must be true of the right-hand side, this proves the lemma for the case $p=q$, thereby completing our induction proof.

Theorem 2.3: Let A^{rs} be a tensorial concomitant of the type

$$A^{rs}=A^{rs}(g_{ij};g_{ij,h};g_{ij,hk}).$$

Then $A^{rs}{}_{|s}=0$ if, and only if $A^{rs}{}_{|r}=0$.

Proof: On account of the formula[22]

$$A^{rs}{}_{|t}=\tfrac{2}{3}A^{rs;\,ij,hk}R_{hijk|t},$$

it readily follows that the equations $A^{rs}{}_{|s}=0$ and $A^{rs}{}_{|r}=0$ are equivalent to

$$A^{rs;\,ij,hk}+A^{rk;\,ij,sh}+A^{rh;\,ij,ks}=0, \tag{2.5}$$

and

$$A^{rs;\,ij,hk}+A^{ks;\,ij,rh}+A^{hs;\,ij,kr}=0, \tag{2.6}$$

respectively. Consequently it suffices to show that (2.5) implies (2.6). From (2.3) it follows that

$$A^{rs;\,ij,hk}=A^{rs;\,hk,ij},$$

and so $A^{rs;\,ij,hk}$ also satisfies the cyclic identity with respect to the indices sij. We can apply Lemma 2.1 to the pth-order derivative of A^{rs} with respect to $g_{i_{2l-1}j_{2l-1},i_{2l}j_{2l}}$ ($l=1,2,\ldots,p$), viz.,

$$A^{rs;\,i_1j_1;\,i_2j_2;\,i_3j_3,i_4j_4;\,\ldots;i_{2p-1}j_{2p-1},i_{2p}j_{2p}},$$

to deduce that $A^{rs;\,i_1j_1,h_1k_1}$ is a polynomial in $g_{ab,cd}$ of degree no greater than $m-2$, where $m=n'/2$. This polynomial can be expressed in the form

$$A^{rs;\,i_1j_1,i_2j_2}=\sum_{l=0}^{m-2}T^{rsi_1j_1i_2j_2i_3j_3i_4j_4\cdots i_{2l-1}j_{2l-1}i_{2l}j_{2l}}\times R_{i_3i_4j_4}\cdots R_{i_{2l-1}i_{2l}j_{2l-1}j_{2l}},$$

where the coefficients $T^{rsi_1j_1\cdots i_{2l}j_{2l}}$ are tensorial concomitants of g_{ab} alone and enjoy the symmetry properties enumerated in Lemma 2.2. By virtue of this lemma each coefficient satisfies the cyclic identity with respect to the indices ri_2j_2. Therefore, (2.6) holds and the theorem is proved.

Lemma 2.4: If A^{rs} satisfies (1.1) and (1.2), then

$$A^{rs;\,ij,hk}+A^{rk;\,ij,sh}+A^{rh;\,ij,ks}=0, \tag{2.7}$$

$$A^{rl;\,Qhk}+A^{rk;\,Qlh}+A^{rh;\,Qkl}=0, \tag{2.8}$$

$$\tfrac{1}{2}(A^{rh;\,Qk}+A^{rk;\,Qh})+A^{rs;\,Qhk}{}_{|s}=0, \tag{2.9}$$

$$A^{rh;\,Q}+A^{rs;\,Qh}{}_{|s}+A^{rl;\,Rhk}R_R{}^Q{}_{lk}+\tfrac{2}{3}A^{rl;\,Qmk}R_m{}^h{}_{lk}=0, \tag{2.10}$$

and

$$\tfrac{1}{2}R_l{}^r{}_{hk}(A^{lh;\,Qk}-2A^{lh;\,Qkm}{}_{|m})-\tfrac{2}{3}R_l{}^r{}_{hk|m}A^{lh;\,Qkm}=0. \tag{2.11}$$

Proof: Equation (2.7) is the consequence of differentiating (1.2) with respect to $g_{ij,hks}$. To derive (2.8)–(2.10) we first remark that the principal forms $P^r(\xi)$ and $P^{rs}(\xi)$ of $A^{rs}{}_{|s}$ and A^{rs} with respect to ξ are related by

$$P^r(\xi)=[P^{rs}(\xi)]_{|s}.$$

By substituting into this identity from (2.2) and by equating the coefficients of $\xi_{Q|(hkl)}$, $\xi_{Q|(hk)}$, and $\xi_{Q|h}$ and ξ_Q in the resulting equation, we can conclude that the tensorial derivatives $[A^{rs}{}_{|s}]^{;\,Qhkl}$, $[A^{rs}{}_{|s}]^{;\,Qhk}$ and $[A^{rs}{}_{|s}]^{;\,Qh}$ are given by the left-hand sides of (2.8)–(2.10) respectively while $[A^{rs}{}_{|s}]^{;\,Q}=A^{rs;\,Q}{}_{|s}+\tfrac{1}{2}A^{rh;\,Rk}R_R{}^Q{}_{hk}+\tfrac{1}{3}A^{rh;\,Rkl}R_R{}^Q{}_{hk}\,|\,l$.

Equations (2.8)–(2.10) now follow on account of (1.2). Finally, (2.11) arises via the simplification of the identity

$$-[A^{rs}{}_{|s}]^{;\,Q}+[A^{rs}{}_{|s}]^{;\,Qh}{}_{|h}-[A^{rs}{}_{|s}]^{;\,Qhk}{}_{|hk}+[A^{rs}{}_{|s}]^{;\,Qhkl}{}_{|hkl}=0.$$

Lemma 2.5: If A^{rs} satisfies (1.1) and (1.2), then

$$D^{rs;\,Qhk}=0, \tag{2.12a}$$

$$D^{rs;\,Qh}=0, \tag{2.12b}$$

$$D^{rs;\,Q}=0, \tag{2.12c}$$

where $D^{rs}=\tfrac{1}{2}(A^{rs}+A^{sr})$.

Proof: To derive the first of (2.12), we begin by repeatedly differentiating (2.11), first with respect to $g_{ab,cde}$ and then with respect to ρ_{R_1,t_1u_1}, ρ_{R_2,t_2u_2}, $\ldots$, ρ_{R_p,t_pu_p} and $g_{i_1j_1,h_1k_1}$, $g_{i_2j_2,h_2k_2}$, $\ldots$, $g_{i_qj_q,h_qk_q}$. On multiplying the resulting equation by a totally symmetric but otherwise arbitrary tensor ψ_{cde}, we find that

$$[g^{ra}E^{Qb}+g^{rb}E^{Qa}+\psi_{cde}g^{re}D^{ab;\,Qcd}]^{;\,\alpha(p);\,\beta(0,q)}+\sum_{l=1}^{q}[g^{ri_l}F^{h_lk_lQj_lab}+g^{rj_l}F^{h_lk_lQi_lab}+g^{rh_l}F^{i_lj_lQk_lab}+g^{rk_l}F^{i_lj_lQh_lab}]^{;\,\alpha(p);\,\beta(l,q)}-\tfrac{8}{3}R_l{}^r{}_{hk}F^{lhQkab;\,\alpha(p);\,\beta(0,q)}=0, \tag{2.13}$$

where

$$E^{Qb}=\psi_{cde}D^{cd;\,Qeb},\quad F^{lhQkab}=\psi_{cde}D^{lh;\,Qke;ab,cd},$$

$$\alpha(p)=R_1t_1u_1;\,R_2t_2u_2;\cdots;\,R_pt_pu_p,$$

and

$$\beta(l,q)=i_1j_1,h_1k_1;\,i_2j_2,h_2k_2;\cdots;\,(i_lj_l,h_lk_l)\hat{}\,;\cdots;\,i_qj_q,h_qk_q.$$

Moreover, on account of (2.8), it follows from Lemma 2.1 that

$$D^{rs;\,Qhk;\,\alpha(n-1)}=0.$$

Hence, to establish the lemma by mathematical induction, it suffices to show that if

$$D^{rs;\,Qhk;\,\alpha(p+1)}=0, \tag{2.14}$$

where $0\leqslant p\leqslant n-2$, then

$$D^{rs;\,Qhk;\,\alpha(p)}=0. \tag{2.15}$$

In order to derive (2.15) from (2.14) we shall use a second inductive argument. To start, we note that on account of (2.14) $D^{rs;\,Qhk;\,\alpha(p)}$ is independent of $\rho_{Q,ij}$ in which case (2.3) leads to

$$D^{rs;\,Qhk;\alpha(p);\,ab,cd} = D^{rs;\,Qhk;\alpha(p);\,cd,ab}.$$

By appealing once more to Lemma 2.1, we find that

$$E^{Qb;\,\alpha(p);\,\beta(0,q')} = 0 \quad \text{and} \quad F^{i_1j_1\ldots i_lj_lQbh_1k_1\ldots h_lk_l;\,\alpha(p);\,\beta(l,q')} = 0$$

whenever $p+2q' \geqslant n$. Therefore, let us suppose that

$$E^{Qb;\,\alpha(p);\,\beta(0,q+1)} = 0 \quad \text{and} \quad F^{i_1j_1\ldots i_lj_lQbh_1k_1\ldots h_lk_l;\,\alpha(p);\,\beta(l,q+1)} = 0 \tag{2.16}$$

for $p+2q<n$ and proceed to establish the validity of (2.16) with $q+1$ replaced by q. In view of the second of (2.16), multiplication of (2.13) by g_{ra} gives rise to

$$nE^{Qb;\,\alpha(p);\,\beta(0,q)} - \sum_{l=1}^{q} [F^{h_lk_lQbi_1j_1\ldots i_lj_l} + F^{i_1j_1\ldots i_lj_lQbh_1k_1\ldots h_lk_l}]^{;\alpha(p);\,\beta(l,q)} = 0. \tag{2.17}$$

Similarly multiplication of (2.13) by g_{rh_1} yields (on replacing the indices k_1ab by bh_1k_1)

$$-E^{Qb;\,\alpha(p);\,\beta(0,q)} + nF^{i_1j_1;Qbh_1k_1;\,\alpha(p);\,\beta(1,q)} - F^{h_1k_1Qbi_1j_1;\,\alpha(p);\,\beta(1,q)} - \sum_{l=2}^{q} [F^{h_1k_1\ldots h_lk_lQbh_1k_1;\,i_1j_1,\,i_1j_1\ldots i_lj_l} + F^{i_1j_1\ldots i_lj_lQbh_1k_1;\,i_1j_1,\,h_1k_1\ldots h_lk_l}]^{;\,\alpha(p);\,i_1j_2,h_2k_2;\cdots;\,(i_1j_1,h_1k_1)\hat{}\,;\cdots;\,i_qj_q,h_qk_q} = 0. \tag{2.18}$$

By repeatedly permuting all pairs of indices i_lj_l and h_lk_l for $l=1,\ldots,q$ in (2.17) and (2.18) we obtain a homogeneous system of linear equations whose coefficient matrix is non-singular.[23] This implies that (2.16) remains valid with $q+1$ replaced by q and thus, by induction on q,

$$E^{Qb;\,\alpha(p)} = 0 \quad \text{and} \quad F^{ijQbhk;\,\alpha(p)} = 0.$$

It is now an elementary matter to obtain (2.15) from (2.13) (with $q=0$). This completes our original induction argument and establishes (2.12a).

Due to (2.12a), (2.8), (2.9), and Bianchi identities, (2.11) reduces to

$$R_l{}^r{}_{hk} D^{lh;\,Qk} = 0. \tag{2.19}$$

By cycling on the indices rhk in (2.9) and by covariantly differentiating (2.9) with respect to x^r it is found that

$$D^{rh;\,Qk} + D^{kr;\,Qh} + D^{hk;\,Qr} = 0 \tag{2.20}$$

and

$$\tfrac{1}{2}(A^{rh;\,Qk} + A^{rk;\,Qh})_{|r} - \tfrac{1}{2}A^{rs;\,Rhk}R_R{}^Q{}_{rs} - \tfrac{1}{3}A^{kr;Qms}R_m{}^h{}_{rs} = 0. \tag{2.21}$$

Differentiation of (2.21) with respect to $g_{ab,cds}$ leads to

$$D^{rh;\,Qs;\,ab,cd} + D^{rh;\,Qd;\,ab,sc} + D^{rh;\,Qc;\,ab,ds} = 0. \tag{2.22}$$

On account of the symmetry properties (2.20) and (2.22), it is possible to derive (2.12b) from (2.19) by an induction argument similar to that used to obtain (2.12a).

Finally, on noting (2.21), (2.12c) follows directly from the result of symmetrizing (2.10) on the indices r and h.

Lemma 2.6: If C^{rs} is a skew-symmetric divergence-free concomitant of the type (1.1), then

$$P^{rs}(\xi) = V^{rst}{}_{|t}, \tag{2.23}$$

where $P^{rs}(\xi)$ is the principal form of C^{rs} and[24]

$$V^{rst}(\rho;\xi) = \tfrac{3}{2}C^{[rs;\,Qt]u}\xi_{Q|u} + [C^{[rs;\,Qt]} - \tfrac{1}{2}C^{[rs;\,Qt]u}{}_{|u}]\xi_Q.$$

Proof: Let $C^r = C^{rs}{}_{|s}$. Then (2.23) follows immediately from the formula

$$P^{rs}(\xi) = V^{rst}{}_{|t} + \tfrac{3}{2}C^{[r;\,Qs]tu}\xi_{Q|tu} + [\tfrac{4}{3}C^{[r;\,Qs]t} - C^{[r;\,Qs]tu}{}_{|u}]\xi_{Q|t} + [C^{[r;\,Qs]} - \tfrac{2}{3}C^{[r;\,Qs]t}{}_{|t} + \tfrac{1}{2}C^{[r;Qs]tu}{}_{|tu}]\xi_Q$$

which may be verified by direct calculation.

It is now a simple matter to prove the theorem stated in the introduction. Indeed, in view of Lemma 2.5, the tensor[25]

$$C_1^{rs} = \int_0^1 [\tilde{A}^{rs;\,Q}\rho_Q + \tilde{A}^{rs;\,Qh}\rho_{Q|h}] + \tilde{A}^{rs;\,Qhk}\rho_{Q|hk}\,dt,$$

where

$$\tilde{A}^{rs} = A^{rs}(g_{ij}; g_{ij,h}; g_{ij,hk}; t\rho_Q; t\rho_{Q,h}; t\rho_{Q,hk})$$

is skew-symmetric in the indices rs. Moreover, on recalling (2.1) and (2.2) it is easily seen that

$$A^{rs} = A_0^{rs} + C_1^{rs}, \tag{2.24}$$

where $A_0^{rs} = A^{rs}(g_{ij}; g_{ij,h}; g_{ij,hk}; 0; 0; 0)$. Since (1.2) implies that A_0^{rs} is divergence-free with respect to the index s we may refer to Theorem 2.3 to conclude that A_0^{rs} is divergence-free with respect to the index r and can therefore be expressed in the form

$$A_0^{rs} = B^{rs} + C_2^{rs},$$

where B^{rs} and C_2^{rs} are respectively symmetric and skew-symmetric divergence-free concomitants of the type (1.4). Because A^{rs} and A_0^{rs} are divergence-free on the index s, it follows from (2.24) that the same must be true of C_1^{rs}. How-

ever, C_1^{rs} is skew-symmetric in its indices and therefore by setting

$$C^{rs} = C_1^{rs} + C_2^{rs}$$

we arrive at (1.3). Finally, (1.5) follows from Lemma 2.6 upon setting

$$E^{rst} = \int_0^1 V^{rst}(\rho; t\rho)\, dt.$$

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[23]See Ref. 2, Lemmas 2.2 and 4.2.
[24]Square brackets indicate skew-symmetrization over the enclosed lower case indices only.
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Constraint on the compound depolarization factor of aligned ellipsoids[a)]

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The bulk parameters for random distributions of aligned ellipsoidal particles with nonsimilar ellipsoidal exclusion surface (the locus of the minimum separation of particle centers) can be specified by a compound depolarization factor D. It is shown that D is positive for all physically realizable values of the fraction of space occupied by particles.

In recent papers[1,2] we generalized the Maxwell (Clausius, Mossotti, Lorenz, Lorentz) form for the bulk relative parameter (P) for a random distribution of identical spheres (with relative parameter p) to the analogous problem of tensor parameters for aligned ellipsoids and nonsimilar cocentered ellipsoidal exclusion surfaces. In particular, for the case where the principal axes of the ellipsoids, of their tensor parameter, and of the exclusion surface were parallel, corresponding to (145)[1] and (183)[2], we obtained the form

$$P_i-1=\Delta_i=w\delta_i/(1+\delta_i D_i),\quad \delta_i=p_i-1,$$
$$D_i=q_i-wQ_i. \tag{1}$$

Here

$$w=(N4\pi/3V)a_1a_2a_3,\qquad 0\leqslant w\leqslant w_r<1, \tag{2}$$

is the fraction of space V occupied by N ellipsoidal particles with semidiameters a_i; their shape factors q_i are given by Maxwell's depolarization integrals

$$q_i=a_1a_2a_3\int_0^\infty I(a_i,x)\,dx\equiv q_i(a_i),$$
$$1/I(a_i,x)=2(a_1^2+x)\,[(a_1^2+x)(a_2^2+x)(a_3^2+x)\,]^{1/2},$$

$$\sum_{i=1}^{3}q_i=1, \tag{3}$$

and Q_i is an analogous set for the exclusion surface. For the corresponding two-dimensional problem of aligned elliptic cylinders ($a_3\to\infty$),

$$q_1=a_2/(a_1+a_2)=1-q_2,\quad q_3=0, \tag{4}$$

and $w=(N\pi/V)a_1a_2$ with V as a surface. In the following, we show that the compound depolarization factor D_i of (1) is positive for all physically realizable values of w.

For isotropic ($\delta_i=\delta$) spherical particles ($a_i=a$) and spherical exclusion surfaces of radius $2a$ (associated with the usual radially symmetric pair-correlation function for a gas of hard spheres of radius a), we have $q_i=Q_i=\frac{1}{3}$, and (1) reduces to Maxwell's result[3]

$$\Delta=w\delta/[1+\delta\tfrac{1}{3}(1-w)],\quad 0\leqslant w\leqslant w_r<1. \tag{5}$$

Although the upper bound w_r (the densest random packing of identical spheres) has not been determined analytically, several measurement producers[4] give $w_r\approx 0.63$. The analogous problem of circular cylinders, $q_i=Q_i=\frac{1}{2}$, corresponds to the replacement of $\frac{1}{3}$ by $\frac{1}{2}$ in (5); for the upper bound w_r (the densest random packing of identical circular disks on a plane), we have used[5] $w_r\approx 0.84$.

For the analogous problem of aligned ellipsoids (a_i) and similar exclusion surfaces with semidiameters $2a_i$ (corresponding to elliptically symmetric pair correlations of aligned hard ellipsoids with semidiameters a_i), we have $Q_i=q_i(2a_i)=q_i(a_i)$, and (1) reduces to

$$\Delta_i=w\delta_i/[1-\delta_i q_i(1-w)\,]. \tag{6}$$

Since $q_i=|q_i|$ and $w\leqslant w_r<1$, it is clear that for this case the compound depolarization factor $D_i=q_i(1-w)$ is positive. For the more general case (1), the statements after (145)[1] and (183)[2] mentioned positive and negative values of $D_i=q_i-wQ_i$; although negative values are not excluded by $w\leqslant w_r<1$, we now show that only positive values are physically realizable because of an implicit constraint that bounds w below w_r for $Q_i\neq q_i$.

The constraint may be introduced explicitly in the simpler context of spherical particles. Thus, Maxwell's form Δ as in (5) also applies if the exclusion surface is a sphere of radius $2A=2ca>2a$, but for such cases w cannot attain the upper ound w_r. To facilitate discussion, we regard the particles of radius a as coated with a hard transparent shell of thickness $A-a$ (i.e., a shell having the same value for the parameter as the imbedding space). We write the volume fraction of coated particles (henceforth the envelopes of radius A) as $W=w(A/a)^3$ such that

$$0\leqslant W\leqslant W_r=w_r, \tag{7}$$

i.e., the densest packing of the spherical envelopes is that of hard spheres. Consequently, the volume fraction of the scattering particles (the spheres with parameter p) is restricted to[5]

$$0\leqslant w\leqslant w_r a^3/A^3=w_r/c^3,\quad c=A/a>1. \tag{8}$$

Thus, although (5) is appropriate, its range of physical realizability in w is bounded below w_r.

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The same considerations apply for aligned ellipsoidal particles (a_i) and similar envelopes ($A_i = c\,a_i > a_i$), i.e., for $Q_i = q_i(c\,a_i) = q_i(a_i)$; the form Δ_i of (6) applies but w cannot attain w_r. Because the volume fraction of the envelopes satisfies (7), w in (6) is restricted to

$$0 \leqslant w \leqslant w_r \Pi_i a_i / \Pi_i A_i, \quad a_i < A_i \tag{9}$$

which with $A_i = c\,a_i$ reduces to w_r/c^3 as for (8).

For the general case (1), the relation of the volume fraction of the particles to that of their envelopes,

$$w = W \Pi_i a_i / \Pi_i A_i, \quad 0 \leqslant W \leqslant W_r < 1, \ a_i \leqslant A_i, \tag{10}$$

provides the constraint that insures $D_i > 0$ for all realizable values of q_i and Q_i. Thus for elliptic cylinders specified by $q_i(a_i)$ of (4) and nonsimilar envelopes $Q_i = q_i(A_i) \neq q_i(a_i)$, we have

$$\begin{aligned} D_i &= q_i - w Q_i = q_i - W \frac{a_1 a_2}{A_1 A_2} Q_i \\ &= \frac{a_j}{a_1 + a_2} - W \frac{a_1 a_2}{A_1 A_2} \frac{A_j}{(A_1 + A_2)} \end{aligned} \tag{11}$$

with $i = 1,2$ and $j = 2,1$ as the complement. We write

$$D_i = a_1 a_2 \left[\frac{1}{a_i (a_1 + a_2)} - \frac{W}{A_i (A_1 + A_2)} \right] > 0 \tag{12}$$

where the inequality holds whether $a_2 > A_1$ or $a_2 < A_1$ provided that $A_1 \geqslant a_1$, and $A_2 \geqslant a_2$. Similarly for ellipsoidal particles specified by $q_i(a_i)$ of (3) and nonsimilar envelopes $Q_i = q_i(A_i)$, we use (10) in D_i to obtain

$$D_i = q_i - w Q_i = a_1 a_2 a_3 \int_0^\infty [I(a_i, x) - W I(A_i, x)]\, dx > 0. \tag{13}$$

The inequality follows from (3) with $I(a_i, x) \geqslant I(A_i, x)$ for $A_i \geqslant a_i$, and from $W \leqslant W_r < 1$. Thus $D_i > 0$ holds for all realizable cases including oblate particles within prolate envelopes, or prolate within oblate, etc. The greater generality associated with $Q_i \neq q_i$ is that the configurational contribution $w Q_i < q_i$ in (1) may be greater or less than $w q_i$, the contribution for the special case of envelope similar to particle.

We extend the essentials directly to the more general case of noncoincident axes of the corresponding dyadics $\tilde{\mathbf{q}}, \tilde{\mathbf{p}}, \tilde{\mathbf{Q}}$. We write (144)[1] and (182)[2] as

$$\begin{aligned} &\tilde{\boldsymbol{\Delta}} \cdot (\tilde{\mathbf{I}} + \tilde{\mathbf{Q}} \cdot \tilde{\boldsymbol{\Delta}})^{-1} = w \tilde{\boldsymbol{\delta}} \cdot (\tilde{\mathbf{I}} + \tilde{\mathbf{q}} \cdot \tilde{\boldsymbol{\delta}})^{-1} \equiv \tilde{\mathbf{R}}(w, \tilde{\boldsymbol{\delta}}, \tilde{\mathbf{q}}), \\ &\tilde{\boldsymbol{\Delta}} = \tilde{\mathbf{P}} - \tilde{\mathbf{I}}, \quad \tilde{\boldsymbol{\delta}} = \tilde{\mathbf{p}} - \tilde{\mathbf{I}}, \end{aligned} \tag{14}$$

where $\tilde{\mathbf{I}}$ is the identity dyadic and $\tilde{\mathbf{R}}$ is an abbreviation. For an isotropic imbedding space characterized by p_0, the relative dyadic parameters equal $\tilde{\mathbf{P}} = \tilde{\mathbf{P}}'/p_0$, $\tilde{\mathbf{p}} = \tilde{\mathbf{p}}'/p_0$, with the prime indicating nonnormalized values; if the imbedding space is anisotropic ($\tilde{\mathbf{p}}_0$), then $\tilde{\mathbf{P}} = \tilde{\mathbf{P}}' = \tilde{\mathbf{p}}_0^{-1}$, $\tilde{\mathbf{p}} = \tilde{\mathbf{p}}' \cdot \tilde{\mathbf{p}}_0^{-1}$, From (14) we have $\tilde{\boldsymbol{\Delta}} = \tilde{\mathbf{R}} \cdot (\tilde{\mathbf{I}} + \tilde{\mathbf{Q}} \cdot \tilde{\boldsymbol{\Delta}})$; thus $(\tilde{\mathbf{I}} - \tilde{\mathbf{R}} \cdot \tilde{\mathbf{Q}}) \cdot \tilde{\boldsymbol{\Delta}} = \tilde{\mathbf{R}}$, and consequently

$$\tilde{\boldsymbol{\Delta}} = (\tilde{\mathbf{I}} - \tilde{\mathbf{R}} \cdot \tilde{\mathbf{Q}})^{-1} \cdot \tilde{\mathbf{R}} = [\tilde{\mathbf{R}}^{-1} \cdot (\tilde{\mathbf{I}} - \tilde{\mathbf{R}} \cdot \tilde{\mathbf{Q}})]^{-1} = (\tilde{\mathbf{R}}^{-1} - \tilde{\mathbf{Q}})^{-1}. \tag{15}$$

Substituting $\tilde{\mathbf{R}}^{-1} = (\tilde{\mathbf{I}} + \tilde{\mathbf{q}} \cdot \tilde{\boldsymbol{\delta}})(w\tilde{\boldsymbol{\delta}})^{-1} = (\tilde{\boldsymbol{\delta}}^{-1} + \tilde{\mathbf{q}})/w$, we obtain

$$\tilde{\boldsymbol{\Delta}} = w(\tilde{\boldsymbol{\delta}}^{-1} + \tilde{\mathbf{D}})^{-1} = w(\tilde{\mathbf{I}} + \tilde{\boldsymbol{\delta}} \cdot \tilde{\mathbf{D}})^{-1} \cdot \tilde{\boldsymbol{\delta}}, \quad \tilde{\mathbf{D}} = \tilde{\mathbf{q}} - w\tilde{\mathbf{Q}} \tag{16}$$

with $\tilde{\mathbf{D}}$ as the compound depolarization dyadic.

In the system ($\hat{\mathbf{z}}_i = \hat{\mathbf{z}}, \hat{\mathbf{x}}, \hat{\mathbf{y}}$) in which $\tilde{\mathbf{Q}}$ is diagonal, we write

$$\tilde{\mathbf{Q}} = \sum Q_i \hat{\mathbf{z}}_i \hat{\mathbf{z}}_i, \quad \tilde{\mathbf{q}} = \sum q_n \hat{\boldsymbol{\xi}}_n \hat{\boldsymbol{\xi}}_n = \sum q_{ij} \hat{\mathbf{z}}_i \hat{\mathbf{z}}_j \tag{17}$$

and

$$\begin{aligned} &\tilde{\mathbf{D}} = \sum D_{ij} \hat{\mathbf{z}}_i \hat{\mathbf{z}}_j, \\ &D_{ii} = q_{ii} - w Q_i, \quad D_{ij} = q_{ij} \quad \text{for} \quad i \neq j. \end{aligned} \tag{18}$$

We use $\hat{\boldsymbol{\xi}}_i = \hat{\mathbf{r}}, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\varphi}}$ in terms of the direction cosines ($\alpha_i = |\alpha_i| < 1$) of $\hat{\boldsymbol{\xi}}_1 = \hat{\mathbf{r}}$ in $\hat{\mathbf{z}}_i$, i.e.,

$$\begin{aligned} &\hat{\boldsymbol{\xi}}_1 = \sum \alpha_i \hat{\mathbf{z}}_i, \\ &\hat{\boldsymbol{\xi}}_2 = [-(1 - \alpha_1^2)\hat{\mathbf{z}}_1 + \alpha_1 \alpha_2 \hat{\mathbf{z}}_2 + \alpha_1 \alpha_3 \hat{\mathbf{z}}_3]/(1 - \alpha_1^2)^{1/2}, \\ &\hat{\boldsymbol{\xi}}_3 = (-\alpha_3 \hat{\mathbf{z}}_2 + \alpha_2 \hat{\mathbf{z}}_3)/(1 - \alpha_1^2)^{1/2} \end{aligned} \tag{19}$$

and take $a_1 < a_2 < a_3$, so that $q_1 > q_2 > q_3$, in order to show directly that $D_{ij} > 0$ for all i,j.

Thus, from $q_{ij} = \sum q_n (\hat{\mathbf{z}}_i \cdot \hat{\boldsymbol{\xi}}_n)(\hat{\boldsymbol{\xi}}_n \cdot \hat{\mathbf{z}}_j) = q_{ji}$, we obtain

$$\begin{aligned} &q_{11} = q_1 \alpha_1^2 + q_2(1 - \alpha_1^2), \quad q_{12} = q_{21} = \alpha_1 \alpha_2 (q_1 - q_2), \\ &q_{13} = q_{31} = \alpha_1 \alpha_3 (q_1 - q_2), \\ &q_{22} = q_1 \alpha_2^2 + (q_2 \alpha_1^2 \alpha_2^2 + q_3 \alpha_3^2)/(1 - \alpha_1^2), \\ &q_{23} = q_{32} = \alpha_2 \alpha_3 [(q_1 - q_2) + (q_2 - q_3)/(1 - \alpha_1^2)], \\ &q_{33} = q_1 \alpha_3^2 + (q_2 \alpha_1^2 \alpha_3^2 + q_3 \alpha_2^2)/(1 - \alpha_1^2), \quad \sum \alpha_i^2 = 1. \end{aligned} \tag{20}$$

Since all $q_{ij} > 0$, we have $D_{ij} > 0$ for $i \neq j$, and we need consider only D_{ii}.

We write

$$\begin{aligned} &D_{ii} = q_{ii} - w Q_i = a_1 a_2 a_3 \int_0^\infty J_i(x)\, dx, \\ &J_i(x) = \sum I(a_n, x)(\hat{\mathbf{z}}_i \cdot \hat{\boldsymbol{\xi}}_n)^2 - W I(A_i, x). \end{aligned} \tag{21}$$

From I of (3), we see that if $J_i(0) > 0$, then $J_i(x) > 0$. Since the distances (a_{ii}) to points $a_{ii}\hat{\mathbf{z}}_i$ on the particle's surface $\Sigma_n (a_{ii}\hat{\mathbf{z}}_i \cdot \hat{\boldsymbol{\xi}}_n / a_n)^2 = 1$ intersected by $\hat{\mathbf{z}}_i$ satisfy $a_{ii} < A_i$,

$$\frac{1}{a_{ii}^2} = \sum \frac{(\hat{\mathbf{z}}_i \cdot \hat{\boldsymbol{\xi}}_n)^2}{a_n^2} > \frac{1}{A_i^2}, \tag{22}$$

and since $\Pi_i A_i > \Pi_n a_n$, we see that $J_i(0) > 0$. Thus $D_{ii} > 0$, and consequently all $D_{ij} > 0$.

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Asymptotic graph counting techniques in ψ^{2N} field theory

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We discuss two different techniques for obtaining asymptotic estimates of the number of n-vertex graphs in a ψ^{2N} field theory as $n\to\infty$. The first technique relies on difference equations and the second makes use of Lipatov's methods. We show how various topological constraints, such as connectedness and Wick ordering, affect the total number of graphs. We show, for example, that Wick ordering reduces the total number of connected graphs by a factor of $e^{N-1/2}$ as $n\to\infty$.

I. INTRODUCTION

There has been much interest lately in the behavior of Feynman perturbation theory in large order.[1] As n, the order of perturbation theory, approaches ∞ the nth term in the perturbation expansion of ψ^{2N} quantum field theory in D dimensions behaves like

$$n^{an}b^{n}n^{c}d\,[1+O(n^{-1})],$$

where a, b, c, and d are constants. It has been shown that n^{an}, the most rapidly varying component of this behavior, is determined by the number of Feynman graphs and not by the values of the Feynman integrals.[1] Therefore, it is essential to develop techniques for making precise asymptotic estimates of the number of graphs as n, the number of vertices, becomes large.

In this paper we present two different combinatorial methods for counting numbers of graphs having many vertices. The first approach consists of finding a difference equation which relates the number of graphs for different n and then solving this difference equation asymptotically for large n. The second approach uses Lipatov's method to approximate a generating function representation of ψ^{2N} field theory in zero-dimensional space-time.

The crucial idea in graph counting is the *symmetry number* of a graph. The symmetry number of a graph is defined as the reciprocal of the number of ways the graph can be turned into itself by permuting the lines or vertices. In Fig. 1 we give examples of graphs, each with its accompanying symmetry number.

We can now define what we mean by the *number* of graphs. *We count a set of n-vertex graphs in a ψ^{2N} field theory by summing the symmetry numbers of the graphs in that set and then multiplying this result by the factor* $[(2N)!]^n$. We choose this definition of the *number* of graphs in a set because it is the same as the definition of the Feynman amplitude in quantum field theory corresponding to that set of graphs in which the Feynman integrals have all been set equal to 1.

We now summarize the organization and content of this paper. In Sec. II we compute the total number of *unconstrained* graphs having n vertices. We show that there are precisely

$$(2Nn+J-1)!!/n! \tag{1.1}$$

(connected plus disconnected) graphs having n vertices and J external legs in a ψ^{2N} field theory.

In Sec. III we consider the topological constraint of connectedness. The restriction is not very strong: We show that as $n\to\infty$ the ratio of the number of connected graphs to the total number of connected plus disconnected graphs approaches 1.

In Sec. IV we consider the constraint of Wick ordering. Wick ordering eliminates all graphs containing self-loops (lines which emerge from and return to the same vertex) and therefore reduces the total number of graphs in any order. We show that as $n\to\infty$, Wick ordering reduces the number of graphs in a ψ^{2N} theory by a factor of $e^{N-1/2}$.

In Sec. V we use Lipatov's methods to consider the other kinds of topological constraints (eliminating all diagrams with specific kinds of vertex or mass corrections). It is remarkable that imposing any finite number of these topological constraints does not alter the factorial growth of the number of graphs in the theory as $n\to\infty$.

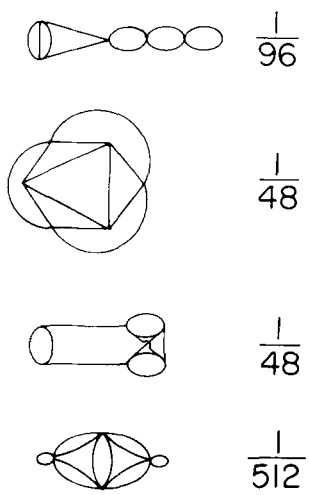

FIG. 1. Four graphs and their accompanying symmetry numbers are shown.

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II. TOTAL NUMBER OF GRAPHS

In this section we compute $A_n(J,2N)$, the total number of graphs (connected and disconnected) having n vertices and J external legs in a ψ^{2N} field theory. Note that J must be an even integer. First, we use a combinatorial approach.[2] There are a total of $2Nn+J$ lines, $2N$ emerging from each vertex and J external lines, that must be connected in all possible ways to make all possible graphs. We begin by choosing any line and connecting it to one of the remaining $2Nn+J-1$ lines. There are $2Nn+J-1$ ways to do this. We are now left with $2Nn+J-2$ free lines. We choose any one of these lines and connect it to one of remaining $2Nn+J-3$ lines. There are $2Nn+J-3$ ways to do this. We continue this process until all lines are connected. Finally, to avoid overcounting we divide by $n!$, the number of arrangements of the vertices. This gives

$$A_n(J,2N)=\frac{(2nN+J-1)!!}{n!}. \tag{2.1}$$

For example, if $J=2$, $N=2$, and $n=2$, (2.1) gives $9!!/2!=3\cdot5\cdot7\cdot9/2$. This result is verified in Fig. 2.

An alternative way to derive (2.1) makes use of the path intergral representation for the J-point Green's function in a ψ^{2N} field theory in D-dimensional space–time:

$$G(x_1,\ldots,x_J)\propto\int d\phi\,\phi(x_1)\cdots\phi(x_J)$$

$$\times\exp\left\{\int\mathscr{L}[\phi(x)]d_Dx\right\}.$$

The case under consideration is particularly simple because all Feynman integrals are 1. This obtains when $D=0$. Furthermore, when $D=0$ the path integral reduces to an ordinary integral:

$$G(g,J,2N)=\int_{-\infty}^{\infty}dx\,x^J\exp(-\tfrac{1}{2}x^2-g\,x^{2N})/\sqrt{2\pi}\,, \tag{2.2}$$

where we have normalized by dividing by $G(0,0,2N)=\sqrt{2\pi}$.

If we now expand $G(g,J,2N)$ into a power series in g, we find that the coefficient of $(-g)^n$ is precisely $(2nN+J-1)!!/n!$.

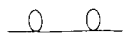
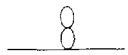
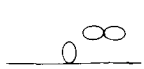
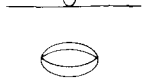
Graph	Symmetry Number	(Symmetry Number)(4!)^2
	$\frac{1}{6}$	96
	$\frac{1}{4}$	144
	$\frac{1}{4}$	144
	$\frac{1}{16}$	36
	$\frac{1}{48}$	12
	$\frac{1}{16}$	36
	$\frac{1}{128}$	$\frac{9}{2}$
Total		$\frac{945}{2}$

FIG. 2. Graphs contributing to $A_2(2,4)$; that is, all graphs having two external legs and two vertices in a ϕ^4 theory. Equation (2.1) predicts that the value of $A_2(2,4)$ is $9!!/2!=945/2$.

III. THE CONNECTEDNESS CONSTRAINT

Suppose we now select from the set of graphs that go to make up $A_n(J,2N)$ just those graphs that are connected. We define $C_n(J,2N)$ as the sum of the connected graphs. How much smaller than $A_n(J,2N)$ is $C_n(J,2N)$?

An exact difference equation relating $A_n(0,2N)$ and $C_n(0,2N)$ is

$$A_n-C_n=\frac{1}{n}\sum_{k=1}^{n-1}k\,C_k\,A_{n-k}, \tag{3.1}$$

where we have suppressed the indices J and N. This equation is merely an enumeration of all the disconnected graphs which constitute A_n-C_n.

The content of (3.1) can be restated in generating function form. We define the connected Green's function $G_{\text{connected}}(g,J,2N)$ in terms of its asymptotic series in powers of g:

$$G_{\text{connected}}(g,0,2N)\sim\sum_{n=1}^{\infty}C_n(0,2N)(-g)^n. \tag{3.2}$$

Then the difference equation (3.1) is exactly equivalent to

$$G_{\text{connected}}(g,0,2N)=\ln G(g,0,2N). \tag{3.3}$$

The simplest way to find the relation between A_n and C_n for large n is to use (3.1). As $n\to\infty$, the largest term in the convolution sum is the last ($k=n-1$). The next largest terms are the $k=1$ and $k=n-2$ terms, and so on. Retaining just the $k=n-1$ term, we have

$$C_n\sim A_n\left[1-\frac{a}{n^{N-1}}-\cdots\right]\quad(n\to\infty), \tag{3.4}$$

where a is a positive constant depending on N:

$$a=(2N-1)!!/2^N N^N. \tag{3.5}$$

For example, if $N=2$ and $n=7$, then $a=3/16$. We know from (2.1) that

$$A_7=27\cdot25\cdot23\cdot21\cdot19\cdot17\cdot15\cdot13\cdot11\cdot3/16$$

and from (3.1) that

$$C_7=27\cdot23201\cdot24^4/7.$$

Thus,

$$C_7/A_7\doteq0.961.$$

This is to be compared with our prediction in (3.4) that

$$1-\frac{3}{16\cdot7}\doteq0.973.$$

From (3.4) we conclude that

$$\lim_{n\to\infty}\frac{C_n(0,2N)}{A_n(0,2N)}=1. \tag{3.6}$$

This shows that eliminating disconnected graphs is not a major effect in large order (large n).

The results is (3.6) is valid even when $J\neq 0$. For example, when $J=2$ (3.1) is replaced by

$$A_n(2,2N)-C_n(2,2N)=\sum_{k=0}^{n-1}C_k(2,2N)A_{n-k}(0,2N), \tag{3.7}$$

where $C_0(2,2N)=1$. Analysis of (3.7) for large n gives (3.6) with 0 replaced by 2. We obtain more complicated convolution equations as J increases, but the result is still that given in (3.6) with 0 replaced by J.

IV. THE WICK-ORDERING CONSTRAINT

Wick ordering is a constraint which eliminates all graphs having self-loops.

A. Difference-equation approach

Consider first the special case of a ψ^4 ($N=2$) theory with $J=0$ (vacuum graphs). For this special class of graphs each graph has precisely $2n$ lines, and, if it is connected and $n>1$, it may have from 0 to n self-loops (at most one self-loop for each vertex). Let $W_{n,k}$ stand for the sum of all connected graphs having n vertices and k self-loops. Then

$$C_n=\sum_{k=0}^{n}W_{n,k}. \tag{4.1}$$

Furthermore, $W_{n,k}$ satisfies the difference equation

$$W_{n,k}=\frac{12}{k}\left[(2n-k-1)\,W_{n-1,k-1}+k\,W_{n-1,k}\right]\quad(k\geqslant 1). \tag{4.2}$$

To derive (4.2), we use the following combinatorial argument: We obtain all of the graphs in the class $W_{n,k}$ by inserting one vertex, with a self-loop attached, to (i) one of the self-loops of each of the graphs of the class $W_{n-1,k}$ (there are k ways to do this because each graph in this class has k self-loops); or to (ii) one of the lines (not a self-loop) of each of the graphs of the class $W_{n-1,k-1}$ (there are $2n-k-1$ ways to do this because each graph in this class has $2n-k-1$ lines that are not self-loops). We must then multiply by $4!=24$ because we have added a new vertex, divide by 2 because that is the symmetry number associated with one self-loop, and divide by k because each graph in $W_{n,k}$ has k self-loops and has therefore been produced k times too often. This reproduces (4.2).

Next we find the approximate solution (4.2) for large n. We will show that

$$\lim_{n\to\infty}C_n/W_{n,0}=e^{3/2}\doteqdot 4.482 \tag{4.3}$$

Substituting (4.2) into (4.1) gives

$$C_n=W_{n,0}+24(n-1)W_{n-1,0}+12(2n-1)\sum_{k=1}^{n-1}\frac{W_{n-1,k}}{k+1}.$$

Substituting (4.2) into this equation gives

$$C_n=W_{n,0}+24(n-1)W_{n-1,0}+12(2n-1)\,12\,(n-2)\,W_{n-2,0}+12^2(2n-1)(2n-2)\sum_{k=1}^{n-2}\frac{W_{n-2,k}}{(k+1)(k+2)}.$$

After substituting (4.2) m times, we obtain

$$C_n=a_nW_{n,0}+a_{n-1}W_{n-1,0}+\cdots+a_{n-m}W_{n-m,0}+b_{n-m}\sum_{k=1}^{n-m}\frac{W_{n-m,k}}{(k+1)(k+2)\cdots(k+m)}, \tag{4.4}$$

where we find using induction that

$$a(n-m)=\frac{2(12)^m(n-m)(2n-1)!}{m!(2n-m)!},$$

$$b(n-m)=\frac{(12)^m(2n-1)!}{(2n-m-1)!}.$$

Finally, we divide both sides of (4.4) by $W_{n,0}$, take n large, define $\lim_{n\to\infty}C_n/W_{n,0}=R$, and recall that, up to corrections of order $1/n$, $C_n\sim(4n-1)!!/n!$ as $n\to\infty$ [see (3.4) and (2.1)]. This converts the series in (4.4) to an infinite sum of the form:

$$R=1+\tfrac{3}{2}+(\tfrac{3}{2})^2/2!+\cdots+(\tfrac{3}{2})^m/m!+\cdots=e^{3/2}$$

and thereby establishes the result in (4.3).

Next, we generalize this argument to the case of ψ^{2N} ($N=3,4,5,\ldots$) theory, still keeping J, the number of external lines 0. For this case there is not one but $N-1$ simultaneous difference equations analogous to (4.2). These difference equations are generated by inserting one vertex with 1 self-loop, or 2 self-loops,..., or $N-1$ self-loops into the various classes of connected graphs having fixed numbers of self-loops. We define $W_{n,k_1,k_2,\ldots,k_{N-1}}$ as the number of n-vertex connected graphs with k_1 vertices having one self-loop, k_2 vertices having 2 self-loops, k_3 vertices having 3 self-loops, and so on. Note that $k_1+k_2+\cdots+k_{N-1}\leqslant n$.

For example, for ψ^6 theory we have two difference equations. Inserting one vertex having two self-loops (see Fig. 3(a) gives

$$W_{n,k_1,k_2}=\frac{90}{k_2}\left[(k_1+1)\,W_{n-1,k_1+1,k_2-1}+2k_2\,W_{n-1,k_1-1,k_2}\right.$$

$$+(3n-k_1-2k_2-1)\ W_{n-1,k_1,k_2-1}\ ] \quad (k_2\geqslant 1)$$

(4.5)

and inserting one vertex having one self-loop (see Fig. 3b) gives

$$W_{n,k_1,0} = \frac{120}{k_1}\ [\tfrac{1}{2}k_1(k_1+1)\ W_{n-1,k_1+1,0} + (2k_1-1)\ W_{n-1,k_1-1,1}$$

$$+k_1(3n-k_1-3)\ W_{n-1,k_1,0} + 4W_{n-1,k_1-3,2}$$

$$+2(3n-k_1-3)\ W_{n-1,k_1-2,1} + \tfrac{1}{2}(3n-k_1-2)$$

$$\times\ [(3n-k_1-3)\ W_{n-1,k_1-1,0} \quad (k_1\geqslant 1).$$

(4.6)

This last equation is complicated because inserting a one-self-loop vertex requires that we cut two lines in a graph. There are many possibilities to consider: cutting two non-self-loops, one non-self-loop and one self-loop, two self-loops, the same self-loop twice, and so on.

The complexity of these difference equations might seem forbidding. However, because we are only interested in asymptotic results for large n, we can make enormous simplifications which reduce the problem almost to triviality. For example, for large n, we may replace (4.2) by the much simpler equation

$$W_{n,k} = \frac{24n}{k}\ W_{n-1,k-1} \tag{4.7}$$

without altering the asymptotic result in (4.3).

Similarly, we may replace the pair of difference equations (4.5) and (4.6), for large n by just *one* much simpler equation

$$W_{n,k_1,0} = \frac{540}{k_1}\ n^2 W_{n-1,k_1-1,0}. \tag{4.8}$$

The generalization to ψ^{2N} theories of (4.7) and (4.8) is

$$W_{n,k_1,0,0,\ldots,0} = \frac{(2N)!(Nn)^{N-1}}{2k_1(2N-3)!!(N-1)!}\ W_{n-1,k_1-1,0,0,\ldots,0}. \tag{4.9}$$

This equation is obtained by inserting a vertex to which is attached a single self-loop (see Fig. 3c). This procedure requires that we cut $N-1$ lines of the existing graph to attach the $2N-2$ free legs of the new vertex. Since there are roughly Nn lines in the original graph, there are roughly $(Nn)^{N-1}/(N-1)!$ different ways to perform these cuts. We multiply by $(2N)!$ because we have added a new vertex. We divide by 2 because the symmetry number for a self-loop is $\frac{1}{2}$ and we divide by $(2N-3)!!$ because this is the number of ways of connecting up to the *pairs* of cut lines [here, we use the same argument that led to (2.1)]. Finally, we divide by k_1 because each graph produced by the vertex insertion has k_1 self-loops and therefore has been produced k times too often.

Next, we iterate (4.9) in precisely the same manner as we iterated (4.2). We begin with the identity

$$C_n(J=0,2N) = \sum_{k_1+k_2+\cdots+k_{N-1}\leqslant N} W_{n,k_1,k_2,\ldots,k_{N-1}}$$

$$\sim \sum_{k_1=0}^{n} W_{n,k_1,0,0,\ldots,0}. \tag{4.10}$$

This asymptotic relation is valid as $n\to\infty$ because $W_{n,k_1,k_2,\ldots,k_{N-1}}$ (one of $k_2,\ldots,k_{N-1}\neq 0$) contributes negligibly to the sum as $n\to\infty$; this is true because the highest power of n in the relevant difference equation is less than $N-1$. Next, we repeatedly substitute (4.9) into (4.10) to obtain

$$C_n(J=0,2N) = W_{n,0,0,\ldots,0} + \sum_{k_1=1}^{n} \frac{\alpha}{k_1}\ W_{n-1,k_1-1,0,0,\ldots,0}$$

$$= W_{n,0,0,\ldots,0} + \alpha\ W_{n-1,0,0,\ldots,0} + \sum_{k_1=1}^{n-1} \frac{\alpha^2}{k_1(k_1+1)}\ W_{n-2,k_1-1,0,0,\ldots,0}$$

$$= W_{n,0,0,\ldots,0} + \alpha\ W_{n-1,0,0,\ldots,0} + \frac{\alpha^2}{2!}\ W_{n-2,0,0,\ldots,0} + \cdots, \tag{4.11}$$

where $\alpha=(2N)!(Nn)^{N-1}/[2(2N-3)!!(N-1)!]$.

However, we know from (2.1) and (3.6) that $C_n(J=0,2N)\sim(2Nn-1)!!/n!$ $(n\to\infty)$ and therefore that

$$\frac{C_n(J=0,2N)}{C_{n-1}(J=0,2N)} \sim \frac{(2Nn)^N}{n} = \beta \quad (n\to\infty). \tag{4.12}$$

Combining this result with that in (4.11) gives

$$\lim_{n\to\infty} \frac{C_n(J=0,2N)}{W_{n,0,0,\ldots,0}}$$

$$= \lim_{n\to\infty} 1+\alpha/\beta+\frac{(\alpha/\beta)^2}{2!}+\frac{(\alpha/\beta)^3}{3!}+\cdots$$

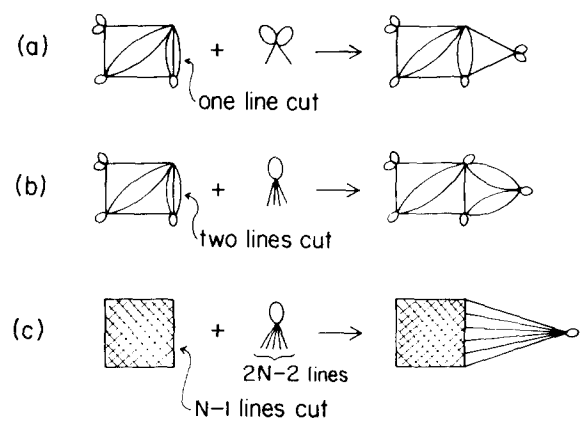


FIG. 3. Insertion of self-loops into graphs. In (a) a vertex having two self-loops is inserted in a ϕ^6 graph and in (b) a vertex having one self-loop is inserted in a ϕ^6 graph. In (c) a vertex having one self-loop is inserted in a ϕ^{2N} graph.

$$= \lim_{n\to\infty} \exp(\alpha/\beta)$$

$$= \lim_{n\to\infty} \exp \frac{(2N)!(Nn)^{N-1}n}{2(2N-3)!!\,(2Nn)^{N}(N-1)!}$$

$$= e^{N-1/2}, \tag{4.13}$$

which reduces to (4.3) when $N=2$.[3]

B. Path-integral approach

The method we use here to impose topological constraints on graphs is quite general. We eliminate those graphs having any given topological structure from the set of all graphs by inserting counterterms (which correspond with the topological structure to be removed) into the exponent in the integrand of (2.2). We refer to the argument of the exponential as the *action*, and we refer to terms which are to be subtracted from the action as *counterterms*.

The insertion of counterterms to remove specific topological structures can be viewed as a renormalization of the graphs of the theory because the graphs have no momentum dependence when $D=0$. For example, for a Wick-ordering subtraction in a ψ^{2N} theory we must subtract off the value of the graph in Fig. 4a. By the Feynman rules for a ψ^{2N} theory in zero-dimensional space–time, the value of a self-loop is $(2N)!(-g)/2$. [The Feynman rules are simply that each vertex has a factor of $-g(2N)!$. The factor of $\frac{1}{2}$ is the symmetry number of a self-loop.] This requires that we add a counterterm to the action of the form

$$\tfrac{1}{2}(2N)!g\frac{x^{2N-2}}{(2N-2)!} = N(2N-1)g\,x^{2N-2}. \tag{4.14}$$

The factor of x^{2N-2} occurs because there are $2N-2$ free legs on the graph in Fig. 4a.

The counterterm in (4.14) miscounts those graphs in which the same vertex is involved in two such subtractions (see Fig. 4b). That is to say, the counterterms also need counterterms to subtract out their effects. The appropriate modification of the action is given by Banks and Bender[3] for the case of Wick ordering (subtracting out all self-loops). The Wick-ordered x^{2N}, written $:x^{2N}:$, is just

$$:x^{2N}: = H_{2N}(x/\sqrt{2})/2^{N},$$

where $H_{2N}(x)$ is a Hermite polynomial. The integrand for counting graphs in the Wick-ordered theory is then

$$\exp(-:x^2/2:-:gx^{2N}:)$$

$$= \exp[-\tfrac{1}{4}H_2(x/\sqrt{2}) - g\,H_{2N}(x/\sqrt{2})/2^{N}]$$

$$= \exp[-x^2/2 + \tfrac{1}{2} - g\,x^{2N} + gN(2N-1)\,x^{2N-2}$$

$$-gN(N-1)(2N-1)(2N-3)\;\; x^{2N-4}/2 + \cdots].$$

Dividing by the $g=0$ case to normalize the path integral, we obtain the generating function for Wick-ordered graphs:

$$(1/\sqrt{2\pi})\int_{-\infty}^{\infty} dx \exp[-\tfrac{1}{2}x^2 - g\,x^{2N} + gN(2N-1)\,x^{2N-2}$$

$$-gN(N-1)(2N-1)(2N-3)\;\; x^{2n-4}/2 + \cdots]. \tag{4.15}$$

We use the idea of Lipatov to find the coefficient of $(-g)^n$ in the expansion of (4.15) when n is large. We expand the terms linear in g into an exponential series, pick out the appropriate term and estimate the resulting integral using Laplace's method. The coefficient of $(-g)^n$ is given by

$$(1/n!\sqrt{2\pi}\,)\int_{-\infty}^{\infty} dx \exp\{-x^2/2 + n\ln[x^{2N}p(x)\,]\},$$

where

$$p(x) = 1 - a_1x^{-2} + a_2x^{-4} + \cdots,$$

$$a_1 = N(2N-1),$$

$$a_2 = N(N-1)(2N-1)(2N-3)/2.$$

The function $f(x) = -x^2/(2n) + \ln[x^{2N}p(x)]$ has a maximum at $x=x_0$, where

$$f'(x_0) = -\frac{x_0}{n} + \frac{2N}{x_0} + \frac{p'(x_0)}{p(x_0)} = 0.$$

When n is large, the approximate location of the maximum is given by

$$x_0^2 \sim 2Nn.$$

The fluctuations about the maximum are controlled by $f''(x_0)$

$$= -\frac{1}{n} + \frac{2N}{x_0^2} + \frac{p''(x_0)p(x_0) - [p'(x_0)\,]^2}{[p(x_0)\,]^2}.$$

Observe that this is negative, which verifies that x_0 is indeed a maximum.

The functions $p(x_0), p'(x_0), p''(x_0)$ are sequences of terms of rapidly decreasing size. Therefore, it is easy to obtain higher-order corrections. (We already know the exact value of the integral for $a_i=0$. We therefore divide out all terms which are independent of the a_i.) The fraction of graphs having n vertices in a Wick-ordered theory compared with the total number of graphs without the Wick-ordering constraint is, by Laplace's method

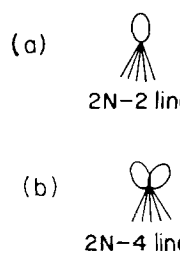


FIG. 4. Subgraphs removed by the Wick-ordering constraint. Note that the counterterm for (4a) oversubtracts (4b). Figure 4a has a symmetry factor of $\frac{1}{2}$ and Figure 4b has a symmetry factor of $\frac{1}{8}$.

$$\left(\frac{2\pi}{nf''(x_0)}\right)^{1/2} e^{nf(x_0)}[(a_i=0)]^{-1}$$

$$\simeq \exp\left\{n\ln p(x_0) - \frac{n x_0^2}{8N}\left[\frac{p'(x_0)}{p(x_0)}\right]^2\right\}\left[1+\frac{a_1}{(2N^2n)}\right]^{-1/2}$$

$$\simeq \exp\left(\frac{-a_1}{2N}\right)\left[1+\frac{2Na_2-(N-1)\,a_1^2-2Na_1}{8nN^3}\right]$$

$$=\exp(-N+\tfrac{1}{2})\left[1-\frac{2N-1}{4n}\right]. \tag{4.16}$$

This is the higher-order in $1/n$ version of (4.13).

Finally, if we repeat the above argument for $J\neq 0$ (graphs with J external legs) then the ratio of Wick-ordered graphs is

$$\exp(-N+\tfrac{1}{2})\left[1-\frac{2N-1}{4n}\left(1-\frac{J}{N}\right)\right]. \tag{4.17}$$

We estimate that the fraction of graphs with no self-loops for $N=2$ and $n=6$ is $e^{-3/2}\doteq 0.22313$ in leading order. The first correction changes this to 0.19523. If we ask the same question for *connected* graphs, the discussion of Sec. III requires that we divide by $(1-\frac{3}{16}\cdot\frac{1}{6})$. Only the denominator is changed because there are no one-vertex connected graphs having no self-loops. This estimated fraction of connected graphs with no self-loops is then 0.2022, which is a good approximation to the exact value of 0.2044 for $n=6$.

V. OTHER TOPOLOGICAL CONSTRAINTS

Consider a constraint which is weaker than Wick ordering. Suppose we wish to exclude those graphs having vertices with two or more self-loops (graphs having no or one self-loop per vertex are allowed) from the set of all graphs. Then we take

$$a_1=0 \quad \text{and} \quad a_2=-N(N-1)(2N-1)(2N-3)/2$$

in the previous Laplace integral. We find that the fraction of graphs having two or more self-loops for each vertex is

$$(N-1)(2N-1)(2N-3)/8Nn. \tag{5.1}$$

Note that there is a factor of $1/n$, which shows that the overwhelming majority of graphs with self-loops do not have more than one self-loop per vertex.

The reason that (5.1) vanishes with n [while (4.17) is $O(1)$ as $n\to\infty$] is that the required counter term has *two* loops (see Fig. 4b) (rather than one as in Fig. 4a). In general, we will see that if the graphical representation of a counterterm has L loops, then the fraction of graphs containing this subgraph will be of order $1/n^{L-1}$

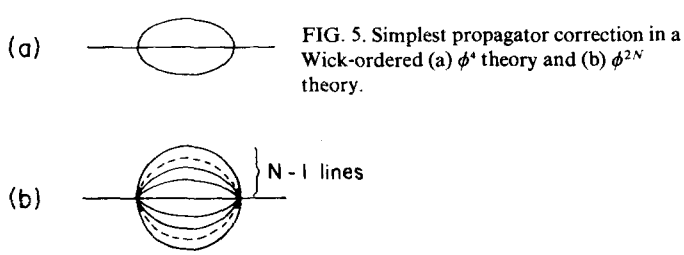


FIG. 5. Simplest propagator correction in a Wick-ordered (a) ϕ^4 theory and (b) ϕ^{2N} theory.

Consider, for example, the propagator bubble graph in Fig. 5. The value of this graph is

$$[(2N)!g]^2/(2N-1)!=2N(2N)!g^2.$$

Thus, a counterterm of the form

$$-N(2N)!g^2x^2$$

is necessary in the action to eliminate all graphs having this subgraph. The stationarity conditions in this case are

$$-x_0=2Ng_0x_0^{2N-1}-2N(2N)!g_0^2x_0=0$$

and

$$-x_0^{2N}-\frac{n}{g_0}-2N(2N)!g_0x_0^2=0.$$

[See (5.4) and (5.5) to see how these equations arise.] We find that the leading contribution (divided by the unconstrained counting) is

$$\exp\left(-\frac{(2N-1)!}{2(2Nn)^{2N-3}}\right)\sim 1-\frac{(2N-1)!}{2(2Nn)^{2N-3}}. \tag{5.2}$$

Thus, for $N=2$, the fraction of graphs having propagator bubbles of the form in Fig. 5a is $3/(4n)$. Since the counterterm has two loops, the fraction of graphs having bubbles is $O(1/n)$.

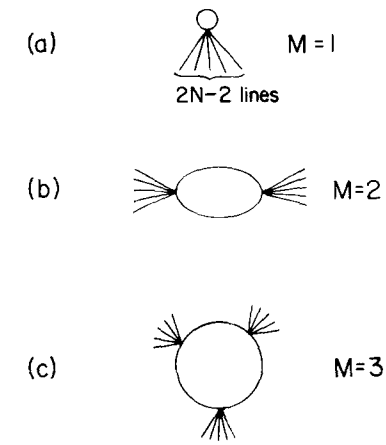


FIG. 6. Examples of subgraphs that occur with nonvanishing probability as n, the number of vertices, tends to ∞. We call these graphs necklace graphs. Each bead or vertex on the necklace has $2N-2$ free lines that connect to the rest of the graph. M is the number of beads.

A. One-loop counterterms

Granting the above assertions, it follows that the only counterterms which eliminate *nonvanishing* fractions of graphs in the many-vertex limit are those whose graphical representations have just one loop. The simplest sorts of counterterms having one loop are shown in Fig. 6. We call these subgraphs necklaces. We now calculate the value of the generic graph of this class, a necklace with M beads. There

are factors of $[-g(2N)!]^M$ from the M vertices, $[M(2M-2)]!/[(2N-2)!]^M$ for the number of ways of combining the remaining lines into a graph having $2N$ lines emerging from each vertex, with all lines indistinguishable, and $(2M)^{-1}$ for circular symmetry. Finally, we include the factor $-x^{M(2N-2)}/[M(2N-2)]!$ to convert the graph into a counterterm, and we obtain the term

$$A_M = -(-g)^M x^{M(2N-2)} [2N(2N-1)]^M / 2M$$

to be added to the action.

Let us examine the integral

$$\int_{-\infty}^{\infty} dx \exp\left[-\tfrac{1}{2}x^2 - g x^{2N} + \sum_{1 \leqslant M \leqslant n} A_M\right]$$

in the limit of large order n. We will compute only the leading order terms. Higher-order corrections vanish for large n like $O(1/n)$. To pick out the coefficient of g^n, we take a contour integral $\oint dg\, g^{-n-1}$, where the contour encloses the cut along the negative real-g-axis, and perform a steepest-descent aproximation on the resulting integral. The coefficient of g^n is

$$\frac{1}{2\pi i}\frac{1}{\sqrt{2\pi}}\oint \frac{dg}{g}\int_{-\infty}^{\infty} dx \times \exp\left[-\tfrac{1}{2}x^2 - g x^{2N} + \sum A_M - n\ln(-g)\right]. \tag{5.3}$$

The leading contribution for large n comes from the saddle point in (x,g) space, which satisfies the two equations

$$0 = -x_0 - 2Ng_0 x_0^{2N-1} - \sum_M (-g_0)^M x_0^{M(2N-2)-1} \times (N-1)[2N(2N-1)]^M, \tag{5.4}$$

$$0 = -x_0^{2N} + \sum_M (-g_0)^{M-1} x_0^{M(2N-2)} \times [2N(2N-1)]^M/2 - n/g_0. \tag{5.5}$$

Dimensional arguments give us the useful expression

$$\tfrac{1}{2}\left[x\frac{d}{dx} - (2N-2)g\frac{d}{dg}\right] \times \left[-\tfrac{1}{2}x^2 - g x^{2N} + \sum A_M - n\ln(-g)\right]\Big|_{\substack{x=x_0\\ g=g_0}} = -\tfrac{1}{2}x_0^2 - g_0 x_0^{2N} - n(N-1) = 0 \tag{5.6}$$

at the saddle point. Substituting

$$x_0^2 = 2Nn(1+\epsilon) \quad \text{and} \quad -g_0 = n(2Nn)^{-N}(1+\delta)$$

into (5.6), where ϵ and δ are $O(1/n)$, we find that in fact $\delta = O(1/n^2)$ and may be neglected to leading order.

With these approximations we find that as $n \to \infty$ the fraction of graphs without a given set of necklace subgraphs is simply

$$\exp\left[-\sum_{M=1}(2N-1)^M/(2M)\right]. \tag{5.7}$$

For $M=1$ this reproduces the leading behavior for the Wick-ordered graphs as derived in (4.13). We see from the form in (5.7) that we can, in leading order, treat any class of subgraphs separately, so that the fraction of graphs without an M-bead necklace is $\exp[-(2N-1)^M/(2M)]$. Note that as $M \to \infty$, this exponential vanishes, showing that all graphs have such a subgraph, as of course they must for M sufficiently large.

B. Distribution of subgraphs

Let us introduce a factor $(1-\alpha_M)$ into the counterterm for the necklace subgraphs

$$-(-g)^M x^{M(2N-2)} [2N(2N-1)]^M (1-\alpha_M)/(2M). \tag{5.8}$$

The α_M then multiplies each occurrence of the given subgraph, so that a graph with subgraphs of M-bead necklaces has a factor of $(\alpha_M)^k$ multiplying it. This factor results from combining $+1$ for any necklace subgraph coming from the expansion of the action, and $-(1-\alpha_M)$ coming from the expansion of the counterterm. This is true for each subgraph, independent of the details of the rest of the graph. Of course, it miscounts overlapping necklaces but this is an $O(1/n)$ effect. For $\alpha_M = 1$ we recover the perturbation series without the contraint on M-bead necklaces. For $\alpha_M = 0$, we have the case treated in part A. To leading order in $1/n$ (the higher-order corrections are very complicated) if there are k subgraphs of the M-bead necklace type, the fraction C_k^M of that type satisfies

$$\sum_k (\alpha_M)^k C_k^M = \exp[-(1-\alpha_M)(2N-1)^M/(2M)]. \tag{5.9}$$

The right side of this equation is simply (5.7) with the extra factor $(1-\alpha_M)$ included in A_M. Equation (5.6) shows that this is the only change resulting from the $(1-\alpha_M)$ factors to leading order in $1/n$. The integral which we are estimating corresponds to the sum of $(\alpha_M)^k$ times the fraction of graphs with k of these M-bead necklace subgraphs, as discussed after (5.7). We have divided out the value for no subtraction, $\alpha_M = 1$. For $\alpha_M = 0$ the sum reduces to the previous case C_0^M, the fraction of graphs with no such subgraph. Differentiating with respect to α_M and setting $\alpha_M = 0$ we find that the fraction of graphs with k M-bead necklaces is

$$C_k^M = \frac{1}{k!}\left[\frac{(2N-1)^M}{2M}\right]^k e^{-(2N-1)^M/(2M)}. \tag{5.10}$$

This is a Poisson distribution. The independence of the different classes of graphs and the independence in each type of subgraph occurring in a many-vertex graph gives a Poisson distribution for each type of subgraph.

In Table I we compare the theoretical distribution in

TABLE I[a]. There are 97 connected diagrams in sixth order ($n=6$) in a ψ^4 theory ($N=2$) having no external legs ($J=0$). In this table we compare the exact fractions of diagrams having a given number W of Wick loops (W ranges from 0 to 6) and a given number L (L ranges from 0 to 6) of propagator corrections (two-bead necklaces as in Fig. 5a) with the asymptotic prediction given in (5.10) that for large n this fraction should be $[(1/W!)(\frac{3}{2})^W e^{-3/2}][(1/L!)(\frac{9}{4})^L e^{-9/4}]$. Although the asymptotic predictions in this paper are valid as $n\to\infty$, we see in this table that $n=6$ is sufficiently large for these predictions to be quite accurate

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$\sum_{\text{all } L}$
$W=0$	0.0235	0.0529	0.0595	0.0446	0.0251	0.0113	0.0042	0.2231
	0.0095	0.0286	0.0643	0.0524	0.0274	0.0143	0.0053	0.2044
$W=1$	0.0353	0.0794	0.0893	0.0670	0.0377	0.0169	0.0063	0.3347
	0.0190	0.0571	0.1428	0.0571	0.0452	0.0190	0.0056	0.3475
$W=2$	0.0265	0.0595	0.0670	0.0502	0.0282	0.0127	0.0048	0.2510
	0.0143	0.0786	0.0999	0.0476	0.0214	0.0089	0.0024	0.2731
$W=3$	0.0132	0.0298	0.0335	0.0251	0.0141	0.0064	0.0024	0.1255
	0.0095	0.0571	0.0357	0.0190	0.0071	0	0	0.1284
$W=4$	0.0050	0.0112	0.0126	0.0094	0.0053	0.0024	0.0009	0.0471
	0.0077	0.0196	0.0089	0.0024	0	0	0	0.0386
$W=5$	0.0015	0.0034	0.0038	0.0028	0.0016	0.0007	0.0003	0.0141
	0.0036	0.0036	0	0	0	0	0	0.0072
$W=6$	0.0004	0.0008	0.0009	0.0007	0.0004	0.0002	0.0001	0.0035
	0.0006	0	0	0	0	0	0	0.0006
$\sum_{\text{all } W}$	0.1054	0.2371	0.2668	0.2000	0.1126	0.0506	0.0190	1
	0.0642	0.2446	0.3517	0.1785	0.1011	0.0422	0.0133	1

[a]The upper number in each square is the asymptotic prediction and the lower number is the exact fraction.

(5.10) for $M=1$ (Wick ordering) and $M=2$ (simple vertex corrections) with the actual distribution of sixth-order ($n=6$) vacuum graphs in a ϕ^4 theory.

Until now we have mostly considered vacuum graphs (graphs with no external legs; that is, $J=0$). However, our leading-order results remain unchanged when there are external legs. If there are J external legs, then the exponent in (5.3) has an extra term of the form $J\ln x$. This term can only affect the large-n behavior by terms of order $1/n$ because x_0^2 and g_0 change by terms of order $1/n$. Thus, the distribution in (5.9) is independent of J. This is not surprising; fixing a few lines of the diagram will not alter the leading-order probability for a given subgraph to occur somewhere in the diagram.

For graphs with many vertices, we now have a simple statistical interpretation of how they are constructed. Although they are complicated structures, the probability of occurrence of any given subgraph is independent, to leading order in $1/n$, of the occurrence of any other subgraph of the same or of a different type. The number of occurrences of a particular subgraph follow a Poisson distribution. The necklace graphs are special subgraphs because they have a nonvanishing probability of occurring as $n\to\infty$; they are a set of measure one. For example, we predict that 1% of all ψ^4 theory Feynman graphs in nth order (n large) are connected graphs having one self-loop, two two-bead necklaces, and two three-bead necklaces.

ACKNOWLEDGMENT

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[2]The counting method used here is not new. It was used by A. Jaffe in Commun. Math. Phys. **1**, 127 (1965).

[3]The result in (4.13) is interesting in view of the result on the large-order behavior of a Wick-ordered gx^{2N} anharmonic oscillator theory obtained by T. Banks and C.M. Bender, J. Math. Phys. **13**, 1320 (1972). Banks and Bender found that the ratio corresponding to (4.13) for the anharmonic oscillator is $\exp[N(2N-1)/(2N-2)]$. This ratio factors into two contributions: $\exp(N-\frac{1}{2})$ (for the diagram counting) times $\exp[(2N-1)/(2N-2)]$ (for the specific oscillator dynamics). Note that for the anharmonic oscillator $D=1$, and not 0 as in this paper.

Analytic solution of a model pulse propagation problem

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A closed form solution is found to a model problem for pulse propagation in a medium that responds hydrodynamically to the pulse. This solution is useful for testing pulse propagation code.

I. INTRODUCTION

Afficionados of the art of numerical computation know that a computer program must be tested in a variety of ways before it can be deemed satisfactory. One of the best tests is to find a model problem for which an analytic solution is possible.

We have recently developed a program for propagation of electromagnetic pulses in a medium which responds hydrodynamically to the energy deposited within it. The electromagnetic propagation code and the hydrodynamic propagation code can be tested separately. However, the codes are used in alternating fashion to integrate over different variables (space and time). Moreover, prediction and correction steps must also alternate so that each code has corrected values of the other variables. We can test the complicated logic involved by specializing from several electromagnetic variables to a single electromagnetic variable E (the pulse energy) and from several hydrodynamic variables to one (the density of the medium). What distinguishes the class of problems we are interested in from others is that there are two timelike variables: z, the distance into the medium (which if divided by the velocity of light c is a time) and $s=t-z/c$, the time back from the leading edge of the pulse.

The simplest model problem we can invent consists of the coupled linear equations

$$\frac{\partial E(z,s)}{\partial z}=-aE-bn, \tag{1.1}$$

$$\frac{\partial n(z,s)}{\partial s}=-cE-dn, \tag{1.2}$$

where a, b, c, and d are constants, and the equations are to be solved subject to the initial conditions

$$n(z,0)=n_0(z), \tag{1.3}$$

$$E(0,s)=E(s), \tag{1.4}$$

where $n_0(z)$ describes the density of the medium before the pulse hits it, and $E(s)$ describes the shape of the pulse at the input plane.

The solution of first-order coupled linear equations would appear to be trivial. However, the reader may conclude from the answers

$$E(z,s)=e^{-az}\left[E(s)+\int_0^s e^{-d(s-s')}\left(\frac{bcz}{s-s'}\right)^{1/2}\times I_1(2[bcz(s-s')]^{1/2})E(s')\,ds'\right]$$
$$-b\,e^{-ds}\int_0^z e^{-a(z-z')}I_0(2[bcs(z-z')]^{1/2})n_0(z')\,dz', \tag{1.5}$$

$$n(z,s)=-c\,e^{-az}\int_0^s e^{-d(s-s')}I_0(2[bcz(s-s')]^{1/2})E(s')\,ds'$$
$$+e^{-ds}\left[n_0(z)+\int_0^z e^{-a(z-z')}\left(\frac{bcs}{z-z'}\right)^{1/2}\times I_1(2[bcs(z-z')]^{1/2})n_0(z')\,dz'\right] \tag{1.6}$$

(where I_0 and I_1 are modified Bessel functions of order 0 and 1) that the solution of the model problem is not completely trivial.

Even for the special case in which the initial density is uniform,

$$n_0(z)=n_0=\text{constant},$$

nontrivial solutions result. The part of $E(z,s)$ proportional to n_0 simplifies to

$$E(z,s)_n=-b\,e^{-ds}(n_0/a)\,e^{-az}\sum_{k=1}^{\infty}\left(\frac{a^2z}{bcs}\right)^{k/2}\times I_k(2[bcsz]^{1/2}). \tag{1.7}$$

Similarly, the part of $n(z,s)$ proportional to n_0 reduces to

$$n(z,s)_n=n_0e^{-(az+ds)}\sum_{k=0}^{\infty}\left(\frac{a^2z}{bcs}\right)^{k/2}I_k(2[bcsz])^{1/2}, \tag{1.8}$$

a result not simply proportional to $E_n(z,s)$ because the sums have different limits.

We have given the results already, in a form adequate for testing pulse programs. The remainder of this paper is devoted to a derivation of these results.

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II. LAPLACE TRANSFORM SOLUTION

Although Eqs. (1.1) and (1.2) appear to describe the time evolution of a pair of coupled linear equations this is not the case because two independent variables are involved. There is no point, then, in diagonalizing the two-by-two matrix. A more fruitful procedure is to introduce the Laplace transform on the variable s,

$$\hat{E}(z,p)=\int_0^\infty \exp(-ps)\,E(z,s)\,ds, \tag{2.1}$$

$$\hat{n}(z,p)=\int_0^\infty \exp(-ps)\,n(z,s)\,ds. \tag{2.2}$$

The energy equation takes the same form as before,

$$\frac{\partial \hat{E}(z,p)}{\partial z}=-a\,\hat{E}(z,p)-b\hat{n}(z,p), \tag{2.3}$$

but the density equation reduces to the algebraic form

$$p\hat{n}(z,p)-n(z,0)=-c\hat{E}(z,p)-d\hat{n}(z,p). \tag{2.4}$$

Thus we can solve for the transformed density

$$\hat{n}(z,p)=\frac{n_0(z)-c\,\hat{E}(z,p)}{p+d} \tag{2.5}$$

in terms of the initial density $n_0(z)\equiv n(z,0)$ and the transformed energy. The differential equation for the energy, with this result inserted, takes the form

$$\frac{\partial \hat{E}(z,p)}{\partial z}=-\alpha(p)\,\hat{E}(z,p)-\frac{b}{p+d}\,n_0(z), \tag{2.6}$$

where

$$\alpha(p)\equiv a-\frac{bc}{p+d}. \tag{2.7}$$

Thus the transformed energy has the solution

$$\hat{E}(z,p)=e^{-\alpha(p)z}\hat{E}(0,p) -\frac{b}{p+d}\int_0^z e^{\alpha(p)(z'-z)}n_0(z')\,dz'. \tag{2.8}$$

If this result is inserted into Eq. (2.5), the solution for the transformed density is found to be

$$\hat{n}(z,p)=-\frac{c}{p+d}e^{-\alpha(p)z}\hat{E}(0,p) +\left(\frac{n_0(z)}{p+d}+\frac{bc}{(p+d)^2}\int_0^z n_0(z')\,e^{-\alpha(p)(z-z')}\,dz'\right). \tag{2.9}$$

The first terms in Eqs. (2.8) and (2.9) will be denoted $\hat{E}_E(z,p)$, $\hat{n}_E(z,p)$ since they are sensitive to the initial energy distribution $E(s)$, and the second terms will be denoted $\hat{E}_n(z,p)$, $\hat{n}_n(z,p)$ since they are sensitive to the initial density $n_0(z)$.

III. PULSE SHAPE DEPENDENT TERMS

The first terms in Eqs. (2.8) and (2.9) depend on $\hat{E}(0,p)$, that is, on the initial pulse shape. By means of the convolution theorem

$$L^{-1}\hat{f}(p)\hat{g}(p)=\int_0^s f(s')g(s-s')\,ds', \tag{3.1}$$

and the shifting theorem

$$L^{-1}\hat{g}(p+d)=e^{-ds}L^{-1}\hat{g}(p), \tag{3.2}$$

where L^{-1} denotes the inverse Laplace transform, the inverse of these terms can be written

$$E(z,s)_E=\exp(-az)\int_0^s G(y,s-s')E(0,s')\,ds', \tag{3.3}$$

$$n(z,s)_E=-\exp(-az)\int_0^s g(s-s')\,E(0,s')\,ds'. \tag{3.4}$$

The subscript reminds us that we are only writing down the terms that depend on the initial pulse shape $E(0,s)$. The factors G and g are given by

$$\exp(s,d)G(y,s)=L^{-1}\exp(y/p)=\delta(s)+L^{-1}[\exp(y/p)-1] =\delta(s)+H(s)\sqrt{y/s}\,I_1(2\sqrt{sy}), \tag{3.5}$$

where $y=bcz$, $H(s)$ is the Heaviside unit function, and

$$g(s)=\exp(-ds)L^{-1}\frac{c}{p}\exp\left(\frac{y}{p}\right) =c\exp(-ds)I_0(2\sqrt{sy}). \tag{3.6}$$

These inverse Laplace transforms may be found as (31) and (35), with $\nu=0$ in Table 5.5 of Ref. 1. These integrals were independently evaluated with the help of the generating function

$$\exp[sp+(y/p)]=\sum_{k=-\infty}^{\infty}[(s/y)^{1/2}p\,]^k I_k(2\sqrt{sy}), \tag{3.7}$$

and the application of a convergence factor $m^2/[m^2-(p+d)^2]$ to $\hat{E}(z,p)$ to eliminate the delta function in Eq. (3.5) and insure the validity of the convolution theorem. When the limit $m\to\infty$ was taken, the results reduced to those obtained directly from the table. Equations (3.5) and (3.6) agree with the pulse shape dependent portion of the results, Eqs. (1.5) and (1.6) quoted in the Introduction.

IV. DENSITY DEPENDENT TERMS

The inverse Laplace transform of the terms in Eq. (2.9) that involve $n_0(z)$ can [with the help of the shifting theorem, Eq. (3.2)] be written in the form

$$n(z,s)_n=\exp(-ds)n_0(z)+\exp(-ds)\int_0^z n_0(z') \times\exp[-a(z-z')]R(z-z')\,dz', \tag{4.1}$$

where

$$R(z)=L^{-1}(bc/p^2)\exp[bcz/p]=(bcs/z)^{1/2}I_1(2(bcsz)^{1/2}). \tag{4.2}$$

[See Table 5.5, (35) of Ref. 1 with $\nu=1$.] Equations (4.1) and (4.2) agree with the result, Eq. (1.6), quoted for the part of $n(z,s)$ that contains $n_0(z)$.

The density dependent part of $E(z,s)$ may be written using Eq. (2.8) and the shifting theorem, Eq. (3.2) as

$$E(z,s)_n=-b\exp(-ds)\int_0^z \exp[-a(z-z')]n_0(z')\,dz'F, \tag{4.3}$$

where F is the inverse Laplace transform

$$F\equiv L^{-1}\{(1/p)\exp[bc(z-z')/p]\}$$

$$=I_0(2[bc(z-z')])^{1/2}). \tag{4.4}$$

The results, Eqs. (3.9), (3.15), (4.3), and (4.4) combine to give the complete answer, Eq. (1.5), for $E(z,s)$ quoted in the Introduction.

V. DENSITY DEPENDENT TERMS: UNIFORM CASE

The case in which the initial density is a constant

$$n(z)=n_0, \tag{5.1}$$

leads to simplified formulas which are most easily obtained by direct use of this assumption from the beginning. If Eqs. (2.8) and (2.9) are integrated over z', the density dependent terms are given by

$$\hat{E}(z,p)_n=-\frac{bn_0}{a}\frac{1-\exp[-az+y/(p+d)]}{p+d-p_0}, \tag{5.2}$$

$$\hat{n}(z,p)_n=\frac{n_0}{p+d-p_0}\left\{1-\frac{p_0}{p+d}\exp\left[-\left(a-\frac{bc}{p+d}\right)z\right]\right\}, \tag{5.3}$$

where $p_0=bc/a$.

After application of the shifting theorem, Eq. (3.2), the associated inverse Laplace transforms may be written

$$E(z,s)_n=\frac{bn_0}{a}e^{-ds}L^{-1}\frac{1-\exp[y(1/p-1/p_0)]}{p_0-p}, \tag{5.4}$$

$$n(z,s)_n=n_0e^{-ds}L^{-1}\frac{1}{p-p_0}\left\{1-\frac{p_0}{p}\exp\left[y\left(\frac{1}{p}-\frac{1}{p_0}\right)\right]\right\}. \tag{5.5}$$

In both cases, no singularity occurs at $p=p_0$. Thus the integration path may be contracted to an infinitesimal circle around the essential singularity at $p=0$. When this is done, the first term which is nonsingular in each case makes no contribution. Thus we may write

$$E(z,s)_n=-\frac{bn_0}{a}e^{-(ds+az)}\frac{1}{2\pi i}\int\frac{\exp[sp+(y/p)]}{p_0-p}\,dp, \tag{5.6}$$

$$n(z,s)_n=n_0e^{-(ds+az)}\frac{1}{2\pi i}\int\frac{p_0}{p}\frac{\exp[sp+(y/p)]}{p_0-p}\,dp. \tag{5.7}$$

The integrals may then be evaluated by means of their residues at $p=0$. These are easily obtained by using the generating function, Eq. (3.7), and expanding $(1-p/p_0)^{-1}$ in a power series in p. The results then agree with Eqs. (1.7) and (1.8) quoted in the Introduction. The results for Eq. (5.7) may also be obtained from those for Eq. (5.6) by noting that

$$\frac{p_0}{p}\frac{1}{p_0-p}=\frac{1}{p_0-p}+\frac{1}{p}.$$

The second term is the one previously evaluated in Eq. (3.6).

VI. SOME INTEGRAL IDENTITIES

A comparison between Eqs. (1.5) and (1.7) leads to an integral identity. If one makes the transformation of variables

$$x=(2az)^{1/2},\quad \sigma=(2bcs/z)^{1/2},\quad t=[2a(z-z')]^{1/2},$$

this identity reduces to the indefinite integral

$$\int_0^x e^{-t^2/2}I_0(\sigma t)t\,dt=e^{-x^2/2}\sum_{k=0}^{\infty}\left(\frac{x}{\sigma}\right)^{k+1}I_{k+1}(\sigma x) \tag{6.1}$$

found in Luke[2]. A comparison between Eqs. (1.6) and (1.8), with the same transformation leads to

$$1+\sigma\int_0^x e^{-t^2/2}I_1(\sigma t)\,dt=e^{-x^2/2}\sum_{k=0}^{\infty}\left(\frac{x}{\sigma}\right)^{k}I_k(\sigma x). \tag{6.2}$$

Equation (6.2) may also be derived by multiplying Eq. (6.1) by σ and integrating on σ from 0 to σ with the help of the relations

$$\int_0^{\sigma}I_0(\sigma' t)t\sigma'\,d\sigma'=\sigma I_1(\sigma t),$$

$$\int_0^{\sigma}\sigma'\left(\frac{x}{\sigma'}\right)^{k+1}I_{k+1}(\sigma' x)\,d\sigma'=\left(\frac{x}{\sigma}\right)^{k}I_k(\sigma x),$$

$$\lim_{\sigma\to\infty}\sum_{k=0}^{\infty}\left(\frac{x}{\sigma}\right)^{k}I_k(\sigma x)=\sum_{k=0}^{\infty}\frac{(x^2/2)^k}{k!}=\exp x^2.$$

In any case, we have found simple derivations of these indefinite integrals as a by-product of our general calculation.

VII. DISCUSSION OF THE SOLUTION

The contribution to the total solution proportional to the input $E(s)$ pulse may be obtained by setting $n_0(z)=0$. The solution is best understood in terms of the impulse response to a delta function input pulse $E(s)=\delta(s)$. For this case, we obtain

$$E(z,s)=e^{-az}\delta(s)+e^{-az}e^{-ds}\left(\frac{bcz}{s}\right)^{1/2}I_1(2(bczs)^{1/2}), \tag{7.1}$$

$$n(z,s) = -c\, e^{-az} e^{-ds} I_0(2(bczs)^{1/2}). \tag{7.2}$$

Thus the energy pulse $E(z,s)$ contains a delta function pulse whose amplitude diminishes exponentially with z, plus a pulse whose length in s expands with z. The density $n(z,s)$ contains a similar pulse. At large times the shape of these pulses is determined by the asymptotic form of the modified Bessel functions. Ignoring slowly varying algebraic factors, the shape of these pulses is determined by

$$\exp[-az - ds + 2(bczs)^{1/2}]. \tag{7.3}$$

see Figs. 1 and 2 for E and n, respectively. This pulse decays if the stability condition

$$ad - bc > 0, \tag{7.4}$$

is obeyed.

The distance s from the leading edge $s=0$ of the pulse at which this broad pulse has a maximum is given by

$$s = bcz/d^2. \tag{7.5}$$

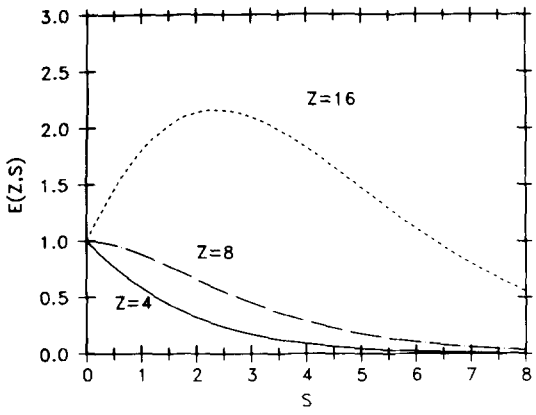

FIG. 1. The pulse shape $E(z,s)$ of Eq. (7.1) is plotted in normalized form

$$E(Z,S) \equiv \frac{E(z,s)}{E(0,s)} = e^{-S} \frac{I_1(2(AZS)^{1/2})}{(AZS)^{1/2}}$$

against S for several Z, where $Z=az$, $S=ds$, and $A \equiv bc/ad$ is chosen to be 0.5. For large enough Z, a maximum appears as suggested by the asympotic shape, Eq. (7.3).

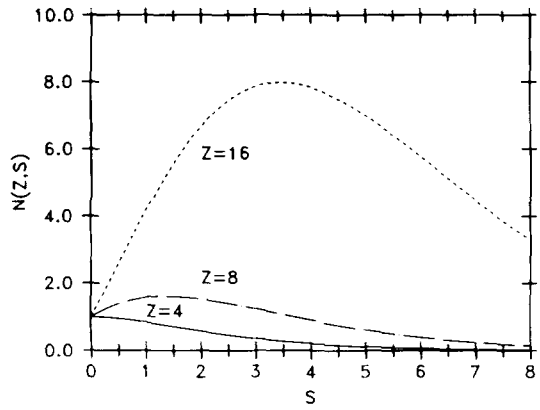

FIG. 2. The pulse shape $n(z,s)$ of Eq. (7.2) is plotted in normalized form

$$N(Z,S) \equiv \frac{n(z,s)}{n(0,s)} = e^{-S} I_0(2(AZS)^{1/2})$$

against S for several Z, where $Z=az$, $S=ds$, and $A \equiv bc/ad$ is chosen to be 0.5.

This simple result neglects the algebraic prefactors (mentioned earlier) which have only a minor influence on the result.

As mentioned in the Introduction, this model problem has been used to test the logical structure and computational properties of a code to handle pulse propagation. The numerical results will be reported in a paper describing the propagation problem and its numerical results.

ACKNOWLEDGMENT

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[1] A. Erdelyi, *Bateman Manuscript Project, Tables of Integral Transformations* (McGraw-Hill, New York, 1954), Vol. I.
[2] Y.L. Luke, *Integrals of Bessel Functions* (McGraw-Hill, New York, 1962), [See 12.2 (20) with $\nu \to 0^+$.]

The transport equation with anisotropic scattering in finite slab geometry[a)]

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We consider one-speed neutron transport or monochromatic radiative transfer in a slab of finite width, with particles incident on both faces. The scattering kernel is represented as a finite sum of Legendre polynomials. An exact expression is obtained for the expansion coefficients of the flux in a singular eigenfunction representation. It involves the X and Y functions of Chandrasekhar and the q_l and s_l polynomials of Sobolev. Case's full- and half-range expansions are obtained as limits when the slab thickness becomes zero or infinite, respectively. Orthogonality relations for the singular eigenfunctions and their adjoints are given. Also, we derive a number of orthogonality relations of the Inönü-type involving moments of the eigenfunctions. Expressions for surface densities, currents, and higher order Legendre moments of the surface fluxes are obtained. Singular integral transform relations between the Chandrasekhar ϕ and ψ functions and the polynomials $g_l(\nu)$, are given. Also, we give the solution of slab problems with one face having diffuse or specular reflecting boundary conditions.

I. INTRODUCTION

In this paper we consider a boundary value problem for the one-speed neutron transport equation, or the analogous radiative transfer equation. The scattering kernel is represented as a finite sum of Legendre polynomials. The flux $\Psi(x,\mu)$ is determined in a slab of finite width $0\leqslant x\leqslant\tau$ with particles incident on both faces, i.e., $\Psi(0,\mu)$ and $\Psi(\tau,-\mu)$ are given for $\mu>0$ The flux is represented in a singular eigenfunction expansion of the form[1-3]

$$\Psi(x,\mu)=\int_\sigma A'(\nu)\phi(\nu,\mu)\,e^{-x/\nu}\begin{pmatrix}1, & \nu>0\\ e^{\tau/\nu}, & \nu<0\end{pmatrix}d\nu. \qquad (1.1)$$

Here, the notation is standard, and is reviewed below. Our main result is that the expansion coefficients $A'(\nu)$ are given exactly by

$$A'(\nu)=\frac{1}{N(\nu)}\int_{-1}^{1}\mu\,\tilde{\phi}(\nu,\mu)\begin{pmatrix}\Psi(0,\mu), & \mu>0\\ \Psi(\tau,\mu), & \mu<0\end{pmatrix}d\mu. \qquad (1.2)$$

Here, $\tilde{\phi}(\nu,\mu)$ is a function similar in form to $\phi(\nu,\mu)$. It is expressed in terms of the Chandrasekhar X and Y functions[4] and the Sobolev[5] polynomials $q_l(\mu)$ and $s_l(\mu)$. In the limits $\tau\to 0$ and $\tau\to\infty$, the above expressions reduce to Case's full-range and half-range expansions, respectively.

The general result above leads to a variety of orthogonality relations involving moments of $\phi(\nu,\mu)$ and $\tilde{\phi}(\nu,\mu)$. Also, expressions for the Legendre moments of the flux both on the surfaces and in the interior of the slab are obtained. Finally, the general result is easily modified to solve problems with a reflecting boundary.

The results given here represents, in a sense, a culmination of a long series of works by many investigators: Expressions for surface fluxes (but not internal fluxes) were obtained for some versions of this problem by workers in radiative transfer theory using methods based on nonlinear integral equations.[4-6] Expressions for internal fluxes were obtained by neutron transport theorists using Fourier transform[7,8] and singular eigenfunction expansion methods[1-3] for many less-general versions of the above problem (isotropic scattering, semi-infinite media, approximate results, etc.). In the present paper we obtain expressions for surface fluxes and internal fluxes. These results hold for finite or semi-infinite slabs, and for general N-term anisotropic scattering.

The plan of this paper is as follows: In Sec. II we summarize relevant results from the theories of radiative transfer and neutron transport. In Sec. III we derive the expression for the expansion coefficients. In Sec. IV, the limiting cases of zero and infinite slab thickness are examined. In Sec. V, expressions for surface fluxes and various relations involving them are derived. In Sec. VI, we derive various orthogonality relations involving the singular eigenfunctions or their moments. In Sec. VII, we consider problems with reflecting boundary conditions. We conclude with a brief discussion in Sec. VIII.

II. SUMMARY OF PREVIOUS RESULTS

This paper draws upon a variety of results from the theories of radiative transfer and neutron transport. This material is found in many different sources, written in varied notation. Thus, it is convenient to summarize essential material here in a consistent notation.

The transport equation for one-speed neutrons in plane geometry with azimuthal symmetry is[2]

$$\frac{\partial}{\partial x}\Psi(x,\mu)$$

$$+\frac{1}{\mu}\left(\Psi(x,\mu)-\tfrac{1}{2}\int_{-1}^{1}p(\mu,\mu')\,\Psi(x,\mu')\,d\mu'\right)=0. \qquad (2.1)$$

Here, x is distance measured in mean free paths and μ is the

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cosine of the angle between the neutron velocity and the positive x axis. The neutron flux is denoted by $\Psi(x,\mu)$, and $p(\mu',\mu)d\mu$ is the mean number of secondary neutrons emerging from a collision with direction cosines in $d\mu$ if the original direction cosine was μ'. We consider the case of anisotropic scattering of arbitrary finite order N,

$$p(\mu,\mu')=\sum_{l=0}^{N}\omega_l P_l(\mu)P_l(\mu'),\quad N<\infty\ . \tag{2.2}$$

Here, $P_l(\mu)$ denotes the Legendre polynomials and ω_l a set of expansion coefficients determined by theory or experiment.

We consider a slab of either finite or semi-infinite thickness, $0\leqslant x\leqslant\tau\leqslant\infty$. The slab is required to be subcritical. This is always true if $\omega_0<1$, and for finite τ it is also true if ω_0 is not too much greater than 1.

Astrophysical applications have motivated studies of the reflection and transmission properties of slabs, and many results have been obtained by Ambarzumian,[6] Chandrasekhar,[4] Busbridge,[9] Sobolev,[5] and others. The simplest problem of this type has a conical beam of neutrons with a given direction cosine μ_0 incident on the slab face at $x=0$. This problem is described by Eq. (2.1) with the boundary conditions

$$\Psi(0,\mu)=\delta(\mu-\mu_0),\quad \mu>0,$$

$$\Psi(\tau,\mu)=0,\quad \mu<0. \tag{2.3}$$

We shall call this Problem 0, and denote the corresponding flux by $\Psi_0(x,\mu)$. The reflected flux is $\Psi_0(0,\mu)$, $\mu<0$, and the transmitted flux is $\Psi_0(\tau,\mu)$, $\mu>0$. Chandrasekhar[4] defined two new functions, $S(\mu,\mu_0)$ and $T(\mu,\mu_0)$ in terms of these unknown fluxes by writing

$$\Psi_0(0,-\mu)=\frac{1}{2\mu}S(\mu,\mu_0),\quad \mu>0,$$

$$\Psi_0(\tau,\mu)=\delta(\mu-\mu_0)\,e^{-\tau/\mu_0}+\frac{1}{2\mu}T(\mu,\mu_0),\quad \mu>0. \tag{2.4}$$

In the latter equation, the first term on the right represents neutrons which pass through the slab without collision; the second term represent neutrons which experience one or more collisions.

Chandrasekhar also introduced functions $\phi_k(\mu_0)$ and $\psi_k(\mu_0)$ which are the Legrende moments of $\Psi_0(x,\mu)$ at $x=0$ and $x=\tau$, i.e.,

$$\psi_k(\mu_0)=\int_{-1}^{1}P_k(\mu)\Psi_0(0,\mu)\,d\mu\ ,$$

$$\phi_k(\mu_0)=\int_{-1}^{1}P_k(\mu)\Psi_0(\tau,\mu)\,d\mu\ . \tag{2.5}$$

(These are Chandrasekhar's definitions of ψ and ϕ. In Sobolev's work, the roles of ψ and ϕ are interchanged.) Use of Eqs. (2.3) and (2.4) in Eq. (2.5) leads to alternative definitions of $\psi_k(\mu_0)$ and $\phi_k(\mu_0)$ in terms of the S and T functions,

$$\psi_k(\mu_0)=P_k(\mu_0)+\frac{(-1)^k}{2}\int_0^1 S(\mu,\mu_0)P_k(\mu)\frac{d\mu}{\mu}, \tag{2.6}$$

$$\phi_k(\mu_0)=P_k(\mu_0)\,e^{-\tau/\mu_0}+\tfrac{1}{2}\int_0^1 T(\mu,\mu_0)P_k(\mu)\frac{d\mu}{\mu}. \tag{2.7}$$

Conversely, it was shown by Chandrasekhar that $S(\mu,\mu_0)$ and $T(\mu,\mu_0)$ are determined by the first N of the ϕ and ψ functions:

$$S(\mu,\mu_0)=\frac{\mu\mu_0}{\mu+\mu_0}\sum_{l=0}^{N}(-1)^l\omega_l \times[\psi_l(\mu)\psi_l(\mu_0)-\phi_l(\mu)\phi_l(\mu_0)\,], \tag{2.8}$$

$$T(\mu,\mu_0)=\frac{\mu\mu_0}{\mu-\mu_0}\sum_{l=0}^{N}\omega_l[\phi_l(\mu)\psi_l(\mu_0)-\psi_l(\mu)\phi_l(\mu_0)\,]. \tag{2.9}$$

The ϕ and ψ functions are solutions of a pair of nonlinear integral equations. One of these follows by substituting (2.8) into (2.6),

$$\psi_k(\mu)-P_k(\mu)=\frac{\mu}{2}\sum_{l=0}^{N}(-1)^{l+k}\omega_l\int_0^1\frac{P_k(\mu')}{\mu+\mu'}\times[\psi_l(\mu)\psi_l(\mu')-\phi_l(\mu)\phi_l(\mu')\,]d\mu'. \tag{2.10}$$

The other equation follows when (2.9) is substituted into (2.7).

It was discovered by Chandrasekhar (for special cases) and Sobolev (in general) that the $(2N+2)$ functions $\phi_k(\mu)$ and $\psi_k(\mu)$ $(k=0,1,\cdots,N)$ can be expressed in terms of two transcendental functions, $X(\mu)$ and $Y(\mu)$, and two sets of polynomials, $q_k(\mu)$ and $s_k(\mu)$. Specifically,[5]

$$\psi_k(\mu)=X(\mu)q_k(\mu)+(-1)^kY(\mu)s_k(-\mu),$$

$$\phi_k(\mu)=X(\mu)s_k(\mu)+(-1)^kY(\mu)q_k(-\mu), \tag{2.11}$$

The X and Y functions are solutions of the nonlinear integral equations[4]

$$X(\mu)=1+\frac{\mu}{2}\int_0^1\frac{g(\mu',\mu')}{\mu+\mu'}[X(\mu)X(\mu')-Y(\mu)Y(\mu')]\,d\mu', \tag{2.12}$$

$$Y(\mu)=e^{-\tau/\mu}+\frac{\mu}{2}\int_0^1\frac{g(\mu',\mu')}{\mu-\mu'}[\,Y(\mu)X(\mu')-X(\mu)Y(\mu')]d\mu'. \tag{2.13}$$

Here, $\frac{1}{2}g(\mu,\mu)$ is the so-called "characteristic function," which is defined in terms of a more general function $g(\mu,\nu)$. The latter function is defined by

$$g(\mu,\nu)=\sum_{l=0}^{N}\omega_l P_l(\mu)\,g_l(\nu). \tag{2.14}$$

The coefficients ω_l are the same as in Eq. (2.2). The $g_l(\nu)$ are a set of polynomials[4,8,10] generated from the recurrence relation

$$(l+1)\,g_{l+1}(\nu)=(2l+1-\omega_l)\,\nu\,g_l(\nu)-l\,g_{l-1}(\nu) \tag{2.15}$$

beginning with $g_0(\nu)=1$. They have parity $(-1)^l$.

The X and Y functions are required to satisfy both Eqs. (2.12) and (2.13) and a set of linear constraints. The latter are expressed in terms of the zeros of a dispersion function $\Lambda(z)$ defined as

$$\Lambda(z)=1-\frac{z}{2}\int_{-1}^{1}\frac{g(\mu',\mu')}{z-\mu'}\,d\mu'. \tag{2.16}$$

This function has $2J\leqslant 2N+2$ zeros ν_j occurring in pairs.[11] The constraints on the X and Y functions are, for $j=1,2,\cdots,2J$,

$$1-\frac{\nu_j}{2}\int_0^1\frac{g(\mu',\mu')X(\mu')}{\nu_j-\mu'}\,d\mu'=\frac{\nu_j}{2}\,e^{-\tau/\nu_j}\int_0^1\frac{g(\mu',\mu')Y(\mu')}{\nu_j+\mu'}\,d\mu'. \tag{2.17}$$

The X and Y functions are also solutions of a pair of linear singular integral equations[9]:

$$\lambda(\mu)X(\mu)+\frac{\mu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\mu-\mu'}\,d\mu'+\left(\frac{\mu}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\mu+\mu'}\,d\mu'\right)e^{-\tau/\mu}=1, \tag{2.18}$$

$$\lambda(\mu)Y(\mu)+\frac{\mu}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\mu-\mu'}\,d\mu'+\left(\frac{\mu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\mu+\mu'}\,d\mu'\right)e^{-\tau/\mu}=e^{-\tau/\mu}. \tag{2.19}$$

These equations hold for $\mu\in(0,1)$, with $\lambda(\mu)$ defined as

$$\lambda(\mu)=\tfrac{1}{2}[\Lambda^+(\mu)+\Lambda^-(\mu)]=\tfrac{1}{2}\lim_{\epsilon\to 0^+}[\Lambda(\mu+i\epsilon)+\Lambda(\mu-i\epsilon)]. \tag{2.20}$$

Either Eqs. (2.12) and (2.13) or Eqs. (2.18) and (2.19) can be used to give an analytic continuation of $X(\mu)$ and $Y(\mu)$ to the complex z plane. In this event, $\lambda(\mu)$ is replaced by $\Lambda(z)$ and, from Eqs. (2.18) and (2.19), the extended functions satisfy the reflection property

$$Y(-z)=e^{\tau/z}X(z). \tag{2.21}$$

It is worth noting that the constraints, Eqs. (2.17), are nothing more than the requirements that the analytic continuations of Eqs. (2.18) and (2.19) hold in the complex plane at the points $z=\nu_j$, where $\Lambda(z)$ vanishes. Finally, the polynomials $q_l(\mu)$ and $s_l(\mu)$ in Eq. (2.11) satisfy a pair of integral equations[5]

$$q_l(\mu)=\left\{\frac{\mu}{2}\int_0^1\frac{X(\mu')[q_l(\mu')g(\mu,\mu')-q_l(\mu)g(\mu',\mu')]}{\mu'-\mu}\,d\mu'+(-1)^l\frac{\mu}{2}\int_0^1\frac{Y(\mu')[s_l(-\mu')g(\mu,\mu')-s_l(-\mu)g(\mu',\mu')]}{\mu'-\mu}\,d\mu'+g_l(\mu)\right\}, \tag{2.22}$$

$$s_l(\mu)=\left\{\frac{\mu}{2}\int_0^1\frac{X(\mu')[s_l(\mu')g(\mu,\mu')-s_l(\mu)g(\mu',\mu')]}{\mu'-\mu}\,d\mu'+(-1)^l\times\frac{\mu}{2}\int_0^1\frac{Y(\mu')[q_l(-\mu')g(\mu,\mu')-q_l(-\mu)g(\mu',\mu')]}{\mu'-\mu}\,d\mu'\right\}. \tag{2.23}$$

In summary, the complete solution of Problem 0 is obtained as follows: The coefficients ω_l are determined from the scattering properties of the slab and the polynomials $g_l(\nu)$ are computed from (2.15). The function $g(\nu,\mu)$ is then given by (2.14). The dispersion function $\Lambda(z)$ is computed from (2.16) and its zeros ν_j are located, generally numerically. The X and Y functions must then be obtained as solutions of Eqs. (2.12) and (2.13) subject to the constraints (2.17). These solutions are known to exist, and to be unique, for subcritical slabs.[12] Closed-form expressions are not known for these functions, in general, except for the case $\tau=\infty$, but analyticity properties can be deduced and numerical methods can be used to generate $X(\mu)$ and $Y(\mu)$ to high accuracy. The polynomials $q_l(\mu)$ and $s_l(\mu)$ can then be determined from Eqs. (2.22) and (2.23). These equations appear cumbersome, but substitution of the polynomial expressions

$$q_l(\mu)=\sum_{n=0}^{N}q_{ln}\mu^n,\qquad s_l(\mu)=\sum_{n=0}^{N}s_{ln}\mu^n, \tag{2.24}$$

leads to $2N+2$ algebraic equations for the coefficients q_{ln} and s_{ln}. These equations can then be solved by standard methods. The functions $\psi_k(\mu)$ and $\phi_k(\mu)$ follow from Eq. (2.11); then, $S(\mu,\mu_0)$ and $T(\mu,\mu_0)$ are given by (2.8) and (2.9). Finally, the reflected and transmitted intensities for Problem 0 are given by (2.4).

It is important to realize that all of the functions $S, T, X, Y, \phi, \psi, q_l, s_l$ are implicitly dependent on the slab thickness τ.

In the limit $\tau\to\infty$, the results simplify since the transmitted flux $\Psi(\tau,\mu)$ goes to zero. Thus, from (2.5), the functions $\phi_k(\mu_0)\to 0$. The limit of the X function as $\tau\to\infty$ is Chandrasekhar's H function.[4] This function satisfies the equation

$$H(\mu)=1+\frac{\mu}{2}\int_0^1 \frac{g(\mu',\mu')H(\mu)H(\mu')}{\mu+\mu'}\,d\mu'. \tag{2.25}$$

Also, $H(\mu)$ satisfies the set of constraints

$$1-\frac{\nu_j}{2}\int_0^1 \frac{g(\mu',\mu')H(\mu')}{\nu_j-\mu'}\,d\mu'=0. \tag{2.26}$$

The latter equation holds for those ν_j with $\mathrm{Re}\,\nu_j>0$. Also,[4] when $\tau\to\infty$

$$\psi_k(\mu)\to H(\mu)q_k(\mu). \tag{2.27}$$

The polynomials $q_k(\mu)$ in the limit $\tau\to\infty$ were studied extensively by Busbridge.[9] We recall[4] that the H function has an analytic continuation to the complex z plane which provides a Wiener-Hopf factorization of $\Lambda(z)$:

$$\Lambda(z)=\frac{1}{H(z)H(-z)} \tag{2.28}$$

The procedure summarized above is seen to lead to expressions for the emergent surface fluxes $\Psi_0(0,-\mu)$ and $\Psi_0(\tau,\mu)$, $\mu>0$, but no expressions are obtained for the internal flux $\Psi_0(x,\mu)$, $0<x<\tau$. Since the internal flux is needed in neutron transport problems, workers in that field have developed alternative methods of analysis to study Eq. (2.1). Most relevant to the present paper is the singular eigenfunction representation of the flux $\Psi(x,\mu)$. This representation was first derived in its present form by Case[1] for isotropic scattering. His results were soon generalized by Mika[11] and by Kuščer and McCormick[13] to include anisotropic scattering. The main result of these analyses is that the neutron flux $\Psi(x,\mu)$ has the representation

$$\Psi(x,\mu)=\sum_{j=1}^{2J} A(\nu_j)\phi(\nu_j,\mu)\,e^{-x/\nu_j} + \int_{-1}^{1} A(\nu)\phi(\nu,\mu)e^{-x/\nu}\,d\nu. \tag{2.29}$$

Here, the ν_j are the zeros of $\Lambda(z)$, as above. The "discrete eigenfunctions" $\phi(\nu_j,\mu)$ are given by

$$\phi(\nu_j,\mu)=\frac{\nu_j}{2}\frac{g(\nu_j,\mu)}{\nu_j-\mu}, \tag{2.30}$$

with $g(\nu,\mu)$ given by (2.14). The "continuum eigenfunctions" are given by

$$\phi(\nu,\mu)=\frac{\nu}{2}\frac{g(\nu,\mu)}{\nu-\mu}+\lambda(\nu)\delta(\nu-\mu). \tag{2.31}$$

The integral in Eq. (2.29) is interpreted as a Cauchy principal value. The $A(\nu_j)$ and $A(\nu)$ are a set of expansion coefficients which must be determined from boundary conditions. In discussing expressions for $A(\nu)$ it is convenient to condense notation in Eq. (2.29) by writing it as

$$\Psi(x,\mu)=\int_\sigma A(\nu)\phi(\nu,\mu)\,e^{-x/\nu}\,d\nu. \tag{2.32}$$

Here, σ denotes the union of the ν_j and the continuum $(-1,1)$. It is, in fact,[14] the spectrum of the inverse of the operator in the second term of Eq. (2.1). The symbol $\int_\sigma d\nu$ in Eq. (2.32) denotes integration along $(-1,1)$ plus summation over the ν_j.

The $\phi(\nu,\mu)$ are normalized so that

$$\int_{-1}^{1}\phi(\nu,\mu)\,d\mu=1,\quad \nu\in\sigma. \tag{2.33}$$

If we define $g_n(\nu)$ by

$$g_n(\nu)=\int_{-1}^{1}P_n(\mu)\phi(\nu,\mu)\,d\mu,\quad \nu\in\sigma, \tag{2.34}$$

then it follows by multiplying Eq. (2.31) by $(\nu-\mu)P_n(\mu)$ and integrating over μ that these $g_n(\nu)$ satisfy the relation, Eq. (2.15). Thus, Eq. (2.34) provides an alternative to Eq. (2.15) as a definition of the g polynomials.

The work of Case, Mika, and Kuščer and McCormick is concerned with the so-called "full-range" and "half-range" expansions. The former arises if $\Psi(0,\mu)$ is given for $(-1<\mu<1)$, i.e., if

$$\int_\sigma A(\nu)\phi(\nu,\mu)d\nu=\Psi(0,\mu)\quad\text{(known)},\quad \mu\in(-1,1) \tag{2.35}$$

In this case, $A(\nu)$ is given by[1,11]

$$A(\nu)=\frac{1}{N(\nu)}\int_{-1}^{1}\mu\phi(\nu,\mu)\Psi(0,\mu)\,d\mu \tag{2.36}$$

Here, $N(\nu)=-N(-\nu)$ is a normalization factor given by

$$N(\nu_j)=\frac{\nu_j^2}{2}g(\nu_j,\nu_j)\Lambda'(\nu_j),\quad j=1,2,\cdots,2J,$$

$$N(\nu)=\nu\Lambda^+(\nu)\Lambda^-(\nu),\quad \nu\in(-1,1) \tag{2.37}$$

The half-range expansion arises in the albedo problem for a half-space. In that case, the boundary conditions for Eq. (2.1) are

$$\Psi(0,\mu)=\text{(known)},\quad 0<\mu<1,$$

$$\Psi(\infty,\mu)=0,\quad -1<\mu<1. \tag{2.38}$$

Now, $A(\nu)$ is given by[13]

$$A(\nu)=\begin{cases}\dfrac{1}{N(\nu)}\displaystyle\int_0^1\mu\frac{H(\mu)}{H(\nu)}\phi^+(\nu,\mu)\Psi(0,\mu)\,d\mu, & \nu\in\sigma_+,\\ 0, & \nu\in\sigma_-.\end{cases} \tag{2.39}$$

Here, $\sigma_\pm$ denote the parts of σ having positive and negative real parts, respectively. The function $\phi^+(\nu,\mu)$ is given by

$$\phi^+(\nu,\mu)=\begin{cases}\dfrac{\nu_j}{2}\dfrac{g^+(\nu_j,\mu)}{\nu_j-\mu}, & j=1,2,\cdots,2J,\\ \dfrac{\nu}{2}\dfrac{g^+(\nu,\mu)}{\nu-\mu}+\lambda(\nu)\delta(\nu-\mu), & \nu\in(-1,1).\end{cases} \tag{2.40}$$

Here,

$$g^{\dagger}(\nu,\mu)=\sum_{l=0}^{N}(-1)^{l}\omega_{l}q_{l}(-\nu)q_{l}(\mu), \tag{2.41}$$

where the $q_l(\mu)$ are the Busbridge q polynomials,[9] i.e., the q polynomials for the case $\tau\to\infty$.

The full- and half-range expansions are special cases of representations appropriate to finite slab problems. For a slab of thickness τ with neutrons incident on both faces, Eq. (2.32) leads to

$$\int_{\sigma}A(\nu)\phi(\nu,\mu)\,d\nu=\Psi(0,\mu)(\text{known}),\quad \mu>0,$$

$$\int_{\sigma}A(\nu)\phi(\nu,\mu)\,e^{-\tau/\nu}\,d\nu=\Psi(\tau,\mu)\ (\text{known}),\quad \mu<0. \tag{2.42}$$

These equations are dual singular integral equations for $A(\nu)$. For the case of isotropic scattering, a respresentation of $A(\nu)$ was given by Gibbs,[15] who used a technique of Vekua[16] to recast singular integral equations of semigeneral form into a matrix Hilbert problem. The X and Y functions appear in the solution of the corresponding homogeneous Hilbert problem, and the final result has the form

$$A(\nu)=\frac{1}{N(\nu)}\int_{-1}^{1}\mu W(\tau,\nu,\mu)\phi(\nu,\mu)\begin{pmatrix}\Psi(0,\mu), & \mu>0\\ \Psi(\tau,\mu), & \mu<0\end{pmatrix}d\mu. \tag{2.43}$$

Here, $W(\tau,\nu,\mu)$ is a weight function related to the X and Y functions. It is the extension of this result to the case of anisotropic scattering, which will be given in the present paper.

III. EXPANSION COEFFICIENTS

The method used below to derive expressions for $A(\nu)$ makes use of the known results for the reflected intensity for a finite slab and uses the full-range expansion to relate $A(\nu)$ to the S function. This approach was first suggested by Pahor[17] for half-space problems. Also, for finite slabs with isotropic scattering, it has been used by Pahor and Zweifel[18] and by Gibbs.[19] Here, we consider the general case of finite slabs with anisotropic scattering. We again consider Problem 0, so that $\Psi_0(0,\mu)$ is given by (2.3) and (2.4). We denote the corresponding $A(\nu)$ by $A_0(\nu)$. The full-range expansion, Eqs. (2.35) and (2.36), then gives a representation of $\Psi_0(x,\mu)$, with

$$A_0(\nu)=\frac{1}{N(\nu)}\left[\mu_0\phi(\nu,\mu_0)-\tfrac{1}{2}\int_0^1 S(\mu,\mu_0)\phi(\nu,-\mu)\,d\mu\right]. \tag{3.1}$$

While this result expresses $A_0(\nu)$ in terms of the S function, and thus indirectly in terms of X and Y functions and q_l and s_l polynomials, it is not in the most useful form for mathematical insight, for computational convenience, or for more general boundary conditions. Thus, a number of manipulations will be made to put the expression for $A_0(\nu)$ in a more suitable form.

In the following development, two new functions related to the X and Y functions will be needed. For $z\notin(-1,0)$, these are defined by

$$W_1(z)=1-\frac{z}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{z+\mu'}\,d\mu', \tag{3.2}$$

$$W_2(z)=\frac{z}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{z+\mu'}\,d\mu', \tag{3.3}$$

For the case of isotropic scattering and $z\in(0,1)$, essentially these functions have been tabulated by Sobouti.[20] Some identities relating $W_1(z)$, $W_2(z)$ and the X and Y functions follow from the extensions of Eqs. (2.12) and (2.13) or Eqs. (2.18) and (2.19) to the complex plane. Thus, from Eq. (2.12) we deduce that

$$X(z)W_1(z)+Y(z)W_2(z)=1. \tag{3.4}$$

Equation (2.13) leads to the same result when the reflection property, Eq. (2.21), is used. Equations (2.18) and (2.19) lead to

$$W_1(-z)=e^{-\tau/z}W_2(z)+\Lambda(z)X(z), \tag{3.5}$$

$$W_2(-z)=e^{-\tau/z}W_1(z)-\Lambda(z)Y(z), \tag{3.6}$$

By using the above three equations, it follows that

$$\Lambda(z)=W_1(z)W_1(-z)-W_2(z)W_2(-z). \tag{3.7}$$

The form of $\Lambda(z)$ obtained here can perhaps best be understood as the determinant of the matrix obtained when Eqs. (2.42) are reexpressed as a matrix Hilbert problem, as in Ref. 15. As shown below Eq. (3.7) reduces to Eq. (2.28) in the limit $\tau\to\infty$

In obtaining expressions for $A(\nu)$ it is convenient to introduce a function $W(\nu)$ related to $W_1(z)$ and $W_2(z)$ which is defined for all $\nu\in\sigma$. Let

$$W(\nu)=\begin{cases}W_1(\nu), & \nu\in\sigma_+,\\ W_2(-\nu), & \nu\in\sigma_-.\end{cases} \tag{3.8}$$

In the Appendix, we derive two identities relating $W(\nu)$ to the ϕ and ψ functions:

$$(-1)^k\int_0^1\psi_k(\mu)\phi(-\nu,\mu)\,d\mu$$

$$=g_k(\nu)-[(-1)^kW(\nu)q_k(-\nu)$$

$$-W(-\nu)s_k(\nu)]e_{\tau}(\nu), \tag{3.9}$$

and

$$(-1)^k\int_0^1\phi_k(\mu)\phi(-\nu,\mu)\,d\mu$$

$$=[W(-\nu)q_k(\nu)-(-1)^kW(\nu)s_k(-\nu)]e_{\tau}(\nu), \tag{3.10}$$

In the above, we have defined

$$e_{\tau}(\nu)=\begin{cases}1, & \nu\in\sigma_{+},\\ e^{\tau/\nu}, & \nu\in\sigma_{-}.\end{cases} \tag{3.11}$$

Equations (3.9) and (3.10) hold for all $\nu\in\sigma$.

With this preparation, we return to Eq. (3.1) for $A_0(\nu)$. Substituting $S(\mu,\mu_0)$ from (2.8) yields

$$\begin{aligned}N(\nu)A_0(\nu)&=\mu_0\phi(\nu,\mu_0)-\frac{\mu_0}{2}\sum_0^N(-1)^k\omega_k\int_0^1\frac{\mu}{\mu+\mu_0}\phi(\nu,-\mu)\\&\quad\times[\psi_k(\mu)\psi_k(\mu_0)-\phi_k(\mu)\phi_k(\mu_0)]\,d\mu.\end{aligned} \tag{3.12}$$

Using the definitions of $\phi(\nu,\mu)$, Eqs. (2.30) and (2.31), and making a partial fraction expansion, leads to

$$\begin{aligned}\frac{\mu}{\mu+\mu_0}\phi(\nu,-\mu)&=\frac{\nu}{\nu-\mu_0}\left(\phi(\nu,-\mu)-\frac{\mu_0}{2}\frac{g(\nu,-\mu)}{\mu_0+\mu}\right).\end{aligned} \tag{3.13}$$

Using the expansion of $g(\nu,-\mu)$ from Eq. (2.14) and the $(-1)^l$ parity of the Legendre polynomial $P_l(\mu)$ converts Eq. (3.13) into

$$\begin{aligned}\frac{\mu}{\mu+\mu_0}\phi(\nu,-\mu)&=\frac{\nu}{\nu-\mu_0}\left(\phi(\nu,-\mu)\right.\\&\quad\left.-\frac{\mu_0}{2(\mu+\mu_0)}\sum_{k=0}^N(-1)^k\omega_k P_k(\mu)g_k(\nu)\right).\end{aligned} \tag{3.14}$$

Using this result in (3.12), rearranging terms, and noting that $\phi(\nu,-\mu)=\phi(-\nu,\mu)$ leads to

$$\begin{aligned}N(\nu)A_0(\nu)\mu_0&\left[\phi(\nu,\mu_0)-\frac{\nu}{2(\nu-\mu_0)}\left(\sum_{k=0}^N\omega_k(-1)^k\right.\right.\\&\times\left.\int_0^1\phi(-\nu,\mu)[\Psi_k(\mu)\psi_k(\mu_0)-\phi_k(\mu)\phi_k(\mu_0)]\,d\mu\right)\\&+\frac{\nu}{2(\nu-\mu_0)}\sum_{k=0}^N\omega_k g_k(\nu)\left(\frac{\mu_0}{2}\sum_{l=0}^N\omega_l(-1)^{k+l}\right.\\&\left.\left.\times\int_0^1\frac{P_k(\mu)}{\mu+\mu_0}[\psi_k(\mu)\psi_k(\mu_0)-\phi_k(\mu)\phi_k(\mu_0)]\,d\mu\right)\right].\end{aligned} \tag{3.15}$$

From Eq. (2.10), the sum over l in Eq. (3.15) is seen to be $\psi_k(\mu_0)-P_k(\mu_0)$. The remaining integral in (3.15) can be expressed in terms of the function $W(\nu)$ by using Eqs. (3.9) and (3.10). Making these simplifications, cancelling common terms, and using the definition of $\phi(\nu,\mu)$ leads to

$$N(\nu)A_0(\nu)=\mu_0\tilde{\phi}(\nu,\mu_0)e_{\tau}(\nu),\quad \nu\in\sigma,\quad \mu_0>0. \tag{3.16}$$

Here, we have defined

$$\tilde{\phi}(\nu,\mu)=\frac{\nu}{2(\nu-\mu)}\tilde{g}(\nu,\mu)+\lambda(\nu)\delta(\nu-\mu),\quad \nu\in\sigma,\quad \mu>0. \tag{3.17}$$

(For $\nu=\nu_j, j=1,2,\ldots,2J$, the delta function term is zero.) The function $\tilde{g}(\nu,\mu)$ is defined for $\mu>0$ by

$$\begin{aligned}\tilde{g}(\nu,\mu)&=W(\nu)\sum_{k=0}^N(-1)^k\omega_k\\&\quad\times[\psi_k(\mu)q_k(-\nu)-\phi_k(\mu)s_k(-\nu)]+W(-\nu)\\&\quad\times\sum_{k=0}^N\omega_k[\phi_k(\mu)q_k(\nu)-\psi_k(\mu)s_k(\nu)].\end{aligned} \tag{3.18}$$

An equivalent expression for $\tilde{g}(\nu,\mu)$ follows by writing the ϕ and ψ functions in terms of X and Y functions as in Eq. (2.11). For $\mu>0$ and $\nu\in\sigma$,

$$\begin{aligned}\tilde{g}(\nu,\mu)&=X(\mu)\left(W(\nu)\sum_{k=0}^N(-1)^k\omega_k[q_k(\mu)q_k(-\nu)\right.\\&\quad-s_k(\mu)s_k(-\nu)]+W(-\nu)\sum_{k=0}^N\omega_k[q_k(\nu)s_k(\mu)\\&\quad\left.-s_k(\nu)q_k(\mu)]\right)+Y(\mu)\left(W(\nu)\sum_{k=0}^N\omega_k\right.\\&\quad\times[q_k(-\nu)s_k(-\mu)-s_k(-\nu)q_k(-\mu)]\\&\quad+W(-\nu)\sum_{k=0}^N(-1)^k\omega_k[q_k(\nu)g_k(-\mu)\\&\quad\left.-s_k(\nu)s_k(-\mu)]\right).\end{aligned} \tag{3.19}$$

The above equations define $\tilde{\phi}(\nu,\mu)$ for $\mu>0$. It is convenient to extend this definition to negative values of μ by defining

$$\tilde{\phi}(\nu,-\mu)=\tilde{\phi}(-\nu,\mu),\quad \mu>0,\quad \nu\in\sigma. \tag{3.20}$$

This definition implies that $\tilde{g}(\nu,\mu)$ must be extended to negative μ as

$$\tilde{g}(\nu,-\mu)=\tilde{g}(-\nu,\mu),\quad \mu>0,\quad \nu\in\sigma. \tag{3.21}$$

It is also of interest to evaluate $\tilde{g}(\mu,\mu)$. From Eq. (3.19), when $\mu>0$ we have

$$\begin{aligned}\tilde{g}(\mu,\mu)&=[X(\mu)W_1(\mu)+Y(\mu)W_2(\mu)]\\&\quad\times\sum_{k=0}^N(-1)^k\omega_l(q_k(\mu)q_k(-\mu)-s_k(\mu)s_k(-\mu)).\end{aligned} \tag{3.22}$$

The factor in square brackets is unity by Eq. (3.4). The remaining sum was considered by Sobolev,[5] who showed it to be equal to $g(\mu,\mu)$. Thus (3.22) reduces to

$$\tilde{g}(\mu,\mu)=g(\mu,\mu), \quad \mu>0. \tag{3.23}$$

By Eq. (3.21), this result also holds for $\mu<0$.

The solution of Problem 0 above is given by Eq. (2.32) with $A(\nu)$ given by Eq. (3.16). With this preparation we now consider more general boundary conditions. First, consider Problem I, defined by the boundary conditions

$$\Psi(0,\mu)=f(\mu)=\text{known}, \quad 0<\mu<1,$$

$$\Psi(\tau,\mu)=0, \quad -1<\mu<0. \tag{3.24}$$

We denote the solution of this problem by $\Psi_I(x,\mu)$ and the corresponding expansion coeficients by $A_I(\nu)$. Clearly, Problem I is a superposition of problems of type 0. Thus,

$$A_I(\nu)=\int_0^1 A_0(\nu)f(\mu_0)\,d\mu_0, \tag{3.25}$$

i.e., using Eqs. (3.16) and (3.24),

$$A_I(\nu)=\frac{e_\tau(\nu)}{N(\nu)}\int_0^1 \mu\,\tilde{\phi}(\nu,\mu)\,\Psi_I(0,\mu)\,d\mu. \tag{3.26}$$

Now, consider Problem II defined by the boundary conditions

$$\Psi(0,\mu)=0, \quad 0<\mu<1, \quad \Psi(\tau,\mu)=f(-\mu), \quad -1<\mu<0. \tag{3.27}$$

By symmetry, the solutions of Problems I and II are related by

$$\Psi_{II}(x,\mu)=\Psi_I(\tau-x,-\mu). \tag{3.28}$$

Substituting the corresponding representations from Eq. (2.32) leads to the conclusion that

$$A_{II}(\nu)=A_I(-\nu)\,e^{\tau/\nu}. \tag{3.29}$$

Substituting $A_I(-\nu)$ from Eq. (3.26) and using Eq. (3.27) leads to

$$A_{II}(\nu)=\frac{e_\tau(\nu)}{N(\nu)}\int_{-1}^0 \mu\,\tilde{\phi}(\nu,\mu)\,\Psi_{II}(\tau,\mu)\,d\mu. \tag{3.30}$$

Finally, we consider our most general boundary value problem, Problem III, defined by Eqs. (2.42), i.e.,

$$\Psi(0,\mu) \text{ known}, \quad \mu>0,$$

$$\Psi(\tau,\mu) \text{ known}, \quad \mu<0. \tag{3.31}$$

By linearity,

$$\Psi_{III}(x,\mu)=\Psi_I(x,\mu)+\Psi_{II}(x,\mu). \tag{3.32}$$

Thus,

$$A_{III}(\nu)=A_I(\nu)+A_{II}(\nu). \tag{3.33}$$

Using (3.26) and (3.30) in (3.33) gives the final result

$$A(\nu)=\frac{e_\tau(\nu)}{N(\nu)}\int_{-1}^1 \mu\,\tilde{\phi}(\nu,\mu)\begin{pmatrix}\Psi(0,\mu), & \mu>0\\ \Psi(\tau,\mu), & \mu<0\end{pmatrix}d\mu. \tag{3.34}$$

A somewhat more symmetrical result is obtained by defining

$$A(\nu)=A'(\nu)e_\tau(\nu). \tag{3.35}$$

Then, Eqs. (2.32) and (3.34) become

$$\Psi(x,\mu)=\int_\sigma A'(\nu)\phi(\nu,\mu)\,e^{-x/\nu}e_\tau(\nu)d\nu, \tag{3.36}$$

$$A'(\nu)=\frac{1}{N(\nu)}\int_{-1}^1 \mu\,\tilde{\phi}(\nu,\mu)\begin{pmatrix}\Psi(0,\mu), & \mu>0\\ \Psi(\tau,\mu), & \mu<0\end{pmatrix}d\mu. \tag{3.37}$$

These results are identical to (1.1) and (1.2), and provide an exact representation of the solution of the general boundary value problem of Eq. (3.31) for the transport equation with anisotropic scattering. The function $\tilde{\phi}(\nu,\mu)$ is defined by Eqs. (3.17) and (3.20). The function $W(\nu)$ which occurs in $\tilde{g}(\nu,\mu)$ is defined by Eqs. (3.8), (3.2), and (3.3). The computation of the remaining functions in $\tilde{\phi}(\nu,\mu)$—the X and Y functions and q_l and s_l polynomials—is discussed in Sec. II above.

IV. SOME LIMITING CASES

In this section, we examine some simplifications which occur when the slab thickness τ approaches 0 or ∞, or when the scattering is isotropic.

In the limit as slab thickness goes to zero there is no scattering in the slab; thus, from Eqs. (2.4), the S and T functions are zero. From Eqs. (2.7) and (2.7) it follows that, as $\tau\to 0$,

$$\psi_k(\mu_0)\to P_k(\mu_0), \tag{4.1}$$

$$\phi_k(\mu_0)\to P_k(\mu_0). \tag{4.2}$$

For $\tau=0$, Eqs. (2.21) and (3.4) imply that $X(\mu)=Y(\mu)=1$ is a solution of Eqs. (2.12) and (2.13). From the definition of $A(z)$, Eq. (2.16), it follows that the constraints, Eqs. (2.17), are also satisfied by these solutions. Since the X and Y functions are uniquely determined by Eqs. (2.12) and (2.13) and the constraints, it follows that as $\tau\to 0$

$$X(\mu)\to 1, \tag{4.3}$$

$$Y(\mu)\to 1. \tag{4.4}$$

From Eq. (2.11), it then follows that as $\tau\to 0$,

$$P_k(\mu)\to q_k(\mu)+(-1)^k s_k(-\mu), \tag{4.5}$$

$$P_k(\mu)\to s_k(\mu)+(-1)^k q_k(-\mu), \tag{4.6}$$

By subtracting Eq. (2.23) from (2.22) and using Eqs. (4.3)–(4.6), it follows that as $\tau\to 0$,

$$q_k(\mu)-s_k(\mu)\to g_k(\mu). \tag{4.7}$$

Finally, from Eqs. (3.4), (4.3), and (4.4) it follows that as $\tau\to 0$

$$W_1(z)\to 1-W_2(z)\to 1-\frac{z}{2}\int_0^1 \frac{g(\mu',\mu')}{z+\mu'}\,d\mu'. \tag{4.8}$$

Now, consider Eq. (3.18) for $\tilde{g}(\nu,\mu)$. Using Eqs. (4.1), (4.2), (4.7), and (4.8), and the definition of $W(\nu)$, it follows that for $\tau\to 0$,

$$\tilde{g}(\nu,\mu)\to\sum_{l=0}^{N}\omega_l P_l(\mu)g_l(\nu)=g(\nu,\mu)\,. \tag{4.9}$$

Thus, from Eqs. (3.17) and (2.31) it follows that

$$\tilde{\phi}(\nu,\mu)\to\phi(\nu,\mu). \tag{4.10}$$

Thus, the general expansion of $\Psi(x,\mu)$, Eqs. (3.36) and (3.37) reduces to the full-range expansion, Eqs. (2.35) and (2.36) in the limit $\tau\to 0$.

The limit $\tau\to\infty$ produces different results. For a semi-infinite slab, clearly $\Psi_0(\tau,\mu)\to 0$. From Eq. (2.5), this implies that as $\tau\to\infty$,

$$\phi_k(\mu)\to 0. \tag{4.11}$$

In this same limit, we note that $X(\mu)=H(\mu)$, $Y(\mu)=0$ satisfy Eqs. (2.12) and (2.13) identically [from the H equation, Eq. (2.25)]. In addition, Eq. (2.26) shows that the constraints, Eq. (2.17), are satisfied. Since this determines the X and Y functions uniquely we have, for $\tau\to\infty$,

$$X(\mu)\to H(\mu), \tag{4.12}$$

$$Y(\mu)\to 0. \tag{4.13}$$

Equations (2.11) now imply that

$$\psi_k(\mu)\to H(\mu)q_k(\mu)\,, \tag{4.14}$$

$$s_k(\mu)\to 0. \tag{4.15}$$

Equations (2.22) now reduces to

$$q_l(\mu)\to\frac{\mu}{2}\int_0^1 \times\frac{H(\mu')[q_l(\mu')g(\mu,\mu')-q_l(\mu)g(\mu',\mu')\,]}{\mu'-\mu}\times d\mu'+g_l(\mu). \tag{4.16}$$

This is the equation satisfied by the Busbridge q polynomials.[17] The functions $W_l(\nu)$ are determined from Eqs. (4.13), (3.2), (4.12), and (3.3):

$$W_1(z)\to 1/H(z), \tag{4.17}$$

$$W_2(z)\to 0. \tag{4.18}$$

From Eq. (3.8) it now follows that as $\tau\to\infty$,

$$W(\nu)\to\begin{cases}1/H(\nu), & \nu\in\sigma_+,\\ 0, & \nu\in\sigma_-.\end{cases} \tag{4.19}$$

Finally, using the above results in Eq. (3.18) gives, for $\mu>0$,

$$\tilde{g}(\nu,\mu)\to\begin{cases}\dfrac{H(\mu)}{H(\nu)}\displaystyle\sum_{k=0}^{N}(-1)^k\omega_k q_k(\mu)q_k(-\nu), & \nu\in\sigma_+,\\ 0, & \nu\in\sigma_-.\end{cases} \tag{4.20}$$

Thus, from Eq. (3.17), as $\tau\to\infty$ we have for $\mu>0$

$$\tilde{\phi}(\nu,\mu)\to\begin{cases}\dfrac{H(\mu)}{H(\nu)}\phi^{\dagger}(\nu,\mu), & \nu\in\sigma_+,\\ 0, & \nu\in\sigma_-.\end{cases} \tag{4.21}$$

Here, $\phi^{\dagger}(\nu,\mu)$ is the function defined by Eq. (2.40). The extension of Eq. (4.21) to $\mu<0$ is given by Eq. (3.20). This result reduces Eqs. (3.36) and (3.37) to the half-range result of Kuščer and McCormick,[13] Eq. (2.39).

An additional limiting case in which simplifications occur even for finite τ is the case of isotropic scattering. Now, only the $l=0$ term is present in Eq. (2.14), so

$$g(\mu,\nu)\to\omega_0. \tag{4.22}$$

With this simplification, it is easily verified that a solution of Eqs. (2.22) and (2.23) is

$$q_0(\mu)=1, \tag{4.23}$$

$$s_0(\mu)=0. \tag{4.24}$$

Thus, from Eqs. (2.11),

$$\psi_0(\mu)=X(\mu), \tag{4.25}$$

$$\phi_0(\mu)=Y(\mu). \tag{4.26}$$

With the above simplifications, Eq. (3.18) yields

$$\tilde{g}(\nu,\mu)\to\omega_0[X(\mu)W(\nu)+Y(\mu)W(-\nu)]. \tag{4.27}$$

This defines $\tilde{g}(\nu,\mu)$ for $\mu>0$, with the extension to $\mu<0$ given by Eq. (3.21). From Eqs. (3.21) and (4.22) it follows that

$$\frac{1}{\omega_0}\tilde{g}(\mu,\mu)\to 1. \tag{4.28}$$

Now, we define

$$W(\tau,\nu,\mu)=\frac{1}{\omega_0}\tilde{g}(\nu,\mu). \tag{4.29}$$

Using Eqs. (3.17), (4.27), and (4.28) we find that

$$\tilde{\phi}(\nu,\mu)\to W(\tau,\nu,\mu)\left(\frac{\omega_0\nu}{2(\nu-\mu)}+\lambda(\nu)\delta(\nu-\mu)\right). \tag{4.30}$$

Thus, Eqs. (3.37) reduces to

$$A'(\nu)=\frac{1}{\mu(\nu)}\int_{-1}^{1}\mu W(\tau,\nu,\mu)\phi(\nu,\mu)\begin{pmatrix}\Psi(0,\mu), & \mu>0\\ \Psi(\tau,\mu), & \mu<0\end{pmatrix}dN. \tag{4.31}$$

This is the same result obtained earlier by Gibbs[19] for the case of isotropic scattering.

Finally, it is of interest to examine the expression for $\Lambda(z)$ in terms of the functions $W_1(z)$ and $W_2(z)$, Eq. (3.7). Since $\Lambda(z)$, defined by Eq. (2.16), is independent of the slab thickness τ, Eq. (3.7) gives a family of representations of $\Lambda(z)$ for $0\leqslant\tau\leqslant\infty$. In the limiting case $\tau\to\infty$, the limiting forms of $W_1(z)$ and $W_2(z)$ from Eqs. (4.17) and (4.18) may be used in Eq. (3.7) to obtain the Wiener–Hopf factorization of $\Lambda(z)$, as in Eq. (2.28).

In contrast, when the limit $\tau \to 0$ is taken in Eq. (3.7), we use Eq. (4.8) to deduce that

$$\Lambda(z)=1-\frac{z}{2}\int_0^1 \frac{g(\mu',\mu')}{z+\mu'}\,d\mu'-\frac{z}{2}\int_0^1 \frac{g(\mu',\mu')}{z-\mu'}\,d\mu'. \quad (4.32)$$

Replacing μ' by $-\mu'$ in the second integral leads to Eq. (2.16) which is the defining integral for $\Lambda(z)$. Thus, interestingly, both the defining integral for $\Lambda(z)$ and the Wiener–Hopf factorization of $\Lambda(z)$ are seen to be special cases of the more general expression, Eq. (3.7).

V. SURFACE FLUXES

The representation of $\Psi(x,\mu)$ in Eq. (3.36) is useful in deriving expressions for Legendre moments of the surface fluxes. These are defined by

$$M_k(x)=\int_{-1}^{1} P_k(\mu)\Psi(x,\mu)\,d\mu, \quad x=0,\tau. \quad (5.1)$$

The lowest order moments, $k=0,1$, represent the product of the neutron density and velocity, and the neutron current, respectively. In deriving expressions for $M_k(0)$ and $M_k(\tau)$, we use several identities involving the ϕ and ψ functions. The first two of these are obtained directly from the definitions, Eqs. (2.5), by substituting the representation of $\Psi_0(x,\mu)$ from Eqs. (3.36) and (3.16). For $\mu_0>0$, this yeids

$$\Psi_k(\mu_0)=\int_{-1}^{1} P_k(\mu)\left(\int_\sigma \mu_0\tilde{\phi}(\nu,\mu_0)\phi(\nu,\mu)e_\tau(\nu)\frac{d\nu}{N(\nu)}\right)d\mu, \quad (5.2)$$

$$\phi_k(\mu_0)=\int_{-1}^{1} P_k(\mu)\times\left(\int_\sigma \mu_0\tilde{\phi}(\nu,\mu_0)\phi(\nu,\mu)e_\tau(-\nu)\frac{d\nu}{N(\nu)}\right)d\mu, \quad (5.3)$$

Interchanging orders of integration and using the fact that the Legendre moments of $\phi(\nu,\mu)$ are the $g_k(\nu)$ gives

$$\Psi_k(\mu_0)=\mu_0\int_\sigma \tilde{\phi}(\nu,\mu_0)g_k(\nu)e_\tau(\nu)\frac{d\nu}{N(\nu)}, \quad \mu_0>0, \quad (5.4)$$

$$\phi_k(\mu_0)=\mu_0\int_\sigma \tilde{\phi}(\nu,\mu_0)g_k(\nu)e_\tau(-\nu)\frac{d\nu}{N(\nu)}, \quad \mu_0>0. \quad (5.5)$$

In the above expressions, $\mu_0>0$. It is also of interest to evaluate the integrals on the right-hand sides of (5.4) and (5.5) for $\mu_0<0$. To do this, we replace ν by $-\nu$ in these integrals and then use the relation (3.20) and Eqs. (5.4) and (5.5) to obtain

$$\mu_0\int_\sigma \tilde{\phi}(\nu,\mu_0)g_k(\nu)e_\tau(\nu)\frac{d\nu}{N(\nu)}$$

$$=(-1)^k\phi_k(-\mu_0), \quad \mu_0<0, \quad (5.6)$$

$$\mu_0\int_\sigma \tilde{\phi}(\nu,\mu_0)g_k(\nu)e_\tau(-\nu)\frac{d\nu}{N(\nu)}$$

$$=(-1)^k\psi_k(-\mu_0), \quad \mu_0<0. \quad (5.7)$$

Expressions for the moments now follow by substituting the representation of $\Psi(x,\mu)$, Eq. (3.36), into Eq. (5.1) and interchanging orders of integration to get

$$M_k(x)=\int_\sigma A'(\nu)\,g_k(\nu)e^{-x/\nu}e_\tau(\nu)\,d\nu. \quad (5.8)$$

Substituting $A'(\nu)$ from Eq. (3.37) and interchanging integrations again yields

$$M_k(x)=\int_{-1}^{1}\begin{pmatrix}\Psi(0,\mu), & \mu>0\\ \Psi(\tau,\mu), & \mu<0\end{pmatrix}\times\left(\mu\int_\sigma \tilde{\phi}(\nu,\mu)g_k(\nu)e^{-x/\nu}\frac{e_\tau(\nu)d\nu}{N(\nu)}\right)d\mu. \quad (5.9)$$

Setting $x=0$ and $x=\tau$, and using Eqs. (5.4) through (5.7) then gives

$$M_k(0)=\int_{-1}^{1}\begin{pmatrix}\Psi(0,\mu)\psi_k(\mu), & \mu>0\\ \Psi(\tau,\mu)(-1)^k\phi_k(-\mu), & \mu<0\end{pmatrix}d\mu, \quad (5.10)$$

$$M_k(\tau)=\int_{-1}^{1}\begin{pmatrix}\Psi(0,\mu)\phi_k(\mu), & \mu>0\\ \Psi(\tau,\mu)(-1)^k\psi_k(-\mu), & \mu<0\end{pmatrix}d\mu. \quad (5.11)$$

These expressions for the surface moments can also be derived directly from the definitions of the ϕ and ψ functions, using superposition arguments.

Equations (5.10) and (5.11) express the surface moments in terms of ϕ and ψ functions and thus, via Eqs. (2.11), in terms of X and Y functions and q_l and s_l polynomials. For $k=0$ and $k=1$, these results have been noted by Kuščer and McCormick.[21] The above results extend theirs to all $k>0$, while Eq. (5.9) gives the moments at any internal point $0<x<\tau$.

VI. ORTHOGONALITY AND SINGULAR INTEGRAL TRANSFORMS

The general expansion of Eqs. (3.36) and (3.37) is equivalent to an integral transform pair, in the following sense. Define the two functions

$$f(\mu)=\begin{cases}\Psi(0,\mu), & \mu>0,\\ \Psi(\tau,\mu), & \mu<0,\end{cases} \quad (6.1)$$

$$e_\tau(\nu,\mu)=\begin{cases}e_\tau(\nu), & \mu>0,\\ e_\tau(-\nu), & \mu<0.\end{cases} \quad (6.2)$$

Then Eqs. (3.36) and (3.37) imply that

$$f(\mu)=\int_\sigma A'(\nu)\phi(\nu,\mu)\, e_\tau(\nu,\mu)\, d\nu, \tag{6.3}$$

$$A'(\nu)=\frac{1}{N(\nu)}\int_{-1}^{1}\mu\,\tilde{\phi}(\nu,\mu)f(\mu)\, d\mu \tag{6.4}$$

Thus, $f(\mu)$ and $A'(\nu)$ are singular integral transforms of one another. These equations follow rigorously[22] if $\mu f(\mu)$ belongs to the class H^* on $(-1,1)$ or, with more analysis,[23] if $\mu f(\mu)$ belongs to $L_p(-1,1)$ with $p>1$. Formal results may be obtained by applying the transforms to functions which are not in these spaces. Thus, if we consider $f(\mu)=\delta(\mu-\mu')$, Eq. (6.4) yields, formally, $A'(\nu)=\mu'\,\tilde{\phi}(\nu,\mu')/N(\nu)$. Substituting this result in Eq. (6.3) leads to

$$\delta(\mu-\mu')=\int_\sigma \mu'\tilde{\phi}(\nu,\mu')\phi(\nu,\mu)\, e_\tau(\nu,\mu)\,\frac{d\nu}{N(\nu)}. \tag{6.5}$$

In a similar fashion, by choosing $A'(\nu)$ to be a delta function we obtain the expression

$$\delta(\nu-\nu')=\frac{1}{N(\nu)}\int_{-1}^{1}\mu\,\tilde{\phi}(\nu,\mu)\phi(\nu',\mu)\, e_\tau(\nu',\mu)\, d\mu\,. \tag{6.6}$$

[This is shorthand notation consistent with Eq. (2.29). For $\nu=\nu_i$ and $\nu'=\nu_j$, the δ function is actually a Kronecker δ.] These formal orthogonality relations are correct in the sense that if $f(\mu)$ belongs to one of the above spaces, then multiplying Eq. (6.5) by $f(\mu')$, integrating over μ', and interchanging orders of integration on the right-hand side leads to Eqs. (6.3) and (6.4), which is the correct result. The same result is obtained by multiplying Eq. (6.6) by $A'(\nu')$ and integrating over $\nu'\in\sigma$.

A transform pair which is, in a sense, adjoint to Eqs. (6.3) and (6.4) can be derived formally by multiplying Eq. (6.5) by $(\mu/\mu')g(\mu)$, integrating over μ, interchanging orders of integration and defining

$$B(\nu)=\int_{-1}^{1}\mu\phi(\nu,\mu)g(\mu)e_\tau(\nu,\mu)\, d\mu\,. \tag{6.7}$$

This sequence of operations yields

$$g(\mu)=\int_\sigma B(\nu)\tilde{\phi}(\nu,\mu)\,\frac{d\nu}{N(\nu)}. \tag{6.8}$$

The transform pair in Eqs. (6.7) and (6.8) is similar to the one in Eqs. (6.3) and (6.4) with the roles of $\phi(\nu,\mu)$ and $\tilde{\phi}(\nu,\mu)$ interchanged. It has been derived here formally. A rigorous verification that Eq. (6.8) is a consequence of Eq. (6.7), and vice versa, would require solving each equation as a singular integral equation for $B(\nu)$ or $g(\mu)$. This procedure would require the same restrictions on $g(\mu)$ that are required for $f(\mu)$ in Eq. (6.3).

A number of additional results which have the character of orthogonality relations can be derived from the above transform pairs, or from Eqs. (6.5) and (6.6). These results may be useful in evaluating certain integrals which arise in applications of the general theory. As an illustration, we multiply Eq. (6.5) by $(\mu/\mu')\,P_l(\mu)\,P_m(\mu')$ and integrate over μ and μ'. We interchange orders of the (regular) integrations over μ and μ' with the (singular) integration over ν. We define the functions

$$\tilde{g}_m(\tau,\nu)=\int_{-1}^{1}P_m(\mu')\,\tilde{\phi}(\nu,\mu')\, d\mu', \tag{6.9}$$

$$g_l(\tau,\nu)=\int_{-1}^{1}\mu\,P_l(\mu)\phi(\nu,\mu)e_\tau(\nu,\mu)\, d\mu\,. \tag{6.10}$$

Then, from the orthogonality properties of the Legendre polynomials, we obtain

$$\int_\sigma g_l(\tau,\nu)\,\tilde{g}_m(\tau,\nu)\,\frac{d\nu}{N(\nu)}=\frac{2}{2l+1}\delta_{lm}. \tag{6.11}$$

This relation also follows directly from the transform pair of Eqs. (6.3) and (6.4) by choosing $f(\mu)=P_m(\mu)/\mu$ then multiplying Eq. (6.3) by $\mu P_l(\mu)$ and integrating over μ. It is of interest to examine Eq. (6.11) in the limits $\tau\to 0$ and $\tau\to\infty$. By using Eqs. (4.10) and (2.34), we deduce from Eq. (6.9) that, as $\tau\to 0$,

$$\tilde{g}_m(\tau,\nu)\to g_m(\nu)\,. \tag{6.12}$$

To evaluate $g_l(\tau,\nu)$, we use the recursion relations for the Legendre polynomials and for the $g_l(\nu)$ [Eq. (2.15)] to deduce from Eq. (6.10) that as $\tau\to 0$

$$g_l(\tau,\nu)\to\left(1-\frac{\omega_l}{2l+1}\right)\nu\, g_l(\nu)\,. \tag{6.13}$$

Thus, for $\tau\to 0$, Eq. (6.11) becomes

$$\int_\sigma g_l(\nu)\,g_m(\nu)\,\frac{\nu d\nu}{N(\nu)}=\left(\frac{2}{2l+1-\omega_l}\right)\delta_{lm}. \tag{6.14}$$

This relation has already been derived by Inönü.[24]

In the limit $\tau\to\infty$ we have, instead, the following results. From Eq. (6.2)

$$e_\tau(\nu,\mu)\to\begin{cases}1, & \mu>0, \quad \nu\in\sigma_+ \text{ or } \mu<0, \quad \nu\in\sigma_-,\\ 0, & \text{other.}\end{cases} \tag{6.15}$$

Thus, from Eq. (6.10), we find

$$g_l(\tau,\nu)\to g_l(\infty,\nu)\equiv\int_0^1\mu\,P_l(\mu)\phi(\nu,\mu)\, d\mu, \quad \nu\in\sigma_+ \tag{6.16}$$

and, by replacing μ by $-\mu$ in Eq. (6.10),

$$g_l(\tau,\nu)\to-(-1)^l g_l(\infty,-\nu), \quad \nu\in\sigma_-. \tag{6.17}$$

From Eqs. (4.21) and (3.20) we have, for $\tau\to\infty$,

$$\tilde{\phi}(\nu,\mu)\to\begin{cases}\dfrac{H(\mu)}{H(\nu)}\phi^{\dagger}(\nu,\mu), & \mu>0, \quad \nu\in\sigma_+,\\ \dfrac{H(-\mu)}{H(-\nu)}\phi^{\dagger}(-\nu,-\mu), & \mu<0, \quad \nu\in\sigma_-,\\ 0, & \text{other.}\end{cases} \tag{6.18}$$

In evaluating $\tilde{g}_m(\tau,\nu)$ in the limit $\tau\to\infty$, we also need the result[3,25]

$$\int_0^1 H(\mu)P_m(\mu)\,\phi^{\dagger}(\nu,\mu)\,d\mu=(-1)^m q_m(-\nu), \quad \nu\in\sigma_+. \tag{6.19}$$

Here, q_m denotes the Busbridge q-polynomial. Using Eqs. (6.13) and (6.19) in (6.10) now leads to

$$\tilde{g}_m(\tau,\nu)\to\begin{cases}\dfrac{1}{H(\nu)}(-1)^m q_m(-\nu), & \nu\in\sigma_+,\\ \dfrac{1}{H(-\nu)}q_m(\nu), & \nu\in\sigma_-.\end{cases} \tag{6.20}$$

Finally, we use the results, Eqs. (6.16) and (6.20) in Eq. (6.11). Writing the integral over σ as separate integrals over σ_+ and σ_-, and replacing ν by $-\nu$ in the latter, leads to

$$\int_{\sigma_+} q_m(-\nu)\,g_l(\infty,\nu)\,\frac{d\nu}{H(\nu)N(\nu)}=\frac{(-1)^m}{2l+1}\delta_{ml}. \tag{6.21}$$

This relation, which expresses the biorthogonality of the $q_m(-\nu)$ and the $g_l(\infty,\nu)$ [defined by Eq. (6.16)] on σ_+, with weight $1/H(\nu)N(\nu)$, appears to be new.

Clearly, the above results Eqs. (6.11), (6.14), and (6.21), are not the most general relations possible. Indeed, rather than multiplying Eq. (6.5) by $(\mu/\mu')\,P_l(\mu)\,P_m(\mu')$, as we did in deriving Eq. (6.11), other powers of μ/μ', or even other orthogonal functions besides P_l, along with any appropriate weight factors, could have been chosen. Thus, it is possible to derive a very large class of relations of the form Eq. (6.11), where $g_l(\tau,\nu)$ and $\tilde{g}_m(\tau,\nu)$ denote appropriate integrals with respect to μ of $\phi(\nu,\mu)$ and $\tilde{\phi}(\nu,\mu)$.

Results analogous to the above can also be obtained by using Eq. (6.6) instead of Eq. (6.5). For example, multiply Eq. (6.6) by $g_l(\nu)\,g_m(\nu')\nu'/N(\nu')$ and integrate over ν and ν' (over σ). Define

$$p_m(\tau,\mu)=\int_\sigma \nu' g_m(\nu')\phi(\nu',\mu)e_\tau(\nu',\mu)\,\frac{d\nu'}{N(\nu')}, \tag{6.22}$$

$$\tilde{p}_l(\tau,\mu)=\mu\int_\sigma g_l(\nu)\,\tilde{\phi}(\nu,\mu)\frac{d\nu}{N(\nu)}. \tag{6.23}$$

Then, use Eq. (6.14) to deduce that

$$\int_{-1}^1 \tilde{p}_l(\tau,\mu)\,p_m(\tau,\mu)d\mu=\left(\frac{2}{2l+1-\omega_l}\right)\delta_{lm}. \tag{6.24}$$

By arguments analogous to those used above, it is readily verified that in the limit $\tau\to 0$ both p_m and $\tilde{p}_l$ reduce to multiples of Legendre polynomials and Eq. (6.24) becomes the well-known orthogonality relation for these functions. Similarly, for $\tau\to\infty$, it is easily shown that

$$p_m(\tau,\mu)\to p_m(\infty,\mu)=(-1)^m p_m(\infty,-\mu)$$

$$\equiv\int_{\sigma_+}\nu g_m(\nu)\phi(\nu,\mu)\frac{d\nu}{N(\nu)}, \quad \mu>0, \tag{6.25}$$

and

$$\tilde{p}_l(\tau,\mu)\to\begin{cases}H(\mu)q_l(\mu), & \mu>0,\\ (-1)^l H(-\mu)\,q_l(-\mu), & \mu<0.\end{cases} \tag{6.26}$$

Finally, Eq. (6.24) reduces to

$$\int_0^1 H(\mu)q_l(\mu)\,p_m(\infty,\mu)\,d\mu=\left(\frac{1}{2l+1-\omega_l}\right)\delta_{lm}. \tag{6.27}$$

Thus, the Busbridge q polynomials and the functions $p_m(\infty,\mu)$ defined by Eq. (6.25) form a biorthogonal set on (0,1) with weight function $H(\mu)$. This result is also new.

The point of the above development has been to indicate that a large number of integrals that may arise in applications can be evaluated by using appropriate orthogonality relations easily derived from the singular integral transform pairs Eqs. (6.3) and (6.4) or (6.7) and (6.8). These relations extend the results of Inönü,[24] derived implicitly for $\tau=0$, to include all $0\leqslant\tau\leqslant\infty$.

Finally, we note one additional result which generalizes previous work. In the limit $\tau\to\infty$, it is known[13] that the polynomials $g_k(\nu)$ satisfy

$$g_k(\nu)=\int_0^1 H(\mu)q_k(\mu)\phi(\nu,\mu)\,d\mu. \tag{6.28}$$

Here, $q_k(\mu)$ denotes the Busbridge polynomial.[9] The corresponding relation for the case of finite τ is obtained from Eqs. (5.4) and (5.5) above. Define

$$K_k(\mu_0)=\begin{cases}\psi_k(\mu_0), & \mu_0>0,\\ (-1)^k\phi_k(-\mu_0), & \mu_0<0.\end{cases} \tag{6.29}$$

Then, from Eqs. (5.4) and (5.5),

$$\frac{1}{\mu_0}K_k(\mu_0)=\int_\sigma g_k(\nu)\,e_\tau(\nu)\,\tilde{\phi}(\nu,\mu_0)\frac{d\nu}{N(\nu)}. \tag{6.30}$$

Interpreting this result as a singular integral transform and using the inversion formula, Eq. (6.7), leads to

$$g_k(\nu)=\int_{-1}^1\phi(\nu,\mu)\begin{pmatrix}1, & \mu>0\\ e^{-\tau/\nu}, & \mu<0\end{pmatrix}K_k(\mu)\,d\mu. \tag{6.31}$$

This result, which expresses the polynomials $g_k(\nu)$ as a transform of the ϕ and ψ functions, reduces to Eq. (6.28) in the limit $\tau\to\infty$, and to Eq. (2.34) in the limit $\tau\to 0$.

VII. REFLECTING BOUNDARIES

In applications of radiative transfer theory to finite atmospheres, it is often necessary to consider boundary conditions more general than those of Eq. (2.42). In particular, a common problem has radiation incident on one boundary and reflected from the other, i.e.,

$$\Psi(0,\mu)=f(\mu) \text{ known}, \quad \mu>0,$$

$$\Psi(\tau,-\mu)=R\,\Psi(\tau,\mu), \quad \mu>0. \tag{7.1}$$

Here, R denotes a reflection operator. In this section, we indicate how the above methods may be adapted to solve this problem in two special cases. In the first, total specular reflection is assumed, i.e.,

$$R_1\Psi(\tau,\mu)=\Psi(\tau,\mu). \tag{7.2}$$

In the second, diffuse reflection with an albedo is assumed, i.e.,

$$R_2\Psi(\tau,\mu)=2a\int_0^1 \mu'\Psi(\tau,\mu')\,d\mu'. \tag{7.3}$$

This second case is often called the Lambert reflecting ground, and simply states that the current of photons incident on the bounary $x=\tau$ is absorbed, and a fraction $a<1$ is reemitted in random directions over the hemisphere $\mu<0$.

The problem for the reflection opeator R_1 is most easily solved by appealing to symmetry: Consider a slab of width 2τ with the flux satisfying the boundary conditions

$$\Psi(0,\mu)=f(\mu), \quad \mu>0,$$

$$\Psi(2\tau,\mu)=f(-\mu), \quad \mu<0. \tag{7.4}$$

By symmetry, the solution of this problem satisfies

$$\Psi(x,\mu)=\Psi(2\tau-x,-\mu). \tag{7.5}$$

In particular, for $x=\tau$ this requires that

$$\Psi(\tau,\mu)=\Psi(\tau,-\mu), \tag{7.6}$$

which is just the condition (7.2). Thus, to solve the problem of transport in a slab of width τ with specular reflection at $x=\tau$, one simply solves the problem in a slab of width 2τ with the boundary conditions of Eq. (7.4). This is a special case of the problem solved in Sec. III above [Eqs. (3.36) and (3.37)], except that all functions depending on slab thickness must now be evaluated for a slab of thickness 2τ.

The problem for the reflection operator R_2 is solved directly. Define

$$J_+(\tau)=\int_0^1 \mu'\Psi(\tau,\mu')\,d\mu'. \tag{7.7}$$

Then, the boundary condition of Eq. (7.3) becomes

$$\Psi(\tau,-\mu)=2aJ_+(\tau). \tag{7.8}$$

Assuming temporarily that $J_+(\tau)$ is known, we write the flux as in Eq. (3.36)

$$\Psi(x,\mu)=\int_\sigma A'(\nu)\phi(\nu,\mu)\,e^{-x/\nu}e_\tau(\nu)\,d\nu, \tag{7.9}$$

where, from Eqs. (3.37), (7.1), and (7.8)

$$A'(\nu)=\frac{1}{N(\nu)}\left(\int_0^1 \mu\,\tilde{\phi}(\nu,\mu)f(\mu)\,d\mu\right.$$

$$\left.+2aJ_+(\tau)\int_{-1}^0 \mu\,\tilde{\phi}(\nu,\mu)\,d\mu\right). \tag{7.10}$$

To condense notation, let

$$A'_1(\nu)=\frac{1}{N(\nu)}\int_0^1 \mu\,\tilde{\phi}(\nu,\mu)f(\mu)\,d\mu, \tag{7.11}$$

$$A'_2(\nu)=\frac{1}{N(\nu)}\int_{-1}^0 \mu\,\tilde{\phi}(\nu,\mu)\,d\mu, \tag{7.12}$$

Correspondingly, for $i=1,2$ let

$$\Psi_i(x,\mu)=\int_\sigma A'_i(\nu)\phi(\nu,\mu)e^{-x/\nu}e_\tau(\nu)\,d\nu, \tag{7.13}$$

Note that the A'_i and $\Psi_i(x,\mu)$ are now known quantities. Using Eqs. (7.9)–(7.13), it follows that

$$\Psi(x,\mu)=\Psi_1(x,\mu)+2aJ_+(\tau)\Psi_2(x,\mu). \tag{7.14}$$

When this expression is substituted into Eq. (7.7), we obtain

$$J_+(\tau)=\frac{J_1(\tau)}{1-2aJ_2(\tau)}. \tag{7.15}$$

Here, we have defined

$$J_i(\tau)=\int_0^1 \mu'\Psi_i(\tau,\mu')\,d\mu' \quad (i=1,2). \tag{7.16}$$

The complete solution of the transport problem with $R=R_2$ is now given by (7.14), where $J_+(\tau)$ is obtained from (7.15), the $J_i(\tau)$ from (7.16), the $\Psi_i(x,\mu)$ from (7.13) and the $A'_i(\nu)$ from (7.11) and (7.12).

VIII. DISCUSSION

The main result of this paper is the representation of the flux $\Psi(x,\mu)$ as an eigenfunction expansion, Eq. (3.36). The coefficients $A'(\nu)$ in that expansion are given by Eq. (3.37) as integrals over the incident surface fluxes. The weighting function $\tilde{\phi}(\nu,\mu)$ in those integrals has a form similar to that of the eigenfunctions $\phi(\nu,\mu)$ themselves. The function $\tilde{g}(\nu,\mu)$ appearing in the definition of $\tilde{\phi}(\nu,\mu)$, Eq. (3.17), is defined in terms of Chandrasekhar ϕ and ψ functions or, alternatively, in terms of X and Y functions and Sobolev polynomials.

The above results extend and unify much previous work. The full-range and half-range eigenfunction expansions are obtained as special cases of the present expansion in the limits of zero and infinite slab thickness. Also, the present results show how the functions arising in the invariant imbedding study of surface fluxes in transport theory (X, Y *et al.*) are related to the singular eigenfunctions occurring in the representation of the internal flux.

Finally, the biorthogonality relations, Eqs. (6.5) and (6.6), which follow from the properties of the eigenfunctions, generalize those obtained earlier for the half-space problem.[13] Integral moments of these relations lead to orthogonality relations for moments of the eigenfunctions. In special cases they reduce to known results for Legendre polynomials and for Inönü's polynomials, and in general [Eqs. (6.11) and (6.24)] they provide results which may be useful for simplifying integrals which arise in applications.

In closing, we note that while the analysis of the present paper has been carried out for the case of azimuthal symmetry, this does not seem to be an essential limitation. More generally, the flux is expanded in a Fourier series in the azimuthal angle ϕ. The equations for the coefficients $\Psi_m(x,\mu)$ of $e^{im\phi}$ in that expansion then uncouple, and each coefficient satisfies an equation analogous to Eq. (2.1). The main differences in the required analyses are the presence of associated Legendre functions $P_l^m(\mu)$ in the equations, and weighting functions $(1-\mu^2)^{m/2}$ in the integrals over μ. For the half-space problem, the eigenfunction expansion results have been given by Kuščer and McCormick.[13] For the surface fluxes, including the case of finite slabs, the corresponding results involving X and Y functions are given by Sobolev.[5] Apart from some notational complexity, the extension of the present work to include azimuthal dependence thus seems straightforward.

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APPENDIX: SOME USEFUL IDENTITIES

Here, we derive the identities, Eqs. (3.9) and (3.10). We begin with the equations satisfied by the q_l and s_l polynomials, Eqs. (2.22) and (2.23). These were originally derived for $0<\mu<1$; however, since both sides of these equations are polynomials in μ, they hold throughout the complex μ-plane. Replacing μ by $-\nu$, multiplying by $(-1)^l$ and using the parity of the $g_l(\nu)$ converts Eqs. (2.22) and (2.23) into

$$-(-1)^l q_l(-\nu)=(-1)^l\frac{\nu}{2}\int_0^1 X(\mu')[q_l(\mu')g(-\nu,\mu') - q_l(-\nu)g(\mu',\mu')]\frac{d\mu'}{\nu+\mu'} + \frac{\nu}{2}\int_0^1 Y(\mu')[s_l(-\mu')g(-\nu,\mu') - s_l(\nu)g(\mu',\mu')]\frac{d\mu'}{\nu+\mu'} + g_l(\nu) \tag{A1}$$

and

$$-(-1)^l s_l(-\nu)=(-1)^l\frac{\nu}{2}\int_0^1 X(\mu')[s_l(\mu')g(-\nu,\mu') - s_l(-\nu)g(\mu',\mu')]\frac{d\mu'}{\nu+\mu'} + \frac{\nu}{2}\int_0^1 Y(\mu') \times [q_l(-\mu')g(-\nu,\mu') - q_l(\nu)g(\mu',\mu')]\frac{d\mu'}{\nu+\mu'}. \tag{A2}$$

Regrouping terms and using the expressions (2.11) for the ϕ and ψ functions leads to

$$g_l(\nu)-(-1)^l\frac{\nu}{2}\int_0^1\psi_l(\mu')g(-\nu,\mu')\frac{d\mu'}{\nu+\mu'} = (-1)^l q_l(-\nu)\left(1-\frac{\nu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu'\right) - s_l(\nu)\left(\frac{\nu}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu'\right) \tag{A3}$$

and

$$-(-1)^l\frac{\nu}{2}\int_0^1\frac{\phi_l(\mu')g(-\nu,\mu')}{\nu+\mu'}d\mu' = (-1)^l s_l(-\nu)\left(1-\frac{\nu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu'\right) - q_l(\nu)\left(\frac{\nu}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu'\right) \tag{A4}$$

From the definition of $\phi(\nu,\mu)$, Eq. (2.31), we have

$$\frac{\nu}{2}\frac{g(-\nu,\mu')}{\nu+\mu'} = \phi(-\nu,\mu') - \lambda(\nu)\delta(\nu+\mu'). \tag{A5}$$

Using this result in Eqs. (A3) and (A4), and appealing to Eq. (2.11) leads to

$$g_l(\nu)-(-1)^l\int_0^1\psi_l(\mu')\phi(-\nu,\mu')d\mu' = (-1)^l q_l(-\nu)\left(1-\frac{\nu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu' - \lambda(\nu)X(-\nu)\theta(-\nu)\right) - s_l(\nu)\left(\frac{\nu}{2}\times\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu' + \lambda(\nu)Y(-\nu)\theta(-\nu)\right) \tag{A6}$$

and

$$-(-1)^l\int_0^1\phi_l(\mu')\phi(-\nu,\mu')d\mu' = (-1)^l s_l(-\nu)\left(1-\frac{\nu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\nu+\mu'}d\mu'\right.$$

$$-\lambda(\nu)X(-\nu)\theta(-\nu)\Big)-q_l(\nu)\left(\frac{\nu}{2}\right.$$

$$\times\left.\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\nu+\mu'}\,d\mu'+\lambda(\nu)Y(-\nu)\theta(-\nu)\right) \tag{A7}$$

Here $\theta(\nu)$ is a step function defined by

$$\theta(\nu)=\begin{cases}1, & \nu\in(0,1),\\ 0, & \text{other.}\end{cases} \tag{A8}$$

For $\nu\in\sigma_+$ the quantities in brackets on the right-hand sides of Eqs. (A7) and (A8) are $W_1(\nu)$ and $W_2(\nu)$. For $\nu\in(-1,0)$, we refer to the singular integral equations satisfied by the X and Y functions, Eqs. (2.18) and (2.19). With $\mu\to-\nu>0$ we find, since $\lambda(\mu)$ is even, that

$$1-\theta(-\nu)\lambda(\nu)X(-\nu)-\frac{\nu}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{\nu+\mu'}\,d\mu'$$

$$=\frac{-\nu}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{-\nu+\mu'}\,d\mu'\,e^{\tau/\nu}$$

$$=W_2(-\nu)\,e^{\tau/\nu},\quad \nu\in(-1,0) \tag{A9}$$

and

$$\theta(-\nu)\lambda(\nu)\,Y(-\nu)+\frac{\nu}{2}\int_0^1\frac{Y(\mu')g(\mu',\mu')}{\nu+\mu'}\,d\mu'$$

$$=\left(1-\frac{(-\nu)}{2}\int_0^1\frac{X(\mu')g(\mu',\mu')}{-\nu+\mu'}\,d\mu'\right)e^{\tau/\nu}$$

$$=W_1(-\nu)\,e^{\tau/\nu},\quad \nu\in(-1,0) \tag{A10}$$

In deriving the last quantities above, we have used Eqs. (3.2) and (3.3). Finally, we consider $\nu=\nu_j\in\sigma_-$. Now, the terms involving $\theta(-\nu)$ in the above equations are zero. The constraint equations, Eq. (2.17) satisfied by the X and Y functions now show that Eqs. (A9) and (A10) also hold for $\nu=\nu_j\in\sigma_-$. Writing Eqs. (A6) and (A7) in terms of the functions $W(\nu)$ [(Eq. 3.8)] and $e_\tau(\nu)$ [Eq. (3.11)] and using Eqs. (A9) and (A10) for $\nu\in\sigma_-$ leads to Eqs. (3.9) and (3.10). Q.E.D.

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Second-quantization representation for a nonrelativistic system of composite particles. II. Kinematical properties of the multispecies Tani transformation

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In previous publications a first-principles method was developed for constructing second-quantization representations for systems of composite bound states and their constituents. It is based on the introduction of redundant modes ("ideal atom variables") which are given physical content by carrying out a suitable unitary transformation. A single transformed Hamiltonian explicitly and simultaneously exhibits all kinematically possible scattering and reaction channels. Most of the previous results were limited to the case of two fermion composites. This restriction is removed herein, in order to allow a first-principles approach to the many-particle quantum dynamics and statistics of chemical and nuclear reactions. The kinematical aspects of the relevant transformation are examined.

1. INTRODUCTION

In previous publications[1-3] a method was developed for constructing second-quantization representations for systems of composite particles and their constituents from first principles. The method is based on the application of an appropriate unitary transformation to the second-quantized Hamiltonian of the constituents. The transformation is chosen so that the composite bound states appear explicitly in the relevant scattering and reaction terms of the transformed Hamiltonian. Except for some specific calculations for liquid helium[4] and ferromagnetism,[5] the previous results were limited to two-fermion composites. Here we shall remove this restriction in order to obtain a formalism adapted to the treatment of the quantum dynamics and statistics of chemical and nuclear reactions.

The "generalized Tani transformation" method employed allows a natural decomposition of such problems into two parts: (a) evaluation of a transformed Hamiltonian in which the structure of the composite bound states and the kinematics of the scattering and reaction processes involving these bound states are explicitly exhibited in the various terms of the transformed Hamiltonian; (b) treatment of this transformed Hamiltonian by standard methods (Wick's theorem, Green's functions, etc.) We shall be concerned here only with part (a). Furthermore, we shall restrict our attention to elucidation of the general kinematical properties of the relevant multispecies Tani transformation. Explicit evaluation of the various terms in the transformed Hamiltonian is best carried out separately for each specific application (specific choice of composite species involved), in view of the algebraic and notational complexities entailed by a completely general notation.

2. FORMALISM

Consider a nonrelativistic many-particle system composed of various different species of "elementary" constiuents. In applications to quantum theories of solids, liquids, gases, plasmas, chemical physics, etc., these constituents could be chosen to be electrons and nuclei of various species, whereas in an application to low-energy nuclear physics they could be chosen to be nucleons. Let $\psi(x^{(j)})$ and $\psi^{\dagger}(x^{(j)})$ be the second-quantized field annihilation and creation operators for particles of the jth *constituent species*. Here $x^{(j)}=(\mathbf{r}^{(j)},\sigma^{(j)})$ with $\mathbf{r}^{(j)}$ the position vector and $\sigma^{(j)}$ the spin z-component variable for a particle of the jth species; if this species has spin zero, then the argument $\sigma^{(j)}$ is to be omitted. If we adopt the standard convention[6] according to which kinematically independent fermion species anticommute, then these field operators will satisfy the commutation and/or anticommutation rules

$$\psi(x_1^{(j)})\cdot\psi(x_2^{(l)})=\psi^{\dagger}(x_1^{(j)})\cdot\psi^{\dagger}(x_2^{(l)})=0,$$
$$\psi(x_1^{(j)})\cdot\psi^{\dagger}(x_2^{(l)})=\delta_{jl}\delta(x_1^{(j)}-x_2^{(l)}). \tag{1}$$

Here $\delta(x_1^{(j)}-x_2^{(j)})$ stands for the product $\delta(\mathbf{r}^{(j)}-\mathbf{r}_2^{(j)})\,\delta_{\sigma_1(j)}\delta_{\sigma_2(j)}$ of a Dirac delta function of position variables by a Kronecker delta function of spin variables, whereas $A\cdot B$ stands for the graded Lie bracket[7]

$$A(x_1^{(j)})\cdot B(x_2^{(l)})\equiv A(x_1^{(j)})B(x_2^{(l)})$$
$$-(-1)^{p_j p_l}B(x_2^{(l)})A(x_1^{(j)}), \tag{2}$$

which is an anticommutator if the jth and l th species are both fermions, and is otherwise a commutator. The *permutation parity* p_j is defined to be zero (or even) if the jth species are bosons, and unity (or odd) if they are fermions.

These various constiuents species will interact, e.g., through the Coulomb interaction, leading to the possibility of formation of various bound states which define the various *composite species*, which may be atoms, molecules, ions, etc. (or nuclear species in applications to nuclear physics). Suppose that the sth *composite* species consists of $n_s^{(1)}$ particles of the first *constiuent* species, $n_s^{(2)}$ particles of the second constituent species, etc. Then the corresponding bound state wavefunctions may be denoted by $\varphi_{\alpha s}(x_1^{(1)}\cdots x_{n_s^{(1)}}^{(1)}, x_1^{(2)}\cdots x_{n_s^{(2)}}^{(2)},\cdots)$, where α stands for all the quantum numbers necessary to label such a state. These bound states may be

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assumed without loss of generality to satisfy orthonormality relations

$$\langle \alpha s | \beta s' \rangle \equiv \int \varphi^*_{\alpha s}(x_1^{(1)} \cdots x_{n_s^{(1)}}^{(1)}, x_1^{(2)} \cdots x_{n_s^{(2)}}^{(2)}, \cdots) \times \varphi_{\beta s'}(x_1^{(1)} \cdots x_{n_{s'}^{(1)}}^{(1)}, x_1^{(2)} \cdots x_{n_{s'}^{(2)}}^{(2)}, \cdots) \times \prod_j dx_1^{(j)} \cdots dx_{n_{s'}^{(j)}}^{(j)} = \delta_{\alpha\beta}, \tag{3}$$

where $\int dx_i^{(j)} = \Sigma_{\sigma_i^{(j)}} \int d^3 r_i^{(j)}$. In addition they are symmetric (p_j=even) or antisymmetric (p_j=odd) in the arguments of each jth constituent species. However, there is no completeness relation involving the bound states alone, since the total state space includes unbound states (involving constituents not bound into composites) as well. Furthermore, there is in general no simple relation analogous to (3) involving *different* composite species s and s'.

States and observables of the system are in principle expressible soley in terms of the dynamical variables of the various *constituent* species. However, if such a representation is employed then the presence, properties, interactions, etc., of the bound *composite* species are not explicit in the algebra of observables but must be inserted essentially as boundary conditions on the state vectors. For many-particle state vectors representing a system of nonzero density, this is a highly nontrivial problem. The Tani-transformation method[1-3] is designed to avoid this difficulty by use of a unitary transformation which introduces explicit composite-particle dynamical variables to describe the composite bound states but retains the constituent-particle dynamical variables to describe the *unbound* constituents. The definition and properties of the relevant transformation are straightforward generalizations of those considered previously[1-3] for two-fermion composites.

3. COMPOSITE-PARTICLE ANNIHILATION AND CREATION OPERATORS

The second-quantized state vector $|\alpha s\rangle$ representing a single composite particle (bound state) of composite species s and bound-state quantum numbers α is

$$|\alpha s\rangle = A_{\alpha s}{}^\dagger |0\rangle \tag{4}$$

where $|0\rangle$ is the normalized vacuum (no-particle state) and $A_{\alpha s}{}^\dagger$ is the composite-particle creation operation

$$A_{\alpha s}{}^\dagger \equiv \left[\prod_j n_s^{(j)}!\right]^{-1/2} \int \varphi_{\alpha s}(x_1^{(1)} \cdots x_{n_s^{(1)}}^{(1)}, x_1^{(2)} \cdots x_{n_s^{(2)}}^{(2)}, \cdots) \times \prod_j \psi^\dagger(x_1^{(j)}) \cdots \psi^\dagger(x_{n_s^{(j)}}^{(j)})\, dx_1^{(j)}\, dx_{n_s^{(j)}}^{(j)}. \tag{5}$$

The corresponding annihilation operator $A_{\alpha s}$ is defined to be $A_{\alpha s} \equiv (A_{\alpha s}{}^\dagger)^\dagger$. More generally, a state containing only bound composites of various species is a linear combination of composite-particle product states $A_{\alpha_1 s_1}{}^\dagger \cdots A_{\alpha_n s_n}{}^\dagger |0\rangle$.

Inner products between such states involve the commutation relations between the $A_{\alpha s}$ and the $A_{\alpha s}{}^\dagger$. These can be determined by using Wick's theorem to rewrite $A_{\alpha s} A_{\beta s'}$ and $A_{\alpha s} A_{\beta s'}{}^\dagger$ as sums of normally ordered products of the constituent field operators ψ and $\psi^\dagger$. The various terms involve *contractions* which are the graded Lie brackets (1). In this way one finds with (3)

$$\begin{aligned} A_{\alpha s} \cdot A_{\beta s'} &= A_{\alpha s}{}^\dagger \cdot A_{\beta s'}{}^\dagger = 0, \\ A_{\alpha s} \cdot A_{\beta s'}{}^\dagger &= \delta_{\alpha\beta} \delta_{ss'} + C_{\alpha s, \beta s'}, \end{aligned} \tag{6}$$

where the graded Lie bracket notation (2) has been extended to the composite-particle operators in the obvious way:

$$A_{\alpha s} \cdot B_{\beta s'} \equiv A_{\alpha s} B_{\beta s'} - (-1)^{p_s p_{s'}} B_{\beta s'} A_{\alpha s}. \tag{7}$$

The permutation parity p_s of the sth composite species is taken to be even or odd according to whether composite species s contains an even or and odd number of fermion constituents; boson constituents are to be disregarded in this counting. The c-number term $\delta_{\alpha\beta}\delta_{ss'}$ in the second line of (6) is just what would occur if these composite particles were elementary, whereas the operators $C_{\alpha s, \beta s'}$ exhibit the kinematical effects of the composite nature and internal structure of the bound states. They are found to be given by

$$\begin{aligned} C_{\alpha s, \beta s'} = \sum_{\nu^{(1)}=0}^{m_{ss'}^{(1)}} \sum_{\nu^{(2)}=0}^{m_{ss'}^{(2)}} \cdots \int & dx_{\nu^{(1)}+1}{}^{(1)} \cdots dx_{n_s^{(1)}}{}^{(1)}\, dx_{\nu^{(2)}+1}{}^{(2)} \cdots dx_{n_s^{(2)}}{}^{(2)} \cdots dy_{\nu^{(1)}+1}{}^{(1)} \cdots dy_{n_{s'}^{(1)}}{}^{(1)}\, dy_{\nu^{(2)}+1}{}^{(2)} \cdots dy_{n_{s'}^{(2)}}{}^{(2)} \cdots \\ & \times K_{\alpha s, \beta s'}(x_{\nu^{(1)}+1}{}^{(1)} \cdots x_{n_s^{(1)}}{}^{(1)}, x_{\nu^{(2)}+1}{}^{(2)} \cdots x_{n_s^{(2)}}{}^{(2)}, \cdots; y_{\nu^{(1)}+1}{}^{(1)} \cdots y_{n_{s'}^{(1)}}{}^{(1)}, y_{\nu^{(2)}+1}{}^{(2)} \cdots y_{n_{s'}^{(2)}}{}^{(2)}, \cdots) \psi^\dagger(x_{\nu^{(1)}+1}{}^{(1)}) \\ & \times \cdots \psi^\dagger(x_{n_s^{(1)}}{}^{(1)}) \psi^\dagger(x_{\nu^{(2)}+1}{}^{(2)}) \cdots \psi^\dagger(x_{n_s^{(2)}}{}^{(2)}) \cdots \psi(y_{n_{s'}^{(2)}}{}^{(2)}) \cdots) \psi(\nu_{(2)+1}{}^{(2)}) \psi \\ & (y_{n_{s'}^{(1)}}{}^{(1)}) \cdots \psi(y_{\nu^{(1)}+1}{}^{(1)}), \end{aligned} \tag{8}$$

where the "exchange kernels" $K_{\alpha s, \beta s'}$ are defined as

$$K_{\alpha s, \beta s'}(x_{\nu^{(1)}+1}{}^{(1)} \cdots x_{n_s^{(1)}}{}^{(1)}, x_{\nu^{(2)}+1}{}^{(2)} \cdots x_{n_s^{(2)}}{}^{(2)}, \cdots; y_{\nu^{(1)}+1}{}^{(1)} \cdots y_{n_{s'}^{(1)}}{}^{(1)}, y_{\nu^{(2)}+1}{}^{(2)} \cdots y_{n_{s'}^{(2)}}{}^{(2)}, \cdots)$$

$$=(\pm)\left[\prod_j \frac{(n_s^{(j)}!)^{1/2}(n_{s'}^{(j)}!)^{1/2}}{\nu^{(j)}!(n_s^{(j)}-\nu^{(j)})!(n_{s'}^{(j)}-\nu^{(j)})!}\right]$$

$$\times\int \varphi_{\alpha s}^{*}(x_1^{(1)}\cdots x_{\nu^{(1)}}^{(1)} y_{\nu^{(1)}+1}^{(1)}\cdots y_{n_s^{(1)}}^{(1)},\ x_1^{(2)}\cdots x_{\nu^{(2)}}^{(2)} y_{\nu^{(2)}+1}^{(2)}\cdots y_{n_s^{(2)}}^{(2)},\cdots)$$

$$\times\varphi_{\beta s'}(x_1^{(1)}\cdots x_{n_{s'}^{(1)}}^{(1)},\ x_1^{(2)}\cdots x_{n_{s'}^{(2)}}^{(2)},\cdots)dx_1^{(1)}\cdots dx_{\nu^{(1)}}^{(1)}\,dx_1^{(1)}\cdots dx_{\nu^{(2)}}^{(2)}\cdots. \tag{9}$$

Here $m_{ss'}^{(j)}$ is the smaller of $n_s^{(j)}$ and $n_{s'}^{(j)}$; note that $n_s^{(j)}$ or $n_{s'}^{(j)}$ may be zero, in which case the sum over $\nu^{(j)}$ is (8) contains only the term $\nu^{(j)}=0$. If $s=s'$ then the c-number term in (8) (that with $\nu^{(1)}=n_s^{(1)}$, $\nu^{(2)}=n_s^{(2)},\cdots$) is to be omitted, being already explicitly exhibited in (6) as the c-number term $\delta_{\alpha\beta}\delta_{ss'}$. We shall now need the explicit formula for the $(\pm)$ prefactor in (9) here. The term with $\nu^{(1)}=\nu^{(2)}=\cdots=0$ is to be omitted from the summation (8), being already accounted for it in the term $A_{\beta s'}{}^{\dagger}A_{\alpha s}$.

The interpretation of the kernels $K_{\alpha s,\beta s'}$ as arising from exchange of identical constituents between the composite bound states $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ is intuitively clear from their definition. Since such exchange can only occur when the bound-state wavefunctions overlap, we expect that the kernels $K_{\alpha s,\beta s'}$ and hence the operators $C_{\alpha s,\beta s'}$ will vanish in the limit of vanishing overlap. This expectation will be substantiated and generalized by the results which will be established in Sec. 6. It follows that the $A_{\alpha s}$ and $A_{\alpha s}{}^{\dagger}$ behave like *elementary* Bose or Fermi operators in the limit of vanishing overlap. This result is, of course, expected on physical grounds.

In addition to (6) one has commutation and/or anticommunication relations between the constituent ψ and $\psi^{\dagger}$ fields and the composite A and $A^{\dagger}$ operators:

$$\psi(x^{(j)})\cdot A_{\alpha s}=0,$$
$$\psi(x^{(j)})\cdot A_{\alpha s}{}^{\dagger}=C_{\alpha s}(x^{(j)}) \tag{10}$$

with

$$C_{\alpha s}(x^{(j)})=n_s^{(j)}\left[\prod_l n_s^{(l)}!\right]^{-1/2}(-1)^{p_j\Sigma_l{}' p_l n_s^{(l)}}\int\varphi_{\alpha s}(x_1^{(1)}\cdots x_{n_s^{(1)}}^{(1)},\cdots,x_1^{(j-1)}\cdots x_{n_s^{(j-1)}}^{(j-1)},$$

$$x_1^{(j)}x_2^{(j)}\cdots x_{n_s^{(j)}}^{(j)},\ x_1^{(j+1)}\cdots x_{n_s^{(j+1)}}^{(j+1)},\cdots)\prod_l{}'\psi^{\dagger}(x_1^{(l)})\cdots\psi^{\dagger}(x_{n_s^{(l)}}^{(l)})dx_1^{(l)}\cdots dx_{n_s^{(l)}}^{(l)} \tag{11}$$

where the prime on Π_l' implies omission of the factors $\psi^{\dagger}(x_1^{(j)})$ and $dx_1^{(j)}$ in the term with $l=j$. The graded Lie bracket in (10) is defined as

$$\psi(x^{(j)})\cdot B_{\alpha s}=\psi(x^{(j)})B_{\alpha s}-(-1)^{pp'}B_{\alpha s}\psi(x^{(j)}). \tag{12}$$

The operator $C_{\alpha s}(x^{(j)})$ in (10) is a consequence of the lack of kinematical independence between the composite particles and their constituents. It is easy to see that $C_{\alpha s}(x^{(j)})$ vanishes either if the composite species s does not contain constituents of the jth species or if the position vector $\mathbf{r}^{(j)}$ lies outside some finite region $\mathscr{R}_{\alpha s}$ within which the bound state $\varphi_{\alpha s}$ is localized. This will be discussed in more detail, along with its consequences, in Sec. 6.

4. IDEAL STATE SPACE AND TANI TRANSFORMATION

The nontrivial commutation relations (6) and (10) would lead to computational difficulties if one were to employ the $A_{\alpha s}$ and $A_{\alpha s}{}^{\dagger}$ operators as composite-particle dynamical variables. For example, the composite-particle product states $A_{\alpha_1 s_1}{}^{\dagger}\cdots A_{\alpha_n s_n}{}^{\dagger}|0\rangle$ are neither orthornormal nor independent of the constituent product states $\psi^{\dagger}(x_1^{j_1})\cdots\psi^{\dagger}(x_n^{(j_n)})|0\rangle$. A related difficulty is that Wick's theorem only applies to operators satisfying elementary Bose or Fermi commutation or anticommutation relations.

These difficulties can be overcome by carrying out a mapping to an "ideal state space" in which the annihilation and creation operators representing the composite particles satisfy *elementary* Bose or Fermi relations, the effects of the composite structure of the bound states being transferred from the commutation relations to the formulas for the second-quantized operators representing observables (e.g., the Hamiltonian). Such an approach is in the spirit of Dyson's theory[8] of "ideal spin waves" in the Heisenberg model and the Bohm-Pines theory[9] of plasma oscillations.

Define the physical state space $\mathscr{P}$ to be the space of all

normalizable linear combinations of constituent product states $\psi^\dagger(x_1^{(j_1)})\cdots\psi^\dagger(x_n^{(j_n)})|0\rangle$. Also define a *completely independent* state space $\mathscr{C}$, the *ideal composite particle state space*, to be the space of all normalizable linear combinations of *ideal composite particle product states* $a_{\alpha_1 s_1}^\dagger\cdots a_{\alpha_n s_n}^\dagger|0\rangle$ where, *by definition*, the $a_{\alpha s}$ and $a_{\alpha s}^\dagger$ satisfy *elementary* Bose/or Fermi commutation and/or anticommutation rules

$$a_{\alpha s}\cdot a_{\beta s'}=a_{\alpha s}^\dagger\cdot a_{\beta s'}^\dagger=0,$$
$$a_{\alpha s}\cdot a_{\beta s'}^\dagger=\delta_{\alpha\beta}\delta_{ss'}, \tag{13}$$

the graded Lie bracket being defined as in (7). Finally, define the *ideal state space* $\mathscr{I}$ to be the space of all normalizable linear combinations of product states

$$a_{\alpha_1 s_1}^\dagger\cdots a_{\alpha_n s_n}^\dagger\psi^\dagger(x_1^{(j_1)})\cdots\psi^\dagger(x_m^{(j_m)})|0\rangle$$

of both constituents and ideal composite particles. To make this definition meaningful, one must supplement (13) by commutation relations between the $a, a^\dagger, \psi$, and $\psi^\dagger$ operators considered as operators on $\mathscr{I}$. We take them to be "normal commutation relations" [6]

$$\psi(x^{(j)})\cdot a_{\alpha s}=\psi(x^{(j)})\cdot a_{\alpha s}^\dagger=0, \tag{14}$$

where the graded Lie bracket is defined as in (12). It then also follows from (14) and (5) that

$$a_{\alpha s}\cdot A_{\beta s'}=a_{\alpha s}\cdot A_{\beta s'}^\dagger=0 \tag{15}$$

with the graded Lie bracket defined as in (7). The commutation relations (1), (6), and (10) on $\mathscr{P}$ and those (13) on $\mathscr{C}$ are then also extended to $\mathscr{I}$.

The physical state space $\mathscr{P}$ is trivially isomorphic with the subspace $\mathscr{I}_0$ of $\mathscr{I}$ consisting of those states $|\varphi\rangle\in\mathscr{I}$ which satisfy the contrains

$$a_{\alpha s}|\varphi\rangle=0,\ \forall\,\alpha, s,\ |\varphi\rangle\in\mathscr{I}_0. \tag{16}$$

Defining the ideal composite particle occupation-number operators $N_{\alpha s}=a_{\alpha s}^\dagger a_{\alpha s}$, the composite species occupation numbers

$$N_s=\sum_\alpha N_{\alpha s}=\sum_\alpha a_{\alpha s}^\dagger a_{\alpha s}, \tag{17}$$

and the total ideal composite particle number operator

$$N_c=\sum_s N_s=\sum_{\alpha s}N_{\alpha s}=\sum_{\alpha s}a_{\alpha s}^\dagger a_{\alpha s} \tag{18}$$

and noting the positive semidefinite property of all of these occupation numbers, one can equivalently state the constrains (16) in the form

$$N_c|\varphi\rangle=0,\ |\varphi\rangle\in\mathscr{I}_0. \tag{19}$$

The interpretation is that in $\mathscr{I}_0$ the ideal composite particles are "redundant modes" (totally unoccupied), which makes the isomorphism of $\mathscr{I}_0$ with $\mathscr{P}$ trivial and obvious.

We now perform a unitary transformation U, the generalized Tani transformation, which shifts the description of bound composites to the $a_{\alpha s}$ and $a_{\alpha s}^\dagger$, in a sense which will presently be precisely defined. We take U to be the obvious generalization of the previous transformation[1-3] to the multispecies case:

$$U=\exp(\tfrac{1}{2}\pi F),$$
$$F=\sum_{\alpha s}(a_{\alpha s}^\dagger A_{\alpha s}-A_{\alpha s}^\dagger a_{\alpha s}). \tag{20}$$

The kinematical properties and resultant physical interpretation of U relating to the interpretation of asymptotic scattering states will be discussed in Sec. 6. However, we shall first discuss here some simpler properties of U related to the particle-number conservation laws.

Let

$$F_{s'}^-=\sum_\alpha a_{\alpha s'}^\dagger A_{\alpha s'} \tag{21}$$

and let N_j be the number operator for constituent species j:

$$N_j=\int dx^{(j)}\ \psi^\dagger(x^{(j)})\psi(x^{(j)}). \tag{22}$$

Then by (5) one has with (17)

$$N_j F_{s'}^-=F_{s'}^-(N_j-n_{s'}^{(j)}),$$
$$N_s F_{s'}^-=F_{s'}^-(N_s+\delta_{ss'}) \tag{23}$$

and hence

$$\left[\left(N_j+\sum_s n_s^{(j)}N_s\right),F_{s'}^-\right]=0. \tag{24}$$

Combining this with the similar relation for $F_{s'}^+=(F_{s'}^-)^\dagger$, one sees from (20) that the operators $N_j+\Sigma_s n_s^{(j)}N_s$ commute with F and hence with U:

$$\left[\left(N_j+\sum_s n_s^{(j)}N_s\right),U\right]=0. \tag{25}$$

Next let $|\varphi\rangle$ be any state in $\mathscr{I}_0$ which is a simultaneous eigenstate of the N_j for all of the various constituent species, with eigenvalues n_j:

$$N_s|\varphi\rangle=0,\quad N_j|\varphi\rangle=n_j|\varphi\rangle,\quad \forall\ j,|\varphi\rangle\in\mathscr{I}_0. \tag{26}$$

Let $|\varphi)$ be the image of such a state under the transformation (20):

$$|\varphi\rangle=U|\varphi),\ |\varphi)=U^{-1}|\varphi\rangle. \tag{27}$$

Then it follows from (25) and (26) that

$$\left(N_j+\sum_s n_s^{(j)}N_s\right)|\varphi)=n_j|\varphi). \tag{28}$$

The physical interpretation is that in $|\varphi)$ the *total* number of constituents of constituent species j is the sum of the number

of *unbound* constituents of this species (counted by N_j) and the number of such constituents *bound* in the various composites, counted by $n_s^{(j)} N_s$ for the sth *composite* species. Note the shift in the meaning of N_j: *Before* the transformation, i.e., in the state $|\varphi\rangle$, it counts *all* constituents of type j, whereas *after* the transformation, i.e., in the state $|\varphi)$, it counts only *unbound* constituents of this type. Similarly, the commutation property (25) ensures that in the transformed Hamiltonian $U^{-1}HU$, only reaction terms consistent with the conservation of particles of each constituent species will occur. This is a generalization of the property exhibits previously[2,3] for the case of two-fermion composites.

This kinematical property of the multi-species Tani transformation (20) generalizes immediately to *any* physical observable A on the physical state space $\mathscr{P}$ which commutes with the constituent species occupation numbers:

$$[N_j, A] = 0. \tag{29}$$

Recalling that $\mathscr{P}$ is isomorphic with the subspace $\mathscr{I}_0$ of the ideal state space $\mathscr{I}$ and that A, being a physical observable on $\mathscr{P}$, is expressed solely in terms of the constituent fields ψ and $\psi^\dagger$, one sees that A will also commute with the composite species occupation numbers N_s:

$$[N_s, A] = 0. \tag{30}$$

Equations (29) and (30) are valid as operator identities on $\mathscr{I}$. It then follows with (25) that

$$\left[\left(N_j + \sum_s n_s^{(j)} N_s\right), U^{-1}AU\right] = 0. \tag{31}$$

This established a set of superselection rules, one for each constituent species j: For any physical observable A satisfying (29), its generalized Tani transform $U^{-1}AU$ has nonvanishing matrix elements only between states with the same eigenvalue of $N_j + \Sigma_s n_s^{(j)} N_s$. These superselection rules are merely the transforms, under U, of the usual particle number conservation superselection rules. They have important consequences for the kinematical structure of the transformed observables $U^{-1}AU$. For example, as previously noted, $U^{-1}HU$ has terms representing dissociation of a composite particle into its constituents and other terms representing dissociation into smaller composites (plus perhaps free constituents) as well as terms representing the inverse reactions (recombination). In fact, there will be terms *explicitly* exhibiting all kinematically possible reactions, i.e., all reactions compatible with the constituent particle conservation laws; however, no other terms will occur. This shows that the transformation (20) is constructed in such a way as to explicitly exhibit the various possible reaction channels in the transformed Hamiltonian $U^{-1}HU$.

5. SUBSIDIARY CONDITION AND STATISTICAL MECHANICS

States $|\varphi)$ related to states $|\varphi\rangle \in \mathscr{I}_0$ by (27) define a subspace $\mathscr{I}_{\text{phys}}$ of $\mathscr{I}$ which is isomorphic to $\mathscr{I}_0$ and hence to the original physical state space $\mathscr{P}$. One can write symbolically

$$\mathscr{I}_{\text{phys}} = U^{-1}\mathscr{I}_0. \tag{32}$$

$\mathscr{I}_{\text{phys}}$ is the subspace of those states $|\varphi) \in \mathscr{I}$ satisfying a subsidiary condition which is the transform of (19):

$$(U^{-1}N_c U)|\varphi) = 0, \quad |\varphi) \in \mathscr{I}_{\text{phys}}. \tag{33}$$

For any two physical states $|\varphi\rangle, |\varphi'\rangle \in \mathscr{P}$, there are esssentially identical[10] states in $\mathscr{I}_0$, which have images $|\varphi), |\varphi') \in \mathscr{I}_{\text{phys}}$. Any calculation in the physical state space $\mathscr{P}$ is equivalent to a calculation in $\mathscr{I}_{\text{phys}}$. For example, for any observable A one has trivially

$$\langle\varphi|A|\varphi'\rangle = (\varphi|U^{-1}AU|\varphi'). \tag{34}$$

The advantage of carrying out the calculation in $\mathscr{I}_{\text{phys}}$ is that processes involving existence, excitation, and reactions of bound composites are then built explicitly into the algebra of observables and hence exhibited explicitly in $U^{-1}AU$. The subsidiary condition (33) is dynamically consistent in the sense that

$$[U^{-1}HU, U^{-1}N_c U] = 0, \tag{35}$$

since the original Hamiltonian H is a functional only of the constituent-particle fields ψ and $\psi^\dagger$ and hence commutes trivially with N_c.

The definition (19) of $\mathscr{I}_0$ generalizes to an infinite sequence of subspaces $\mathscr{I}_n$ of $\mathscr{I}$, $n = 0,1,2,\cdots$, where $\mathscr{I}_n$ is the space of those states $|\varphi\rangle$ satisfying

$$N_c|\varphi\rangle = n|\varphi\rangle, \quad |\varphi\rangle \in \mathscr{I}_n. \tag{36}$$

The $\mathscr{I}_n$ are disjoint, and their union (n running from 0 to ∞) spans the ideal state space $\mathscr{I}$. If the subsidiary condition (19) is dropped then, since H does not contain any $a_{\alpha s}$ and $a_{\alpha s}^\dagger$ operators, it will have the same eigenvalue spectrum on $\mathscr{I}$ as it does on the subspace $\mathscr{I}_0$, but with a spurious infinite degeneracy of every energy level. Similarly, along with $\mathscr{I}_{\text{phys}} = U^{-1}\mathscr{I}_0$ there is an infinite sequence of disjoint subspaces $U^{-1}\mathscr{I}_n$ whose union is $\mathscr{I}$; each $U^{-1}\mathscr{I}_n$ for $n \geq 1$ can be regarded as a "copy" of $\mathscr{I}_{\text{phys}}$, each state $|\varphi) \in \mathscr{I}_{\text{phys}}$ being imaged, with the same energy, in all the other subspaces $U^{-1}\mathscr{I}_n$. The same argument applies to any other physical observable: one can safely ignore the subsidiary condition in evaluating eigenvalues, so long as the density of states is not required.

On the other hand, the grand partition function

$$Z_1(\beta;\mu_1,\mu_2,\cdots) = \text{Tr}_0 \exp\left[-\beta U^{-1}\left(H - \sum_j \mu_j N_j\right)U\right] \tag{37}$$

does depend on the density of states, and so the trace must be restricted to a basis spanning $\mathscr{I}_{\text{phys}}$; this is the meaning of the zero subscript on Tr_0. Here the N_j are the constituent-species occupation number operators (22) and the μ_j are the corresponding constituent chemical potentials. One can, however, remove the restriction on the trace by defining a generalized partition function

$$\Xi(\beta,\zeta,\mu_1,\mu_2,\cdots)$$
$$=\mathrm{Tr}\ \exp\left[-\beta U^{-1}(H-\lambda\ N_c-\sum_j \mu_j N_j)U\right], \tag{38}$$

where

$$\zeta=\exp(\beta\lambda), \tag{39}$$

and the trace now runs over the whole ideal space $\mathscr{I}$. Then the grand partition function Z can be recovered as the coefficient of the constant term in the expansion of Ξ in powers of ζ, or equivalently as a contour integral

$$Z(\beta;\mu_1;\mu_2,\cdots)=(2\pi i)^{-1}\int \zeta^{-1}\Xi(\beta,\zeta;\mu_1,\mu_2,\cdots)\,d\zeta\ . \tag{40}$$

Note that chemical potentials for the *composite* species do not occur in (37) or (38); there are no constraints on the occupations of the composite species, which adjust their occupations to the equilibrium values as a result of the chemical (or nuclear, etc.) reactions implied by the various reaction terms in $U^{-1}HU$. In cases where one is dealing with a situation where the occupations of one or more composite species are constrained to have values other than those appropriate to complete equilibrium, one would introduce additional terms $-\mu_s N_s$ in (37), where the μ_s are the chemical potentials of only those composite species which have *constrained nonequilibrium* values.

These properties and consequences of the subsidiary condition and resultant decomposition of $\mathscr{I}$ are all straightforward generalizations from the special case of two-fermion composites. Similarly, as in that case the projector P_0 onto $\mathscr{I}_0$ can be written as[2]

$$P_0=:e^{-N_c}:$$
$$=1+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\sum_{\alpha_1 s_1\cdots\alpha_n s_n} a_{\alpha_1 s_1}^{\dagger}\cdots a_{\alpha_n s_n}^{\dagger} a_{\alpha_n s_n}\cdots a_{\alpha_1 s_1}, \tag{41}$$

where the colons denote normal-ordering. The corresponding projector onto $\mathscr{I}_{\mathrm{phys}}$ is $U^{-1}P_0\,U$.

6. BEHAVIOR OF THE TANI TRANSFORM FOR ORTHOGONAL OR NONOVERLAPPING COMPOSITES: ASYMPTOTIC STATES

The generalized Tani transformation (20) was introduced for the purpose of shifting the description of bound composites from the original $A_{\alpha s}$, $A_{\alpha s}^{\dagger}$ operators to the "ideal composite particle operators" $a_{\alpha s}$, $a_{\alpha s}^{\dagger}$ which satisfy *elementary particle* commutation relations (13). In this section we shall investigate the sense in which this shift is effected, along with related questions of the interpretation of the transformed operators and of the asymptotic scattering and reaction states.

Let us first investigate the behavior of the transformation in certain limiting situations. This will be done in the form of a sequence of definitions, lemmas, and theorems.

Definition 1: The composite particle creation operators $A_{\alpha s}^{\dagger}$ and $A_{\beta s'}^{\dagger}$ are said to be *completely orthogonal* (denoted by $A_{\alpha s}^{\dagger}\perp A_{\beta s'}^{\dagger}$) iff the following two conditions are satisfied:

$$A_{\alpha s}\cdot A_{\beta s'}^{\dagger}=0$$
$$[C_{\alpha s,\alpha s}, A_{\beta s'}^{\dagger}]=0. \tag{42}$$

Here $A_{\alpha s}\cdot A_{\beta s'}^{\dagger}$ is the graded Lie bracket (7) occurring in (6). Thus (42) requires the vanishing of the operator $C_{\alpha s,\beta s'}$ if $A_{\alpha s}^{\dagger}$ and $A_{\beta s'}^{\dagger}$ are to be completely orthogonal; however, it does not require the vanishing of $C_{\alpha s,\alpha s}$. Note also that if $A_{\alpha s}^{\dagger}\perp A_{\beta s'}^{\dagger}$, then $\langle \alpha s|\beta s'\rangle=0$ where the states $|\alpha s\rangle$ are defined by (4). However, the converse need not be true; for example, if composite species s and s' contain different numbers of any constituent species[11] then $|\alpha s\rangle$ and $|\beta s'\rangle$ will be orthogonal, but nevertheless $A_{\alpha s}^{\dagger}$ and $A_{\beta s'}^{\dagger}$ may not be completely orthogonal.

Definition 2: $\psi^{\dagger}(x^{(j)})$ and $A_{\alpha s}^{\dagger}$ are said to be *completely orthogonal* [denoted by $\psi^{\dagger}(x^{(j)})\perp A_{\alpha s}^{\dagger}$] iff

$$\psi(x^{(j)})\cdot A_{\alpha s}^{\dagger}=0, \tag{43}$$

where the expression (43) is the graded Lie bracket (12) occurring in (10). Thus (43) requires the vanishing of the operator $C_{\alpha s}(x^{(j)})$.

Lemma 1: $A_{\alpha s}^{\dagger}\perp A_{\beta s'}^{\dagger}$ if the composite species s and s' contain no common constituents, and $\psi^{\dagger}(x^{(j)})\perp A_{\alpha s}^{\dagger}$ if the composite species s does not contain constituents of species j.

Proof: Under the hypotheses of the lemma the operators $C_{\alpha s,\beta s'}$ and $C_{\alpha s}(x^{(j)})$ vanish, since Wick's-theorem contractions can only occur between constituent field operators of the same species. The commutator $[C_{\alpha s,\alpha s}, A_{\beta s'}^{\dagger}]$ vanishes for the same reason.

Definition 3: $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ are said to be *nonoverlapping* iff

$$\varphi_{\alpha s}^{*}(\cdots x\cdots)\,\varphi_{\beta s'}(\cdots x\cdots)=0 \tag{44}$$

for every argument x which refers to a constituent species common to $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$. Note that this must be true as an identity in x and in all the other arguments of $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$. Note also that $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ can be nonoverlapping even when *different* constituent species in $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ occupy the *same* region of space. If $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ contain no common constituents, then they are trivially nonoverlapping, by definition.

Definition 4: $x^{(j)}$ and $\varphi_{\alpha s}$ are said to be *nonoverlapping* iff

$$\varphi_{\alpha s}(\cdots x^{(j)}\cdots)=0 \tag{45}$$

where one or more arguments of $\varphi_{\alpha s}$ referring to the jth constituent species have the *particular* value $x^{(j)}$. If $\varphi_{\alpha s}$ does not contain constituents of species j, then $x^{(j)}$ and $\varphi_{\alpha s}$ are trivially nonoverlapping, by definition.

Lemma 2: $A_{\alpha s}^{\dagger}\perp A_{\beta s'}^{\dagger}$ if $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ are nonoverlapping, and $\psi^{\dagger}(x^{(j)})\perp A_{\alpha s}^{\dagger}$ if $x^{(j)}$ and $\varphi_{\alpha s}$ are nonoverlapping.

Proof: Recalling that the term with $\nu^{(1)}=\nu^{(2)}=\cdots=0$ is omitted from the sum (8), one sees that all of the exchange kernels $K_{\alpha s,\beta s'}$, and hence the operator $C_{\alpha s,\beta s'}$, vanish if (44) is satisfied. The commutator $[C_{\alpha s,\alpha s},A_{\beta s'}{}^{\dagger}]$ is also proportional to products of the form (44) and hence also vanishes. Similarly, it follows from (11) that the operator $C_{\alpha s}(x^{(j)})$ vanishes if (45) is satisfied.

Definition 5: $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ are said to be *strongly orthogonal* iff

$$\int \varphi_{\alpha s}{}^{*}(\cdots x\cdots)\,\varphi_{\beta s'}(\cdots x\cdots)\,dx=0 \tag{46}$$

for every argument x which refers to a constituent species common to $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$. Note that this must be true as an identity in all of the other arguments of $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$, which are *not* integrated over. Note also that if $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ are nonoverlapping, then they are strongly orthogonal, but that the converse need not be true. If $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ contain no common constituent species, then they are trivially strongly orthogonal, by definition.

Lemma 3: $A_{\alpha s}{}^{\dagger}\perp A_{\beta s'}{}^{\dagger}$ if $\varphi_{\alpha s}$ and $\varphi_{\beta s'}$ are strongly orthogonal.

Proof: The proof is only a trivial refinement of that of Lemma 2. One need only note than in the expression (9) for the exchange kernels, the product $\varphi_{\alpha s}{}^{*}(\cdots x\cdots)\,\varphi_{\beta s'}(\cdots x\cdots)$ is integrated over x. Hence (46) is sufficient to ensure vanishing of $C_{\alpha s,\beta s'}$: (44) is not necessary. The same integrals (46) occur in the expression for the commutator $[C_{\alpha s,\alpha s},A_{\beta s'}{}^{\dagger}]$ as a result of Wick's-theorem contractions between the constituent ψ field operators in $C_{\alpha s,\alpha s}$ and the corresponding $\psi^{\dagger}$ field operators in $A_{\beta s'}{}^{\dagger}$; hence this commutator also vanishes.

Theorem 1: If the $A_{\alpha s}{}^{\dagger}$ belonging to different composite species s are completely orthogonal, then

$$UA_{\alpha s}{}^{\dagger}|0\rangle=a_{\alpha s}{}^{\dagger}|0\rangle,\quad \forall(\alpha s). \tag{47}$$

Proof: By (20), (5), and (6) one has under the given hypothesis

$$\begin{aligned}FA_{\alpha s}{}^{\dagger}|0\rangle&=\sum_{\beta s'}a_{\beta s'}{}^{\dagger}A_{\beta s'}A_{\alpha s}{}^{\dagger}|0\rangle\\&=\sum_{\beta}a_{\beta s}{}^{\dagger}A_{\beta s}A_{\alpha s}{}^{\dagger}|0\rangle\\&=\sum_{\beta}a_{\beta s}{}^{\dagger}(\delta_{\alpha\beta}+C_{\beta s,\alpha s})\,|0\rangle\\&=\sum_{\beta}a_{\beta s}{}^{\dagger}\delta_{\alpha\beta}|0\rangle=a_{\alpha s}{}^{\dagger}|0\rangle.\end{aligned} \tag{48}$$

Similarly

$$Fa_{\alpha s}{}^{\dagger}|0\rangle=-\sum_{\beta s'}A_{\beta s'}{}^{\dagger}a_{\beta s'}a_{\alpha s}{}^{\dagger}|0\rangle=-A_{\alpha s}{}^{\dagger}|0\rangle. \tag{49}$$

The desired result (47) then follows[12] as in the simpler case of two-fermion composites. Note that the hypothesis of the theorem was required because[13] $C_{\beta s',\alpha s}|0\rangle$ need not in general vanish for $s\neq s'$; on the other hand $C_{\beta s,\alpha s}|0\rangle$ vanishes for all α,β. Complete orthogonality of different $A_{\alpha s}{}^{\dagger}$ and $A_{\beta s}{}^{\dagger}$ belonging to the *same* composite species s is *not* required for validity of the theorem; however, orthogonality of the different *wavefunctions* $\varphi_{\alpha s}$ and $\varphi_{\beta s}$ (for each given s) is assumed [Eq. (3)].

Theorem 2:

$$U\psi^{\dagger}(x^{(j)})\,|0\rangle=\psi^{\dagger}(x^{(j)})\,|0\rangle. \tag{50}$$

Proof: Every *composite* species contains more than one constituent particle. Then by (10), (11), (14), and (20)

$$F\psi^{\dagger}(x^{(j)})\,|0\rangle=0. \tag{51}$$

The desired result follows immediately.

Theorem 3: Suppose that all of the different $A_{\alpha s}{}^{\dagger}$ occurring in the Tani transformation operator (20) are mutually completely orthogonal and suppose that $(\alpha_1 s_1)\cdots(\alpha_n s_n)$ are any discrete set selected from these (αs). Then

$$UA_{\alpha_1 s_1}{}^{\dagger}\cdots A_{\alpha_n s_n}{}^{\dagger}|0\rangle=a_{\alpha_1 s_1}{}^{\dagger}\cdots a_{\alpha_n s_n}{}^{\dagger}|0\rangle. \tag{52}$$

Proof: The proof is a straightforward generalization of that give previously.[14] Under the hypotheses of the theorem one finds that

$$\begin{aligned}[A_{\alpha_k s_k}{}^{\dagger},F]_{2m}&=(-1)^m A_{\alpha_k s_k}{}^{\dagger}+D_{\alpha_k s_k}{}^{(2m)},\\[A_{\alpha_k s_k}{}^{\dagger},F]_{2m-1}&=(-1)^m a_{\alpha_k s_k}{}^{\dagger}+D_{\alpha_k s_k}{}^{(2m-1)},\end{aligned} \tag{53}$$

for $m=1,2,3,\cdots$, where $[\,]_m$ denotes the multiple commutator of order m and where the $D_{\alpha s}{}^{(m)}$ satisfy[15]:

$$\begin{aligned}&D_{\alpha_k s_k}{}^{(m)}|0\rangle=0,\\&D_{\alpha_k s_k}{}^{(m)}\cdot a_{\alpha_l s_l}=D_{\alpha_k s_k}{}^{(m)}\cdot a_{\alpha_l s_l}{}^{\dagger}=0,\quad k\neq l,\\&D_{\alpha_k s_k}{}^{(m)}\cdot A_{\alpha_l s_l}=D_{\alpha_k s_k}{}^{(m)}\cdot A_{\alpha_l s_l}{}^{\dagger}=0,\quad k\neq l.\end{aligned} \tag{54}$$

Then[14]

$$\begin{aligned}&UA_{\alpha_k s_k}{}^{\dagger}U^{-1}\\&\quad=a_{\alpha_k s_k}{}^{\dagger}\sin\left(\frac{\pi}{2}\right)+A_{\alpha_k s_k}{}^{\dagger}\cos\left(\frac{\pi}{2}\right)+D_{\alpha_k s_k}\\&\quad=a_{\alpha_k s_k}{}^{\dagger}+D_{\alpha_k s_k},\end{aligned} \tag{55}$$

where $D_{\alpha_k s_k}$ satisfies the same conditions (53) as do the $D_{\alpha_k s_k}{}^{(m)}$. Then, noting that $U|0\rangle=|0\rangle$, one has

$$\begin{aligned}&UA_{\alpha_1 s_1}{}^{\dagger}\cdots A_{\alpha_n s_n}{}^{\dagger}|0\rangle\\&\quad=(UA_{\alpha_1 s_1}{}^{\dagger}U^{-1})\cdots(UA_{\alpha_n s_n}{}^{\dagger}U^{-1})\,|0\rangle\\&\quad=(a_{\alpha_1 s_1}{}^{\dagger}+D_{\alpha_1 s_1})\cdots(a_{\alpha_n s_n}{}^{\dagger}+D_{\alpha_n s_n})\,|0\rangle\end{aligned}$$

$$=(a_{\alpha_1 s_1}{}^{\dagger}+D_{\alpha_1 s_1})\cdots(a_{\alpha_{n-1} s_{n-1}}{}^{\dagger}+D_{\alpha_{n-1} s_{n-1}})a_{\alpha_n s_n}{}^{\dagger}|0\rangle$$

$$=\cdots=a_{\alpha_1 s_1}{}^{\dagger}\cdots a_{\alpha_n s_n}{}^{\dagger}|0\rangle. \tag{56}$$

Note that in contradistinction to Theorem 1, complete orthogonality of different $A_{\alpha s}{}^{\dagger}$ belonging to the *same* composite species s is required for the validity of this theorem if $n>1$.

Theorem 4: Let $\{j_1\cdots j_m\}$ be any selection of constituent-species labels such that neither this set nor any of its subsets exhaust all of the constituents making up any of the composite species s, i.e., such that it is not possible to construct any of the composite species from constituents of types $j_1\cdots j_m$. Then

$$U\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle$$

$$=\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle. \tag{57}$$

Proof: By (20) and (14)

$$F\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle$$

$$=\sum_{\alpha s}a_{\alpha s}{}^{\dagger}A_{\alpha s}\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle. \tag{58}$$

Under the given hypothesis, it is not possible to form a Wick's-theorem contraction between *all* of the ψ operators in *any* of the $A_{\alpha s}$ and the given $\psi^{\dagger}$ operators. Hence some of the ψ operators in every $A_{\alpha s}$ will always commute and/or anticommute through all of the $\psi^{\dagger}$ factors so as to annihilate the vacuum. It follows that

$$F\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle=0. \tag{59}$$

The desired result then follows immediately upon expansion of the exponential in (20).

Theorem 5: Assume the validity of the hypotheses of Theorem 3 and suppose in addition that $\{x_1{}^{(j_1)}\cdots x_m{}^{(j_m)}\}$ is some set of constituent-particle arguments which are all nonoverlapping with all of the $\varphi_{\alpha s}$ occurring in the Tani transformation (20). Then

$$UA_{\alpha_1 s_1}{}^{\dagger}\cdots A_{\alpha_n s_n}{}^{\dagger}\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle$$

$$=a_{\alpha_1 s_1}{}^{\dagger}\cdots a_{\alpha_n s_n}{}^{\dagger}\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle. \tag{60}$$

Proof: By the proofs of (55) and (50) one has

$$UA_{\alpha_1 s_1}{}^{\dagger}\cdots A_{\alpha_n s_n}{}^{\dagger}\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle$$

$$=(a_{\alpha_1 s_1}{}^{\dagger}+D_{\alpha_1 s_1})\cdots(a_{\alpha_n s_n}{}^{\dagger}+D_{\alpha_n s_n})$$

$$\times\psi^{\dagger}(x_1{}^{(j_1)})\cdots\psi^{\dagger}(x_m{}^{(j_m)})|0\rangle. \tag{61}$$

Under the hypotheses of the theorem the $D_{\alpha s}$ will commute or anticommute with all of the $\psi^{\dagger}(x^{(j)})$ in (61) and will annihilate the vacuum.[15] The desired result then follows immediately.

Let us now discuss the physical interpretations and implications of these theorems. "Asymptotic scattering states" are states in which all of the particles present are well-separated in the sense that they are described by nonoverlapping wavepackets. Consider such a state of the type $A^{\dagger}\cdots A^{\dagger}\psi^{\dagger}\cdots\psi^{\dagger}|0\rangle$ occurring on the left side of Eq. (60), and suppose that all of thse particles, both composite (described by $A^{\dagger}$ operators) and elementary (described by $\psi^{\dagger}$ operators) are mutually nonoverlapping in the sense of Definitions 3 and 4. Then with Lemma 2 one sees that the hypotheses of Theorem 5 will be satisfied, so that the Tani transformation will redescribe the state in the form $a^{\dagger}\cdots a^{\dagger}\psi^{\dagger}\cdots\psi^{\dagger}|0\rangle$. This verifies that the transformation (20) has the desired effect of redescribing composite bound states in terms of the elementary-particle operators $a_{\alpha s}{}^{\dagger}$. In fact, the hypotheses of the theorem are somewhat weaker; Definition 5 and Lemma 3 show that Theorem 5 is valid in some other cases as well. Of course, in applications to the theory of chemical and nuclear reactions the interacting composite and constituent particles *will* overlap (and more generally will be nonorthogonal) during collisions; indeed, such collisions are essential for the reactions. Nevertheless, the limiting cases described by Theorem 5 and the preceding theorems are essential for the physical interpretation of the various terms in the transformed Hamiltonian $U^{-1}HU$ in terms of scattering and reaction processes with various incoming and outgoing particles (asymptotic states) in one–one correspondence with the corresponding a, $a^{\dagger}$, ψ, and $\psi^{\dagger}$ operators in the corresponding terms of $U^{-1}HU$. The explicit evaluation of such terms, by methods used previously[2-5] in some special cases, will be deferred to subsequent publications.

Theorems 2 and 4 bear on the interpretation of the ψ and $\psi^{\dagger}$ operators in the transformed Hamitonian. They show, together with the other theorems, that in $U^{-1}HU$, ψ and $\psi^{\dagger}$ describe *unbound* constituents, whereas in H they describe *both* unbound constituents *and* all of the constituents bound in composites. Again, the sharp distinction between bound and unbound constituents and between composites of various species breaks down in the transient overlapping configurations formed during reaction processes, for which the hypotheses of the theorems fail. Nevertheless, the theorems set the framework of the physical interpretation through their connection with the asymptotic states.

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[10]Any state $|\varphi\rangle \in \mathscr{P}$ can be represented in the form $|\varphi\rangle = G|0\rangle$ where G is a functional of the constituent-particle field creation operators $\psi^\dagger(x^{(j)})$ for all the constituent species j, and $|0\rangle$ is the vacuum state of $\mathscr{P}$. The corresponding state in $\mathscr{I}_0$ has the form $|\varphi\rangle = G|0\rangle$, where G is exactly the same functional as before but $|0\rangle$ is now the vacuum state of $\mathscr{I}$.
[11]In fact, if $s \neq s'$, then it is necessarily true that composite species s and s' contain different numbers of one or more constituent species; otherwise the two composite species would be the same, by definition.
[12]See Eqs. (16)–(18) of Ref. 2.
[13]For example, if $s' = \mathrm{H}$ (atomic hydrogen) and $s = \mathrm{H}_2$ (molecular hydrogen), then $C_{\beta s', \alpha s}$ will contain a term proportional to the electron field creation operator $\psi^\dagger$ (with no factor ψ on the right) and hence will not annihilate the vacuum.
[14]See Ref. 2, Eqs. (20)–(26) and Appendix A.
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Polynomial basis for Yang–Mills invariants

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It is shown that any polynomial invariant of the SU(2) Yang–Mills field is a polynomial in a basic set of ten invariants, although only nine of them are functionally independent. Polynomial bases for the self-dual and anti-self-dual Yang–Mills fields are also presented.

INTRODUCTION

The physically significant quantities associated with any gauge field must be both Lorentz invariant and gauge invariant. We shall refer to such quantities as invariants. For electromagnetic theory the invariants which depend only on the field strengths at a point (rather than on their derivatives as well) are functions of two independent invariants

$$I_1 = F_{\mu\nu}F^{\mu\nu},$$

$$I_2 = F_{\mu\nu}{}^*F^{\mu\nu},$$

where

$${}^*F_{\mu\nu} = \tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}.$$

Moreover it can be shown that[1] any invariant which is a polynomial in the components $F_{\mu\nu}$ is also a polynomial of I_1 and I_2.

For non-Abelian gauge fields the situation is more complicated. The tensor $F^i_{\mu\nu}$ (i is the internal symmetry index) is not gauge invariant, but transforms according to the adjoint representation of the gauge group. Moreover, not all the gauge-invariant information is contained in $F^i_{\mu\nu}$, since there are[2] gauge-inequivalent fields A^i_μ which give rise to the same $F^i_{\mu\nu}$. Nevertheless, as a first step toward understanding the invariants of a non-Abelian gauge theory, one of us[3] studied the invariants which could be formed from the field strengths $F^i_{\mu\nu}$ of an SU(2) gauge theory. It was shown that there are nine independent invariants, and nine independent polynomials of lowest degree were exhibited. It was then claimed, in analogy with the electromagnetic case, that these nine polynomial invariants formed a polynomial basis, that is, that any invariant polynomial in the $F^i_{\mu\nu}$ could be written as a polynomial of these nine invariants. This claim is not correct.

In this paper, we shall show that although there are nine functionally independent invariants, a polynomial basis must consist of ten elements. We exhibit a choice for these 10 basis elements, and present a reduction algorithm for reducing any polynomial invariant to a polynomial in these ten invariants. We shall also show that for self-dual or anti-self-dual fields, the polynomial basis consists of three independent polynomial invariants.

There is also an elegant group-theoretic approach to this problem which we learned from Professor Louis Michel. We have a basis $(F^i_{\mu\nu})$ for a particular representation of a group ($L\times$SU(2), where L is the Lorentz group). The problem is to determine the number of independent polynomial invariants (and their degree) which can be formed from this basis. We also wish to ascertain whether these independent invariants of lowest degree form a polynomial basis, and if not, what must be added to form the desired polynomial basis. The general theory and its application to our special case is presented in the Appendix.

1. A SIMPLE EXAMPLE

Before plunging into the details of the Yang–Mills case, we illustrate by a simple example how a polynomial basis can have more elements than the number of functionally independent invariants. Suppose we are given three vectors $\mathbf{w}$, $\mathbf{y}$, and $\mathbf{z}$, and we want to construct the lowest degree independent rotationally invariant quantities which can be formed from the components of $\mathbf{w}$, $\mathbf{y}$, and $\mathbf{z}$. The result is the six scalar products

$$w^2,\quad y^2,\quad z^2,\quad \mathbf{w}\cdot\mathbf{y},\quad \mathbf{w}\cdot\mathbf{z},\quad \mathbf{y}\cdot\mathbf{z}. \tag{1}$$

But these do not form a polynomial basis since $\mathbf{w}\cdot\mathbf{y}\times\mathbf{z}$ is a polynomial invariant, but is obviously not a polynomial in the above invariants. Functionally $\mathbf{w}\cdot\mathbf{y}\times\mathbf{z}$ is not independent, since

$$\begin{aligned}(\mathbf{w}\cdot\mathbf{y}\times\mathbf{z})^2 &= w^2y^2z^2 - w^2(\mathbf{y}\cdot\mathbf{z})^2 - y^2(\mathbf{w}\cdot\mathbf{z})^2 - z^2(\mathbf{w}\cdot\mathbf{y})^2 \\ &\quad + 2\,\mathbf{w}\cdot\mathbf{y}\,\mathbf{w}\cdot\mathbf{z}\,\mathbf{y}\cdot\mathbf{z}.\end{aligned} \tag{2}$$

A general polynomial invariant can be written as

$$P_1 + \mathbf{w}\cdot\mathbf{y}\times\mathbf{z}\,P_2, \tag{3}$$

where P_1 is a polynomial in the six invariants of (1).

2. SU(2) YANG-MILLS THEORY

To review terminology, let $F^i_{\mu\nu}$ be the Yang–Mills field at a point [$i=1,2,3$ being the SU(2) or O(3) index and $\mu,\nu=0,1,2,3$ are the Lorentz indices]. An invariant of $F^i_{\mu\nu}$ will mean from now on an algebraic function of $F^i_{\mu\nu}$ which is unchanged by Lorentz or gauge transformations, for all values of $F^i_{\mu\nu}$. A polynomial invariant of $F^i_{\mu\nu}$ is an invariant which is a polynomial in $F^i_{\mu\nu}$. To study the invariants of $F^i_{\mu\nu}$, it is convenient to define[3]

$$J_{ij} = \tfrac{1}{2}F^i_{\mu\nu}F^{j\nu\mu},\quad K_{ij} = \tfrac{1}{2}F^i_{\mu\nu}F^{j\nu\mu*},$$

$$I = \tfrac{1}{6}\epsilon_{ijk}F^i_\mu F^j_\nu F^{k\mu}_\rho,\quad I' = -\tfrac{1}{6}\epsilon_{ijk}F^{i\nu}_\mu{}^* F^{j\rho}_\nu{}^* F^{k\mu}_\rho{}^*, \tag{4}$$

where $F^{*\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\rho\sigma}F_{\rho\sigma}$ ($\epsilon^{0123}=1$). The Lorentz invariant, symmetric 3×3 matrices J and K, transform under

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gauge transformations as

$$J \to OJO^T, \quad K \to OKO^T, \tag{5}$$

where O is a 3×3 orthogonal matrix representing the gauge transformation. A set of nine independent invariants which are polynomials in $F^i_{\mu\nu}$, of the lowest degree are[3]

$$\begin{aligned}&\mathrm{Tr}(J),\ \mathrm{Tr}(K),\ t,\ t',\ \mathrm{Tr}(J^2),\ \mathrm{Tr}(JK),\ \mathrm{Tr}(K^2),\\ &\mathrm{Tr}(J^3),\ \mathrm{Tr}(K^3).\end{aligned} \tag{6}$$

We define a polynomial basis to be a minimal set of polynomial invariants such that an arbitrary polynomial invariant can be written as a polynomial in these invariants. A polynomial basis for the SU(2) gauge field is (6) together with $\mathrm{Tr}(JKJK)$. This follows from

Theorem 1: Any polynomial invariant of the SU(2) Yang–Mills field can be written as

$$P_1 + P_2\mathrm{Tr}(JKJK) + P_3(\mathrm{Tr}(JKJK))^2, \tag{7}$$

where P_i are polynomials in the nine invariants (6).

The proof is a constructive one which proceeds in several steps. First we show for all gauge groups how to reduce every Lorentz-invariant polynomial in the $F^i_{\mu\nu}$ to a polynomial in a finite set of Lorentz scalars [see below, Eq. (17)]. Using properties of the gauge group SU(2), we show that every gauge-invariant polynomial of the Lorentz scalars is a polynomial in t, t', and the elements K_{ij} and J_{ij} defined in (4). Finally we show how all gauge invariant polynomials in K_{ij} and J_{ij} can be written as in (7).

Step 1: *Every Lorentz-invariant polynomial in* $F^i_{\mu\nu}$ *is a polynomial in a finite set of Lorentz scalars.* The proof is more easily presented in the spinor formalism.[4] Define the matrices $\sigma^\mu_{AA'}$, by

$$\begin{aligned}&\sigma^0_{AA'} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \quad \sigma^1_{AA'} = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad \sigma^2_{AA'} = \begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\\ &\sigma^3_{AA'} = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},\end{aligned} \tag{8}$$

and let

$$\psi^i_{AB\,A'B'} = \sigma^\mu_{AA'}\sigma^\nu_{BB'}F^i_{\mu\nu}. \tag{9}$$

From the reality and antisymmetry of $F^i_{\mu\nu}$ it can be shown that,[4]

$$\psi^i_{AB\,A'B'} = \phi^i_{AB}\epsilon_{A'B'} + \epsilon_{AB}\bar{\phi}^i_{A'B'}, \tag{10}$$

where ϵ_{AB} is the Levi–Civita alternating symbol in two dimensions, ϕ^i_{AB} is symmetric in A, B and $\bar{\phi}^i$ is the complex conjugate of ϕ^i. The ϵ tensor is used to raise and lower indices and in this respect is analogous to the metric in tensor calculus. (10) just expresses the well-known result that $F_{\mu\nu}$ belongs to the $(1,0)+(0,1)$ representation of the analytic continuation of the Lorentz group to O(4).

Any Lorentz scalar built from the $\psi^i_{AB\,A'B'}$ must arise by contracting the unprimed and primed indices separately. Hence it must be formed from products of tensors of the form

$$R^{ij\cdots l} = \phi^{iB}_A\phi^{jC}_B\cdots\phi^{lA}_D, \quad \bar{R}^{pq\cdots s} = \bar{\phi}^{pB'}_{A'}\bar{\phi}^{qC'}_{B'}\cdots\bar{\phi}^{sA'}_{E'}. \tag{11}$$

This is obvious group theoretically—to obtain scalars from a product of tensors belonging to $(1,0)+(0,1)$ one must couple the $(1,0)$ pieces and the $(0,1)$ pieces separately to form scalars.

The power of the spinor formalism arises because the indices $A, B, \cdots$ take only two values. It follows easily that

$$\phi^{(iB}_A\phi^{j)C} = \tfrac{1}{4}L^{ij}\delta_A{}^C, \tag{12}$$

where[5]

$$L^{ij} \equiv 2\phi^{iB}_D\phi^{jD}_B = K^{ij} + iJ^{ij} \tag{13}$$

and $(\ )$ denotes symmetrization. Also

$$\phi^{[iB}_A\phi^{jC}_B\phi^{k]D}_C = \tfrac{1}{8}\delta_A{}^D T^{ijk}, \tag{14}$$

where

$$T^{ijk} = 4\phi^{[iC}_B\phi^{jE}_C\phi^{k]B}_E, \tag{15}$$

$[\ ]$ denoting complete antisymmetrization (over the gauge group indices only). Now given a tensor $R^{ijkl\cdots}$ with more than three indices, we can write it as a sum of $R^{[ijk]l\cdots}$, $R^{(ijk)l\cdots}$ and two other tensors which are symmetric in the pairs of indices i,j, and j,k, respectively. It follows then from (11), (12), and (14) that

$$\begin{aligned}R^{ijkl\cdots} = {}&\tfrac{1}{8}T^{ijk}R^{l\cdots} - \tfrac{1}{4}L^{ij}R^{kl\cdots}\\ &+ \tfrac{1}{4}L^{ik}R^{jl\cdots} - \tfrac{1}{4}L^{ik}R^{il\cdots}.\end{aligned} \tag{16}$$

It follows from a repeated application of (16) and its complex conjugate that any tensor which is a product of $R^{ij\cdots}$ and $\bar{R}^{pq\cdots}$ defined in (11), can be written as sums of products of the Lorentz scalars

$$L^{ij}, \quad \bar{L}^{pq}, \quad T^{ijk}, \quad \bar{T}^{pqr}. \tag{17}$$

Hence every polynomial invariant is a gauge invariant polynomial in the Lorentz scalars (17).

Step 2: *For the group* SU(2), *gauge invariant polynomials of the Lorentz scalars are polynomials in* t, t', J^{ij}, K^{ij}. For SU(2), the indices i,j,k take only three values so that since T^{ijk} is completely antisymmetric

$$T^{ijk} = \tau\epsilon^{ijk}, \quad \bar{T}^{ijk} = \bar{\tau}\epsilon^{ijk}, \tag{18}$$

where τ is a Lorentz-gauge defined by

$$\tau \equiv \tfrac{2}{3}\epsilon_{ijk}\phi^{iB}_A\phi^{jC}_B\phi^{kA}_C = t + it', \tag{19}$$

where t and t' are defined in (4). It follows from (13) and the statement below (17) that every polynomial invariant of the SU(2) gauge field is a polynomial in t, t', K_{ij} and J_{ij}.

Step 3: *Every gauge invariant polynomial in* K_{ij} and J_{ij} *can be written as in* (7).

We notice first that a polynomial in J and K has an even number of gauge indices in each term. Since a gauge invariant must be formed by contracting with the invariant tensors δ_{ij} and ϵ_{ijk}, it is clear that there must be an even number of ϵ tensors in such an invariant. But an even number of ϵ tensors can be expressed in terms of the Kronecker deltas using the relation

TABLE I. Inequivalent strings modulo relations (22) and (23).

Degree	Strings
1	J, K
2	J^2, K^2, JK, KJ
3	JKJ, J^2K, JK^2, KJK
4	J^2KJ, $KJKJ$, $JKJK$, J^2K^2, KJK^2
5	$JKJKJ$, J^2KJK, $KJKJK$, $JKJK^2$
6	J^2KJKJ, J^2KJK^2, $KJKJK^2$
7 or more	None

$$\epsilon_{ijk}\epsilon_{lmn}=\begin{vmatrix}\delta_{il} & \delta_{im} & \delta_{in}\\ \delta_{jl} & \delta_{jm} & \delta_{jn}\\ \delta_{kl} & \delta_{km} & \delta_{kn}\end{vmatrix}. \tag{20}$$

It follows that any invariant which is a polynomial in J and K can be written as a sum of products of invariants of the form

$$\mathrm{Tr}(J^\alpha K^\beta J^\gamma K^\delta \cdots), \tag{21}$$

where $\alpha,\beta,\cdots$ are nonnegative integers. We now show by an explicit reduction algorithm that (21) can always be written in the form (7).

The key identities for this reduction are obtained from the Cayley-Hamilton theorem. According to this theorem, the 3×3 matrix $K+\lambda J$ for any λ must satisfy its own characteristic equation. That means that $(K+\lambda J)^3$ can be written as a polynomial in K and J of lower degree, with coefficients involving traces of various powers of $(K+\lambda J)$.

These traces (apart from the factor λ) are polynomials in the invariants in (6), since[3] $\mathrm{Tr}(J^2K)$ and $\mathrm{Tr}(JK^2)$ are expressible in terms of tt', t'^2-t^2, and the remaining invariants of (6). By equating coefficients of λ, we then have

$$\begin{aligned} &K^3\sim 0,\\ &J^3\sim 0,\\ &K^2J\sim -JK^2-KJK,\\ &KJ^2\sim -J^2K-JKJ, \end{aligned} \tag{22}$$

where $A\sim B$ means that $(A-B)$ is a polynomial in J,K of lower degree than the degree of $(A-B)$, and whose coefficients are polynomials in the invariants of (6).

Two more useful identities are obtained by applying the Cayley–Hamilton theorem to JK and KJ. This yields

$$\begin{aligned} &(JK)^3\sim 0,\\ &(KJ)^3\sim 0, \end{aligned} \tag{23}$$

if we adjoin $\mathrm{Tr}(JKJK)$ to the set of allowable coefficients. Note that $\mathrm{Tr}((JK)^3)$ is not an independent variable since

$$\det((JK)^3)=(\det(J)\det(K))^3, \tag{24}$$

and $\det(J)$ or $\det(K)$ is a polynomial in the invariants of (6).

It is now straightforward to show that the complete set of matrices of the form $J^\alpha K^\beta J^\gamma K^\delta\cdots$ ($\alpha,\beta,\gamma,\delta,\cdots$ nonnegative integers), which are inequivalent under identities (22), and (23), is given in Table I. Consequently any invariant string of matrices can be written as a linear combination of the strings of Table I. The coefficients of this polynomial are polynomials in (6), and $\mathrm{Tr}(JKJK)$, which are themselves traces of elements in Table I. Thus traces of elements of Table I form a polynomial basis for invariants constructed from J and K. Those of degrees less than or equal to 3 are polynomials in (6). In degree 4, only $\mathrm{Tr}(JKJK)$ is independent of the previous ones. There are no new invariants of degrees 5 and 6. To reduce $\mathrm{Tr}(J^2KJK^2)$, we need in addition the property that J and K are symmetric. We conclude then that the only new invariant is $\mathrm{Tr}(JKJK)$ [or $\mathrm{Tr}(J^2K^2)$] so that a polynomial basis for Yang–Mills invariants are the ten invariants

$$\begin{aligned} &\mathrm{Tr}(J),\ \mathrm{Tr}(K),\ t,\ t',\ \mathrm{Tr}(J^2),\ \mathrm{Tr}(JK),\ \mathrm{Tr}(K^2),\ \mathrm{Tr}(J^3),\\ &\mathrm{Tr}(K^3),\ \mathrm{Tr}(JKJK). \end{aligned} \tag{25}$$

We note that only nine of the above ten invariants are independent,[3] so that there must be a relation between them. If we define

$$J'=J-\tfrac{1}{3}\mathrm{Tr}(J)I,\quad K'=K-\tfrac{1}{3}\mathrm{Tr}(K)I, \tag{26}$$

then the relation is

$$\mathrm{Tr}^3(J'K'J'K')+a\,\mathrm{Tr}^2(J'K'J'K')+b\,\mathrm{Tr}(J'K'J'K')+c=0 \tag{27}$$

TABLE II. Coefficients in the minimal polynomial relation (27).

```
 a =-5*JK**2/2+J2*K2

 b =-2*K2*J2K**2+2*JK**4+2*JK*J2K*K2J+J2**2*K2**2/4-2*J2*K2J**2
-3*J2*JK**2*K2/2+2*K3*J2*J2K+2*J3*K2*K2J-2*J3*K3*JK

 c =+2*J2K**2*K2J**2-JK**6/2-2*JK**3*J2K*K2J+2*JK**2*K2*J2K**2
-J2**2*JK**2*K2**2/8+J2*JK**4*K2/2+2*J2*JK**2*K2J**2-J2*JK*K2
*J2K*K2J+K3**2*J2**3/9-8*K3*J2K**3/3+K3*J2**2*K2*J2K/3-2*K3
*J2**2*JK*K2J/3-2*K3*J2*JK**2*J2K/3+J3**2*K2**3/9-2*J3**2
*K3**2/3-8*J3*K2J**3/3-2*J3*JK**2*K2*K2J/3-2*J3*JK*K2**2*J2K/3
+J3*J2*K2**2*K2J/3+4*J3*K3*J2K*K2J+10*J3*K3*JK**3/9-J3*K3
*J2*JK*K2/3

We have used the following symbols above

J2=Tr(J'**2) , K2=Tr(K'**2) , J3=Tr(J'**3) , K3=tr(K'**3)
 JK=Tr(J'K') , J2K=Tr(J'**2*K') , K2J=Tr(K'**2*J')

 where J' and K' are the traceless parts of J and K defined in (26).
```

where a, b, and c are given in Table II. Using (27), any power of Tr($JKJK$), greater than two, can be expressed in the form (7). Since we have shown above that any polynomial invariant can be expressed as a polynomial in (6) and Tr($JKJK$), this completes the proof of Step 3 and Theorem 1.

Equation (27) is also the polynomial relation between Tr($JKJK$) and the nine invariants (6), of the lowest degree in Tr($JKJK$). Hence it is not possible to express Tr($JKJK$) as a polynomial in (6). Also, since the invariants (7) are a set of independent, lowest-degree polynomials in $F^i_{\mu\nu}$, it follows that there is no polynomial basis with less than ten invariants.

Consider now the self-dual or anti-self-dual fields ($F^i_{\mu\nu} = \pm i F^{*i}_{\mu\nu}$) which have the spinor forms $\bar{\phi}^i_{A'B'}$ and ϕ^i_{AB} respectively. It follows from the above proof that any polynomial invariant formed from ϕ^i_{AB} (without complex conjugation) is a polynomial in τ and L^{ij}. But since the 3×3 matrix L satisfies its characteristic equation, it follows that any polynomial in L can be expressed as a polynomial in

$$\det L, \quad \mathrm{Tr}(L), \quad \mathrm{Tr}(L^2). \tag{28}$$

However, it can be shown that[5]

$$\det L = -\tau^2. \tag{29}$$

We therefore have the following theorem:

Theorem 2: Any polynomial invariant of the anti-self-dual SU(2) gauge field ϕ^i_{AB} is a polynomial in

$$\tau, \quad \mathrm{Tr}(L), \quad \mathrm{Tr}(L^2), \tag{30}$$

whereas a polynomial invariant of the self-dual SU(2) gauge field $\bar{\phi}^i_{A'B'}$ is a polynomial in

$$\bar{\tau}, \quad \mathrm{Tr}(\bar{L}), \quad \mathrm{Tr}(\bar{L}^2). \tag{31}$$

Unlike in the case of the real Yang–Mills field, the polynomial basis for self-dual and anti-self-dual fields consists of independent invariants.

So far our discussion has been confined to gauge fields defined on Minkowski space–time. It is of course possible to define $F^i_{\mu\nu}$ on a four-dimensional Euclidean space–time E_4. Using the isomorphism between O(4) and SU(2)×SU(2), the spinor form (6) can again be obtained for $F^i_{\mu\nu}$; but in this case ϕ^i_{AB} and $\bar{\phi}^i_{A'B'}$ are real and independent (not complex conjugates of each other) and transform under each of the two SU(2) groups mentioned above. Also (9) must be replaced by $L = K + J$ and (15) by $\tau = l + l'$. It is clear that Theorem 1 and 2 are then valid for an SU(2) gauge field on E_4 as well.

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APPENDIX

In this appendix we sketch the general theory[6] of the polynomial invariants formed from the basis elements of a given representation (not necessarily irreducible) of a compact group G. In particular we show how many independent elements there are and their degree in the original basis. (If the group is semisimple but not compact, its representations are analytic continuations of some compact group. We apply our results to this group and then analytically continue back to the semisimple group.) For concreteness one can focus on the $F^i_{\mu\nu}$ forming a basis for an 18-dimensional representation of O(4)×O(3), or the symmetric matrices J and K of the text forming a 12-dimensional basis of O(3).

Let E denote the basis elements of a representation D of G. G acts in the obvious way on polynomials in E. Homogeneous polynomials of degree n form the basis for a representation $D^{(n)}$ of G, namely the totally symmetric part of

$$\underbrace{D\times D\times\cdots\times D}_{n \text{ times}}.$$

The number of *linearly* independent polynomial invariants of degree n is the number of times the reduction of $D^{(n)}$ contains the identity representation. If we denote this quantity by c_n, the orthogonality of the characters implies that

$$c_n = \int d\mu(g)\,\mathrm{Tr}(D^{(n)}(g)), \tag{A1}$$

where $d\mu(g)$ is the invariant measure on the group normalized to

$$\int d\mu(g) = 1. \tag{A2}$$

It is straightforward combinatorics[7] to show that the generating function

$$f(t) \equiv \sum_{n=0}^{\infty} c_n t^n \tag{A3}$$

can be written as

$$f(t) = \int \frac{d\mu(g)}{\det[1 - tD(g)]}. \tag{A4}$$

If D is reducible, let

$$D = D_1 \oplus D_2 \oplus \cdots \oplus D_m, \tag{A5}$$

where D_i is irreducible. Then define

$$F(t_1, t_2, \ldots, t_m) \equiv \sum_{n_i=0}^{\infty} c_{n_1 n_2 \cdots n_m} t_1^{n_1} t_2^{n_2} \cdots t_m^{n_m} = \int \frac{d\mu(g)}{\prod_{i=1}^m \det[1 - t_i D_i(g)]}. \tag{A6}$$

Then $c_{n_1\cdots n_m}$ represents the number of linearly independent polynomials of degree n_1 in the basis elements belonging to D_1, n_2 in the basis elements belong to D_2, etc.

The Yang–Mills fields $F^i_{\mu\nu}$ form the basis for an 18-dimensional representation of O(4)×O(3), i.e., of O(3)×O(3)×O(3). The representation is reducible, transforming according to $(1,0,1) + (0,1,1)$ where each index labels the angular momentum J of the corresponding O(3) group. $(1,0,1)$ and $(0,1,1)$ are respectively the self-dual and anti-self-dual parts of $F^i_{\mu\nu}$. It is then straightforward but tedious to evaluate (A6) for this case

$$F(t_1,t_2)=\int \frac{d\mu(g_1)\,d\mu(g_2)\,d\mu(g_3)}{\det(1-t_1D^{(1)}(g_1)\times D^{(1)}(g_3))\det(1-t_2D^{(1)}(g_2)\times D^{(1)}(g_3))} \tag{A7}$$

where $d\mu$ now denotes the invariant measure for O(3) while $D^{(1)}$ denotes the $J=1$ representation. The integrals over g_1 and g_2 can be done independently to give

$$F(t_1,t_2)=\frac{(1-t_1+t_1^2)}{(1-t_1)}\,\frac{(1-t_2+t_2^2)}{(1-t_2)}\int \frac{d\mu(g_3)}{\det(1-t_1^2D^{(1)}(g_3))\det(1-t_2^2D^{(1)}(g_3))} \tag{A8}$$

$$=\frac{g(t_1,t_2)}{(1-t_1^2)(1-t_2^2)(1-t_1^3)(1-t_2^3)(1-t_1^4)(1-t_2^4)(1-t_1^2t_2^2)(1-t_1^4t_2^2)(1-t_1^2t_2^4)}$$

where

$$g(t_1,t_2)=1+t_1^4t_2^4+t_1^8t_2^8. \tag{A9}$$

If one expands each of the denominators in (A8), the coefficient of $t_1^m t_2^n$ denotes how many linearly independent invariants can be formed of degree m in the self-dual parts of $F^1_{\mu\nu}$ and of degree n in the anti-self-dual parts. Ignoring the factor $g(t_1,t_2)$, we see that invariants can be formed by combining arbitrary powers of two quadratic invariants, two cubic invariants, three quartic invariants, and two invariants of degree 6. (Here we have not distinguished between self-dual and anti-self-dual parts.) This agrees with the fundamental invariants listed in (6) of the text. However, the presence of $g(t_1,t_2)$ indicates that these do not suffice. There is clearly one more linearly independent polynomial invariant of degree 8 and another of degree 16. These corresponds to $\mathrm{Tr}(JKJK)$ and $\mathrm{Tr}^2(JKJK)$. The absence of a term like $t_1^{12}t_2^{12}$ in $g(t_1,t_2)$ means that $\mathrm{Tr}^3(JKJK)$ is not an independent invariant.

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A new approach to the inverse problem

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The full-range orthogonality theorem concerning the elementary solutions of the equation of transfer is used to develop a solution of the inverse problem for a finite plane-parallel slab.

I. INTRODUCTION

The solution of the inverse problem given recently[1] for a finite slab is an improvement over previous infinite-medium results[2-4]; however, because the reported solution[1] depends on spatial moments of the total flux, more improvement is sought. From an experimental point of view a solution in terms only of surface quantities is what is most desired. Here we wish to report a method by which the desired solution can be established.

II. ISOTROPIC SCATTERING

To study first the simplest inverse problem for radiative transfer or neutron diffusion in a finite slab we consider the equation of transfer

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\psi(x,\mu)=\frac{\omega}{2}\int_{-1}^{1}\psi(x,\mu')\,d\mu', \quad x\in[-a,a], \tag{1}$$

where $\psi(x,\mu)$ is the angular flux, x is the position variable measured in mean-free paths, and ω is the single scattering albedo. Here for a transport problem defined by the boundary conditions

$$\psi(-a,\mu)=f_1(\mu), \quad \mu>0, \tag{2a}$$

and

$$\psi(a,-\mu)=f_2(\mu), \quad \mu>0, \tag{2b}$$

we wish to find ω in terms of $f_1(\mu), f_2(\mu)$ and the exit distributions $\psi(-a,-\mu)$ and $\psi(a,\mu)$, $\mu>0$. This problem was solved recently[5] for $f_1(\mu)=\mu^\beta, \beta=0,1,2,\cdots$, and $f_2(\mu)=0$; however, here we intend to develop a solution to the general problem and to establish a procedure that can readily be generalized to the case of anisotropic scattering.

We begin by expressing $\psi(x,\mu)$ in terms of Case's elementary solutions,[6] i.e.,

$$\psi(x,\mu)=A(\nu_0)\phi(\nu_0,\mu)e^{-x/\nu_0}+A(-\nu_0)\phi(-\nu_0,\mu)e^{x/\nu_0}+\int_{-1}^{1}A(\nu)\phi(\nu,\mu)e^{-x/\nu}\,d\nu, \tag{3}$$

where

$$\phi(\nu_0,\mu)=\frac{\omega}{2}\nu_0\frac{1}{\nu_0-\mu}, \tag{4a}$$

$$\phi(\nu,\mu)=\frac{\omega\nu}{2}Pv\left(\frac{1}{\nu-\mu}\right)+\lambda(\nu)\delta(\nu-\mu), \tag{4b}$$

$$\lambda(\nu)=1-\omega\nu\tanh^{-1}(\nu), \tag{5}$$

and $\pm\nu_0$ are the zeros of

$$\Lambda(z)=1+\frac{\omega}{2}z\int_{-1}^{1}\frac{d\mu}{\mu-z}. \tag{6}$$

In Eq. (3), $A(\nu_0), A(-\nu_0)$, and $A(\nu)$ are expansion coefficients to be determined by the boundary conditions. We shall not need them here. We can now use the full-range orthogonality theorem[6]

$$\int_{-1}^{1}\phi(\xi,\mu)\phi(\xi',\mu)\mu\,d\mu=0, \quad \xi\neq\xi', \tag{7}$$

to deduce from Eq. (3) that

$$\int_{-1}^{1}\phi(-\xi,\mu)\psi(\pm a,\mu)\mu\,d\mu=A(-\xi)N(-\xi)e^{\pm a/\xi}, \quad \xi\in P, \tag{8}$$

and

$$\int_{-1}^{1}\phi(\xi,\mu)\psi(\pm a,\mu)\mu\,d\mu=A(\xi)N(\xi)e^{\mp a/\xi}, \quad \xi\in P, \tag{9}$$

where $N(\pm\xi)$ are normalization constants and $\xi\in P \Rightarrow \xi=\nu_0$ or $\xi=\nu\in(0,1)$. We can now eliminate $A(\pm\xi)N(\pm\xi)$ in Eqs. (8) and (9) to find the equations used recently by Siewert and Benoist[7] to develop the F_N method of solving problems in neutron diffusion, i.e.,

$$\int_{-1}^{1}\phi(\xi,\mu)\psi(-a,-\mu)\mu\,d\mu-e^{-2a/\xi}\times\int_{-1}^{1}\phi(\xi,\mu)\psi(a,-\mu)\mu\,d\mu=0, \quad \xi\in P, \tag{10a}$$

and

$$\int_{-1}^{1}\phi(\xi,\mu)\psi(a,\mu)\mu\,d\mu-e^{-2a/\xi}\times\int_{-1}^{1}\phi(\xi,\mu)\psi(-a,\mu)\mu\,d\mu=0, \quad \xi\in P. \tag{10b}$$

Equations (10) define a system of singular integral equations and constraints that can be used to deduce the exit distributions when ω is given; however, we can use Eqs. (10) here to find ω when we assume we can determine experimentally the exit distributions. Thus if we use Eq. (4b) in Eqs. (10) for $\xi=\nu\in(0,1)$ we can solve immediately for ω; from Eq. (10a) and Eq. (10b), respectively, we obtain

$$\omega=\frac{2}{k_1(\nu)}[\psi(-a,-\nu)-\psi(a,-\nu)e^{-2a/\nu}], \quad \nu\in(0,1), \tag{11a}$$

and

$$\omega=\frac{2}{k_2(\nu)}[\psi(a,\nu)-\psi(-a,\nu)e^{-2a/\nu}], \quad \nu\in(0,1), \tag{11b}$$

where

$$k_1(\nu)=\int_{-1}^{1}T(\mu,\nu)[\psi(-a,-\mu)-\psi(a,-\mu)e^{-2a/\nu}]\mu\,d\mu \tag{12a}$$

and

$$k_2(\nu)=\int_{-1}^{1}T(\mu,\nu)[\psi(a,\mu)-\psi(-a,\mu)e^{-2a/\nu}]\mu\,d\mu \tag{12b}$$

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with

$$T(\mu,\nu)=P\nu\left(\frac{1}{\mu-\nu}\right)+2\tanh^{-1}(\nu)\delta(\mu-\nu), \tag{13}$$

Clearly any value of $\nu\in(0,1)$ can be used in Eqs. (11) to give an explicit result for ω in terms of the exit distributions. The limit as $\nu\to 0$ is particularly interesting; we find

$$\omega=2\psi(-a,0^+)\left[\int_0^1\psi(-a,-\mu)\,d\mu+\int_0^1 f_1(\mu)\,d\mu\right]^{-1} \tag{14a}$$

and

$$\omega=2\psi(a,0^+)\left[\int_0^1\psi(a,\mu)\,d\mu+\int_0^1 f_2(\mu)\,d\mu\right]^{-1}. \tag{14b}$$

It is curious that Eqs. (14a) and (14b) involve, respectively, only the angular distribution at $x=-a$ and $x=a$. It is also obvious that other expressions for ω can be obtained from Eqs. (10) for $\xi=\nu\in(0,1)$; e.g., we can multiply Eqs. (10) for $\xi=\nu\in(0,1)$ by "arbitrary" functions, say $G_1(\nu)$ and $G_2(\nu)$, and integrate over ν to obtain

$$\omega=\frac{2\int_0^1 G_1(\nu)[\psi(-a,-\nu)-\psi(a,-\nu)e^{-2a/\nu}]\,d\nu}{\int_0^1 G_1(\nu)k_1(\nu)\,d\nu} \tag{15a}$$

and

$$\omega=\frac{2\int_0^1 G_2(\nu)[\psi(a,\nu)-\psi(-a,\nu)e^{-2a/\nu}]\,d\nu}{\int_0^1 G_2(\nu)k_2(\nu)\,d\nu}. \tag{15b}$$

III. ANISOTROPIC SCATTERING

Let us now consider the extension of the method discussed in Sec. II to the general case of anisotropic scattering. We start with

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\psi(x,\mu)=\frac{\omega}{2}\sum_{l=0}^{N}(2l+1)f_l P_l(\mu)\int_{-1}^{1}P_l(\mu')\psi(x,\mu')\,d\mu', \tag{16}$$

$$\psi(-a,\mu)=f_1(\mu),\quad \mu>0, \tag{17a}$$

and

$$\psi(a,-\mu)=f_2(\mu),\quad \mu>0. \tag{17b}$$

Here $f_0=1$ and we seek to express $\omega,f_1,f_2,\ldots,f_N$ in terms of the surface quantities $\psi(\pm a,\mu)$. Following the notation of McCormick and Kuščer,[8] we can write

$$\psi(x,\mu)=\sum_{\alpha=0}^{\kappa=1}[A(\nu_\alpha)\phi(\nu_\alpha,\mu)e^{-x/\nu_\alpha}+A(-\nu_\alpha)\phi(-\nu_\alpha,\mu)e^{x/\nu_\alpha}]+\int_{-1}^{1}A(\nu)\phi(\nu,\mu)e^{-x/\nu}\,d\nu, \tag{18}$$

where now we have $\kappa\pm$ pairs of zeros $(\pm\nu_\alpha)$ of

$$\Lambda(z)=1+\frac{\omega}{2}z\int_{-1}^{1}g(\mu,\mu)\,\frac{d\mu}{\mu-z}. \tag{19}$$

We note[8] that

$$\phi(\nu_\alpha,\mu)=\frac{\omega}{2}\nu_\alpha g(\nu_\alpha,\mu)\left(\frac{1}{\nu_\alpha-\mu}\right), \tag{20a}$$

$$\phi(\nu,\mu)=\frac{\omega}{2}\nu g(\nu,\mu)P\nu\left(\frac{1}{\nu-\mu}\right)+\lambda(\nu)\delta(\nu-\mu), \tag{20b}$$

and

$$\lambda(\nu)=1+\frac{\omega}{2}\nu P\int_{-1}^{1}g(\mu,\mu)\,\frac{d\mu}{\mu-\nu}, \tag{21}$$

where

$$g(\nu,\mu)=\sum_{l=0}^{N}(2l+1)f_l g_l(\nu)P_l(\mu). \tag{22}$$

In addition, $P_l(\mu)$ is used to denote Legendre's polynomial and the polynomials $g_l(\mu)$, of order l, are those introduced by Chandrasekhar.[9] Our task of determining ω and the coefficients f_l would be extremely simple were it not for the fact that the $g_l(\nu)$ depend on

$$h_l=(2l+1)(1-\omega f_l); \tag{23}$$

e.g.,

$$g_0(\nu)=1,\quad g_1(\nu)=h_0\nu,\quad g_2(\nu)=\tfrac{1}{2}(h_0h_1\nu^2-1), \tag{24}$$

and, in general,

$$(l+1)g_{l+1}(\nu)=\nu h_l g_l(\nu)-l g_{l-1}(\nu). \tag{25}$$

The full-range orthogonality relation concerning the elementary solutions is of the same form[8] as for the isotropic scattering case, i.e.,

$$\int_{-1}^{1}\phi(\xi,\mu)\phi(\xi',\mu)\mu\,d\mu=0,\quad \xi\neq\xi', \tag{26}$$

and thus we can readily generalize Eqs. (10) to obtain

$$\int_{-1}^{1}\phi(\xi,\mu)\psi(-a,-\mu)\mu\,d\mu-e^{-2a/\xi}\int_{-1}^{1}\phi(\xi,\mu)\psi(a,-\mu)\mu\,d\mu=0,\quad \xi\in P, \tag{27a}$$

and

$$\int_{-1}^{1}\phi(\xi,\mu)\psi(a,\mu)\mu\,d\mu-e^{2a/\xi}\int_{-1}^{1}\phi(\xi,\mu)\psi(-a,\mu)\mu\,d\mu=0,\quad \xi\in P, \tag{27b}$$

for the general case. Here $\xi\in P\Rightarrow\xi\in\{\nu_\alpha\}\cup(0,1)$. If we now enter Eq. (20b) into Eqs. (27) we obtain

$$\int_{-1}^{1}\mathcal{A}(\mu,\nu)[\psi(-a,-\mu)-\psi(a,-\mu)e^{-2a/\nu}]\mu\,d\mu=2[\psi(-a,-\nu)-\psi(a,-\nu)e^{-2a/\nu}] \tag{28a}$$

and

$$\int_{-1}^{1}\mathcal{A}(\mu,\nu)[\psi(a,\mu)-\psi(-a,\mu)e^{-2a/\nu}]\mu\,d\mu=2[\psi(a,\nu)-\psi(-a,\nu)e^{-2a/\nu}] \tag{28b}$$

where

$$\mathcal{A}(\mu,\nu)=\sum_{l=0}^{N}(2l+1-h_l)g_l(\nu)\times\left[P_l(\mu)P\nu\left(\frac{1}{\mu-\nu}\right)+2\delta(\mu-\nu)Q_l(\nu)\right] \tag{29}$$

with

$$Q_l(\nu)=\tfrac{1}{2}P\int_{-1}^{1}P_l(x)\,\frac{dx}{\nu-x}. \tag{30}$$

It is clear that $N+1$ values of $\nu\in(0,1)$ can be chosen to generate, from either Eq. (28a) or Eq. (28b), $N+1$ algebraic equations involving the $N+1$ unknowns; however, the equations are nonlinear! If we let

$$M_1(\mu,\nu)=\psi(-a,-\mu)-\psi(a,-\mu)e^{-2a/\nu} \tag{31a}$$

and

$$M_2(\mu,\nu)=\psi(a,\mu)-\psi(-a,\mu)e^{-2a/\nu}, \tag{31b}$$

then we can write Eqs. (28) as

$$\sum_{l=0}^{N}(2l+1-h_l)g_l(\nu)R_l^{(1)}(\nu)=2M_1(\nu,\nu),\quad \nu\in(0,1), \tag{32a}$$

and

$$\sum_{l=0}^{N}(2l+1-h_l)g_l(\nu)R_l^{(2)}(\nu)=2M_2(\nu,\nu),\quad \nu\in(0,1), \tag{32b}$$

where the known functions are

$$R_l^{(\alpha)}(\nu)=\int_0^1\left[P_l(\mu)Pv\left(\frac{1}{\mu-\nu}\right)+2Q_l(\nu)\delta(\mu-\nu)\right]M_\alpha(\mu,\nu)\mu\,d\mu + (-1)^l\int_0^1 P_l(\mu)M_\alpha(-\mu,\nu)\mu\,\frac{d\mu}{\mu+\nu}. \tag{33}$$

We can consider Eqs. (32) evaluated at selected values of $\nu\in(0,1)$, say $\{\nu_\beta\}$, or multiply the equations by a sequence of convenient functions, say $\{G_\beta(\nu)\}$, and integrate over ν to generate equations to be solved for the h_l. It is rather easy to see that it is sufficient to solve $2N$, for $N>0$, linear algebraic equations to establish the desired h_l. Although the inversion of a $2N\times 2N$ matrix is required here, it is clear that the inverse problem can be solved in this manner. One serious limitation to this solution is the fact that N must be specified before finding the various h_l. The solution given in Ref. 1 did not suffer from this fact, but it did require the flux at all x. Clearly what is desired here is an orthogonality relation that could be used with Eqs. (32) to extract the coefficients h_l. To date, such a relation has not been found.

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SU_2 monopole harmonics

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For a particle of I-spin I in an SU_2 monopole field in five-dimensional Euclidean space, the monopole harmonics are found. They belong to the irreducible representation $(p,q)_5$ where $p = q+2I$. They form a complete set of wave sections.

1. INTRODUCTION

It was pointed out two years ago that the "wavefunction" of a charged particle around a Dirac magnetic monopole should be a wave section.[1] The angular part of wave sections were called monopole harmonics. They have been extremely useful for studying electron–monopole interactions.[2] Now Dirac's monopole has been generalized[3] to an SU_2 monopole. In this paper we develop the corresponding SU_2 monopole harmonics. We shall concentrate on the SU_2 monopole field β of Ref. 3. (The result for the other SU_2 monopole field, field α, is easily obtained from the results of this paper.)

To be more specific we study the angular part of the wave sections of a particle of SU_2 spin I in field β in five-dimensional space. The angular momentum operators $L_{\mu\nu}$ ($\mu, \nu = 1, 2, 3, 4, 5$) have been given explicitly in Ref. 3,

$$L_{\mu\nu} = -L_{\nu\mu} = x_\mu(\partial_\nu + Y_k b_\nu^k) - x_\nu(\partial_\mu + Y_k b_\mu^k) - r^2 f_{\mu\nu}^k Y_k . \tag{1.1}$$

They satisfy the commutation rule

$$[L_{\mu\nu}, L_{\alpha\beta}] = \delta_{\nu\alpha}L_{\mu\beta} - \delta_{\mu\alpha}L_{\nu\beta} - \delta_{\nu\beta}L_{\mu\alpha} + \delta_{\mu\beta}L_{\nu\alpha}, \tag{1.2}$$

which are the commutation rules for the infinitesimal operators of the group SO_5.

There are ten generators $L_{\mu\nu}$. Of these, six are those of the subgroup SO_4. We follow the standard method of decomposing them into two SU_2 algebras:

$$J_1 = \frac{-i}{2}(L_{23} + L_{14}), \quad J_2 = \frac{-i}{2}(L_{31} + L_{24}),$$

$$J_3 = \frac{-i}{2}(L_{12} + L_{34}),$$

$$K_1 = \frac{-i}{2}(L_{23} - L_{14}), \quad K_2 = \frac{-i}{2}(L_{31} - L_{24}),$$

$$K_3 = \frac{-i}{2}(L_{12} - L_{34}). \tag{1.3}$$

They form two sets of commuting angular momenta $\mathbf{J}$ and $\mathbf{K}$:

$$[J_i, K_j] = 0, \quad [J_1, J_2] = iJ_3, \quad [K_1, K_2] = iK_3, \quad \text{etc.} \tag{1.4}$$

Furthermore, they are all Hermitian, since iY_k is Hermitian.

We have thus the following five operators

$$A \equiv \tfrac{1}{2}\sum_{\mu,\nu=1}^{5}(L_{\mu\nu})^2, \quad \mathbf{J}^2, \quad \mathbf{K}^2, \quad J_3, \quad K_3, \tag{1.5}$$

which are all Hermitian and mutually commute. The problem we want to solve is to find the simultaneous eigensections of these five operators, if $L_{\mu\nu}$ is given by (1.1).

2. MATRIX REPRESENTATION OF (1.2)

We find in this section all irreducible matrix representations of (1.2), ignoring (1.1), with $L_{\mu\nu}$ being represented by anti-Hermitian matrices. That is, we find all irreducible representations of the covering group of SO_5. We first diagonalize all five operators (1.5). Because of (1.4) the irreducible representation must contain blocks, each with $(2j+1)(2k+1)$ states, where j and k are defined by

$$\text{diagonal element of } \mathbf{J}^2 = j(j+1), \quad (j = 0, \tfrac{1}{2}, 1, \cdots),$$
$$\text{diagonal element of } \mathbf{K}^2 = k(k+1), \quad (k = 0, \tfrac{1}{2}, 1, \cdots). \tag{2.1}$$

Each such block will be denoted by $(j,k)_4$ and forms an irreducible representation of the subalgebra of $L_{\mu\nu}$, $\mu, \nu = 1, 2, 3, 4$.

Each irreducible representation consists of a collection of such blocks $(j,k)_4$ of states. Some examples are given in Fig. 1. We use the + signs to indicate the collection of blocks.

Theorem 1: Each irreducible representation $(p,q)_5$ is designated by two integers p, q so that $p \geq q \geq 0$. For this irreducible representation, A of (1.5) is diagonal and all diagonal elements are equal to $-\frac{1}{2}p^2 - \frac{1}{2}q^2 - q - 2p$. The states of $(p,q)_5$ are a collection of blocks $(j,k)_4$,

$$(p,q)_5 = \sum \left(\frac{r+s}{2}, \frac{r-s}{2}\right)_4, \tag{2.2}$$

where

$$r = \tfrac{1}{2}(p-q), \tfrac{1}{2}(p-q)+1, \ldots, \tfrac{1}{2}(p+q),$$
$$s = \tfrac{1}{2}(q-p), \tfrac{1}{2}(q-p)+1, \ldots, \tfrac{1}{2}(p-q).$$

[No $(j,k)_4$ occurs more than once in (2.2).] The dimension of the representation is $N \times N$ where

$$N = (1+q)(1+p-q)(1+\tfrac{1}{2}p)[1+\tfrac{1}{3}(p+q)]. \tag{2.3}$$

The proof of this theorem is somewhat tedious and will be omitted. Examples of the sum (2.2) are graphically given in Fig. 1.

We notice that the states with the highest eigenvalue of J_3 in $(p,q)_5$ are in the right-most circle in Fig. 1, i.e., in $(\frac{1}{2}p, \frac{1}{2}q)_4$. This highest eigenvalue is $\frac{1}{2}p$. For states with this eigenvalue for J_3 there is one and only

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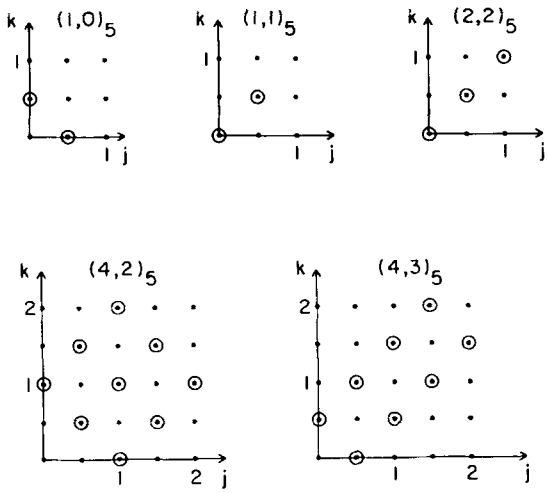

FIG. 1. Examples of the decomposition of irreducible representations $(p, q)_5$ of the covering group of SO_5 into sums of $(j, k)_4$ which are irreducible representations of the covering group of SO_4. $p \geq q \geq 0$ are integers. Each circle represents one $(j, k)_4$. The leading state belongs to the right-most circle, which is always $(\frac{1}{2}p, \frac{1}{2}q)_4$. The circles form a rectangle with the left-most corner at $(0, \frac{1}{2}p - \frac{1}{2}q)_4$.

one with the highest eigenvalue $\frac{1}{2}q$ for K_3. This state will be called the *leading state* of $(p, q)_5$.

In our notation here, p and q are related to that of Ref. 4 by

$$\lambda_1 = p - q, \lambda_2 = q. \tag{2.4}$$

3. SO_5 ORBITAL HARMONICS

The generators $L_{\mu\nu}$ consist of an "orbital" part $\overset{o}{L}_{\mu\nu}$ and an isospin part involving Y_k:

$$\overset{o}{L}_{\mu\nu} = -\overset{o}{L}_{\nu\mu} = x_\mu \partial_\nu - x_\nu \partial_\mu .$$

These orbital operators are $L_{\mu\nu}$ when $Y = 0$. We define $\overset{o}{\mathbf{J}}$ and $\overset{o}{\mathbf{K}}$ in the same way as (1.3). By straightforward evaluation we find

$$\overset{o}{\mathbf{J}}^2 = \overset{o}{\mathbf{K}}^2 \tag{3.1}$$

The operators $\overset{o}{L}_{\mu\nu}$ operate on angular functions in the five-dimensional space. These angular functions decompose into blocks, each belonging to one irreducible representation of SO_5. We shall find in this section these irreducible representations and the angular functions that belong to them. The main result is

Theorem 2: The linearly independent homogeneous polynomials of x_1, x_2, x_3, x_4, x_5 of degree p transform into themselves under a rotation SO_5. The transformation matrix M_p forms a representation of SO_5. M_p decomposes into a sum of irreducible representations,

$$M_p = (p, p)_5 + (p-2, p-2)_5 + (p-4, p-4)_5 + \cdots + [(0, 0)_5 \text{ or } (1, 1)_5]. \tag{3.2}$$

The homogeneous polynomials of degree p belonging to $(p, p)_5$ will be called SO_5 harmonics. The collection of all SO_5 harmonics, for $p = 0, 1, 2, \cdots$, forms a complete set of angular functions.

Proof: (a) We first choose as independent homogeneous polynomials of degree p,

$$(x_1 + ix_2)^a (x_1 - ix_2)^b (x_3 + ix_4)^c (x_3 - ix_4)^d x_5^e, \qquad a + b + c + d + e = p, \tag{3.3}$$

where a, b, c, d, and e are integers ≥ 0. (3.3) is an eigenfunction of $\overset{o}{J}_3$ and $\overset{o}{K}_3$ with eigenvalues

$$\tfrac{1}{2}(a - b + c - d) \quad \text{and} \quad \tfrac{1}{2}(a - b - c + d), \tag{3.4}$$

respectively. Thus the largest eigenvalue of $\overset{o}{J}_3$ is $\frac{1}{2}p$, for states with $a + c = p$, $b = d = e = 0$. Among these, the one with the largest eigenvalue for $\overset{o}{K}_3$ obtains for the case $c = 0$, for which $\overset{o}{K}_3$ has eigenvalue $\frac{1}{2}p$. Thus the leading state of M_p has eigenvalues $\frac{1}{2}p$, $\frac{1}{2}p$ for $\overset{o}{J}_3$, $\overset{o}{K}_3$. This state is contained in M_p exactly once. By Theorem 1, M_p contains $(p, p)_5$ exactly once. Furthermore M_p does not contain any $(p', q')_5$ for which $p' > p$.

(b) We write

$$M_p = (p, p)_5 + O_p .$$

Now $(\sum_1^5 x_\mu^2)$ times the homogeneous polynomials of degree $p - 2$ form a subspace (of M_p) that transforms into itself. Thus M_p contains M_{p-2}. But M_{p-2} contains no (p', q') with $p' > p - 2$, according to (a) above. Hence M_{p-2} is contained entirely in O_p. The dimension of M_p is easily seen to be C_p^{5+p-1}. The dimension of $(p, p)_5$ is $\frac{1}{6}(p+1)(p+2)(2p+3)$. Hence the dimension of O_p is the difference of the two, which is exactly $C_{p-2}^{5+(p-2)-1}$ = dimension of M_{p-2}. Thus

$$M_p = (p, p)_5 + M_{p-2}.$$

We thus obtain (3.2) by iteration.

(c) The completeness of the SO_5 harmonics follows from the completeness of the polynomial functions.

Theorem 3: The SO_5 harmonics Z (which are polynomails) of degree p defined in the last theorem satisfy

$$\left(\sum_1^5 \partial_\mu^2\right) Z = 0. \tag{3.5}$$

Proof: In a straightforward way we find

$$\begin{aligned}
\mathring{A} &= \tfrac{1}{2}\left(\sum_{\mu,\nu=1}^{5} \overset{o}{L}_{\mu\nu}\right)^2 \\
&= \sum_{\mu \neq \nu} [x_\mu \partial_\nu x_\mu \partial_\nu - x_\mu \partial_\nu x_\nu \partial_\mu] \\
&= \sum_{\mu \neq \nu} [x_\mu^2 \partial_\nu^2 - (\partial_\nu x_\nu)(x_\mu \partial_\mu)] \\
&= \sum [x_\mu^2 \partial_\nu^2 - (\partial_\nu x_\nu)(x_\mu \partial_\mu)] - \sum_\mu [x_\mu^2 \partial_\mu^2 - \partial_\mu x_\mu x_\mu \partial_\mu] \\
&= \sum [x_\mu^2 \partial_\nu^2 - (x_\nu \partial_\nu)(x_\mu \partial_\mu)] - 5 \sum_\mu x_\mu \partial_\mu + 2 \sum x_\mu \partial_\mu \\
&= r^2 \sum \partial_\nu^2 - (r\partial_r)^2 - 3(r\partial_r).
\end{aligned} \tag{3.6}$$

Now

$$(r\partial_r) Z = pZ.$$

Using Theorem 1 which shows that $\mathring{A}Z = (-p^2 - 3p)Z$, we arrive at (3.5).

TABLE I. SO_5 harmonic functions for $p=0$, 1, 2. These functions have not been properly normalized.

$(p,p)_5$	j	k	m_j	m_k	Z(unnormalized)
$(0,0)_5$	0	0	0	0	1
$(1,1)_5$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	x_1+ix_2
			$\frac{1}{2}$	$-\frac{1}{2}$	x_3+ix_4
			$-\frac{1}{2}$	$\frac{1}{2}$	x_3-ix_4
			$-\frac{1}{2}$	$-\frac{1}{2}$	x_1-ix_2
	0	0	0	0	x_5
$(2,2)_5$	1	1	1	1	$(x_1+x_2)^2$
			1	0	$(x_1+ix_2)(x_3+ix_4)$
			1	−1	$(x_3+ix_4)^2$
			0	1	$(x_1+ix_2)(x_3-ix_4)$
			0	0	$x_1^2+x_2^2-x_3^2-x_4^2$
			0	−1	$(x_1-ix_2)(x_3+ix_4)$
			−1	1	$(x_3-ix_4)^2$
			−1	0	$(x_1-ix_2)(x_3-ix_4)$
			−1	−1	$(x_1-ix_2)^2$
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$x_5(x_1+ix_2)$
			$\frac{1}{2}$	$-\frac{1}{2}$	$x_5(x_3+ix_4)$
			$-\frac{1}{2}$	$\frac{1}{2}$	$x_5(x_3-ix_4)$
			$-\frac{1}{2}$	$-\frac{1}{2}$	$x_5(x_1-ix_2)$
	0	0	0	0	$5x_0^2-r^2$

Theorem 4: A homogeneous polynomial of $x_1, \ldots, x_5$ of degree p that satisfies (3.5) is a SO_5 harmonic as defined in Theorem 2. It belongs to $(p,p)_5$ under SO_5.

Proof: Let Z' be a polynomial belonging to $(p-2,p-2)_5$ in the decomposition (3.2).

$$(r\partial_r)Z'=pZ'.$$

By Theorem 1,

$$\mathring{A}Z'=[-(p-2)^2-3(p-2)]Z'.$$

Thus (3.6) gives

$$(r^2\textstyle\sum\partial_\nu^2)Z'=[-(p-2)^2-3(p-2)+p^2+3p]Z'$$
$$=(4p+2)Z'.$$

Thus Z' is an eigenfunction of $r^2\sum\partial_\nu^2$ with eigenvalue $4p+2>0$. Similarly, we find the decomposition (3.2) is a decomposition into different eigenvalues of $(r^2\sum\partial_\nu^2)$. The theorem follows.

The (unnormalized) harmonics for $p=0, 1, 2$ are tabulated in Table I.

4. ANGULAR VARIABLES

It is convenient to introduce the angular variables $r, \theta, \xi_1, \xi_2, \xi_3$ defined by Eqs. (18) and (22) of Ref. 3. We can express the operators $L_{\mu\nu}$ in these variables in a straightforward evaluation. We obtain

$$x_i\partial_j-x_j\partial_i=\xi_i\frac{\partial}{\partial\xi_j}-\xi_j\frac{\partial}{\partial\xi_i},$$
$$x_i\partial_4-x_4\partial_i=-\tfrac{1}{2}(1-\xi^2)\frac{\partial}{\partial\xi_i}-\xi_i\left(\xi_j\frac{\partial}{\partial\xi_j}\right), \tag{4.1}$$

$$\mathring{A}\equiv\tfrac{1}{2}\sum_1^5(\mathring{L}_{\mu\nu})^2=\frac{1}{\sin^3\theta}\frac{\partial}{\partial\theta}\left(\sin^3\theta\frac{\partial}{\partial\theta}\right)$$
$$+\frac{(1+\xi^2)^3}{4\sin^2\theta}\frac{\partial}{\partial\xi_i}\frac{1}{1+\xi^2}\frac{\partial}{\partial\xi_i}, \tag{4.2}$$

$$\mathring{B}=\tfrac{1}{2}\sum_1^4(\mathring{L}_{\mu\nu})^2=-2\mathring{\mathbf{J}}^2-2\mathring{\mathbf{K}}^2=\frac{(1+\xi^2)^3}{4}\frac{\partial}{\partial\xi_i}\left(\frac{1}{1+\xi^2}\frac{\partial}{\partial\xi_i}\right), \tag{4.3}$$

where all $i,j=1,2,3$. The Laplacian operator $\sum^5\partial_\mu^2$ can be expressed in the angular and radial variables by combining (3.6) with (4.2), and agrees, of course, with the standard expression obtainable from the metric given in Ref. 3.

The homogeneous polynomials of degree $(2j)$ of x_1, x_2, x_3, and x_4 (without x_5) form a representation of SO_4 rotations of these four coordinates. Breaking the representations into irreducible ones, $(\alpha,\beta)_4$, one obtains $\alpha=\beta$ through the use of (3.1). The largest one is obviously $(j,j)_4$. The states of this irreducible representation are thus equal to

$$(r\sin\theta)^{2j}W_{j,m_j,m_k}(\xi_1,\xi_2,\xi_3),$$

where W will be called azimuthal functions, which are generalizations of the usual azimuthal functions $\exp(im\phi)$. They satisfy

$$\mathring{\mathbf{J}}^2W_{j,m_j,m_k}=\mathring{\mathbf{K}}^2W_{j,m_j,m_k}=j(j+1)W_{j,m_j,m_k},$$
$$\mathring{J}_3W_{j,m_j,m_k}=m_jW_{j,m_j,m_k}, \tag{4.4}$$
$$\mathring{K}_3W_{j,m_j,m_k}=m_jW_{j,m_j,m_k}.$$

Notice that the operators $\mathring{\mathbf{J}}$ and $\mathring{\mathbf{K}}$ are dependent only on ξ_i and $\partial/\partial\xi_i$, as is obvious from (4.1). We shall further define the W's with phases and normalization factors such that the usual formulas

$$(J_1+iJ_2)W_{j,m_j,m_k}=(j-m_j)^{1/2}(j+m_j+1)^{1/2}W_{j,m_j+1,m_k},$$
$$(K_1+iK_2)W_{j,m_j,m_k}=(j-m_k)^{1/2}(j+m_k+1)^{1/2}W_{j,m_j,m_k+1}, \tag{4.5}$$

are valid. Under an SO_4 rotation in x_1, x_2, x_3, x_4, the W function transforms under the irreducible representation $(j,j)_4$.

The harmonic functions of Sec. 3 are thus

$$Z=r^pF(\theta)W_{j,m_j,m_k}. \tag{4.6}$$

Using (4.2), (4.3), (4.4), and Theorem 1 we find

$$(-p^2-3p)Z=\mathring{A}Z=\frac{1}{\sin^3\theta}\frac{\partial}{\partial\theta}\left(\sin^3\theta\frac{\partial}{\partial\theta}\right)Z$$
$$-\frac{4}{\sin^2\theta}j(j+1)Z,$$

or

$$\frac{1}{\sin^3\theta}\frac{\partial}{\partial\theta}\left(\sin^3\theta\frac{\partial}{\partial\theta}\right)F-\frac{4}{\sin^2\theta}j(j+1)F+(p^2+3p)F=0. \tag{4.7}$$

This can be solved using Jacobi polynomials. We shall not go into it here since (4.7) is a special case of a more general equation to be solved in Sec. 6 below.

5. EVALUATION OF J AND K

We have by definition

$$L_{12} = \overset{o}{L}_{12} + Y_k[x_1 b_2^k - x_2 b_1^k] - r^2 f_{12}^k Y_k . \tag{5.1}$$

The field strengths f and the potentials b have been given explicitly in Ref. 3, and in Eqs. (37β) and (34$'\beta$), but in coordinates r, θ, ξ. We want now to evaluate L_{12} in Cartesian coordinates. The evaluation is a straightforward tensor transformation. One obtains, after some algebra, for[3] region a,

$$Y_k(x_1 b_2^k - x_2 b_1^k)$$
$$= -\frac{4(1-\cos\theta)}{(1+\xi^2)^2}\left[\tfrac{1}{2}(1-\xi^2)(\xi_1 Y_2 - \xi_2 Y_1) + \xi^2 Y_3 - \xi_3(\xi\cdot Y)\right],$$
$$r^2 f_{12}^k Y_k = (\text{above}) + Y_3 . \tag{5.2}$$

Thus we obtain the simple formula

$$L_{12} = \overset{o}{L}_{12} - Y_3 . \tag{5.3}$$

Similarly, we start from

$$L_{14} = \overset{o}{L}_{14} + Y_k[x_1 b_4^k - x_4 b_1^k] - r^2 f_{14}^k Y_k \tag{5.4}$$

and evaluate the terms. After some algebra we obtain, for region a,

$$Y_k(x_1 b_4^k - x_4 b_1^k)$$
$$= \frac{4(1-\cos\theta)}{(1+\xi^2)^2}\left[\tfrac{1}{2}(1-\xi^2)(Y_2\xi_3 - Y_3\xi_2) + \xi_1(\xi\cdot Y) + \tfrac{1}{4}(1-\xi^2)^2 Y_1\right],$$
$$r^2 f_{14}^k Y_k = (\text{above}) - Y_1 . \tag{5.5}$$

Thus we obtain the simple formula for region a,

$$L_{14} = \overset{o}{L}_{14} + Y_1 . \tag{5.6}$$

Cyclically permiting 1, 2, 3 in (5.3) and (5.6) and adding, we obtain

Theorem 5:

$$\mathbf{J}^{(a)} = \overset{o}{\mathbf{J}}, \quad \mathbf{K}^{(a)} = \overset{o}{\mathbf{K}} + i\mathbf{Y}, \text{ for}^3 \text{ region } a. \tag{5.7}$$

Notice that $i\mathbf{Y} = \mathbf{I}$ is the isospin of the particle moving in the monopole field β. Similarly we obtain

Theorem 6:

$$\mathbf{J}^{(b)} = \overset{o}{\mathbf{J}} + i\mathbf{Y}, \quad \mathbf{K}^{(b)} = \overset{o}{\mathbf{K}} \text{ for region } b. \tag{5.8}$$

Is the extremely simple form for **J** and **K** given above surprising? It is really not, since the operators **J** and **K** are in the "azimuthal" plane, and the corresponding azimuthal problem for the Dirac monopole results in the very simple formulas (20) of Ref. 1.

It will be proved in Appendix A that in the overlap between regions a and b,

$$\overset{o}{\mathbf{J}} + i\mathbf{Y} = \tau^{-1}\overset{o}{\mathbf{J}}\tau, \quad \overset{o}{\mathbf{K}} = \tau^{-1}(\overset{o}{\mathbf{K}} + i\mathbf{Y})\tau, \tag{5.9}$$

i.e.,

$$\mathbf{J}^{(b)} = \tau^{-1}\mathbf{J}^{(a)}\tau, \quad \mathbf{K}^{(b)} = \tau^{-1}\mathbf{K}^{(a)}\tau,$$

where τ is the representation, for the isospin I in question, of the transition function T. T has been explicitly given in Ref. 3, Eq. (24β). Thus the wave sections in regions a and b are related by

$$\psi^{(b)} = \tau^{-1}\psi^{(a)} \tag{5.10}$$

which is as it should be.

Equation (5.9) is the generalization of

$$(-i\partial_\phi + q) = \exp(-2iq\phi)(-i\partial_\phi - q)\exp(2iq\phi) \tag{5.11}$$

for the gauge transformation between regions a and b in the discussions of Ref. 1 for the Dirac monopole. Compare Eqs. (20) in that reference.

6. EIGENSECTIONS X

Consider a simultaneous eigensection X for all five operators (1.5). Since $L_{\mu\nu}$ satisfies the commutation rules (1.2), we consider an eigensection belonging to $(p,q)_5$, and satisfying

$$\mathbf{J}^2 X = j(j+1)X, \quad \mathbf{K}^2 X = k(k+1)X,$$
$$J_3 X = m_j X, \quad K_3 X = m_k X.$$

In region a, Theorem 5 and (3.1) thus show that $X^{(a)}$ belong to eigenvalue $j(j+1)$ for $\overset{o}{\mathbf{J}}^2 = \overset{o}{\mathbf{K}}^2$, and to eigenvalue $k(k+1)$ for $(\overset{o}{\mathbf{K}} + \mathbf{I})^2$. Consider for fixed j and m_j the states

$$|j, m_j, m_k', m_I\rangle = (W_{j,m_j,m_k'})\chi_{m_I}(s), \tag{6.1}$$

where s is the isospin coordinate, m_I denotes the third component of **I**, and χ is the spin wavefunction. W is the azimuthal function defined in Sec. 4. Using Clebsch–Gordon coefficients for combining states with different m_k' and m_I, we define linear combinations of (6.1) to obtain an eigenstate U of $(\overset{o}{\mathbf{K}} + \mathbf{I})^2$ and $\overset{o}{K}_3 + I_3$ with eigenvalues $k(k+1)$ and m_k. The state will be written as U_{j,k,m_j,m_k}. Thus

$$X^{(a)} = G^{(a)}(\theta)\, U_{j,k,m_j,m_k}(\xi, s). \tag{6.2}$$

We have

$$|k - j| \le I. \tag{6.3}$$

To determine $G^a(\theta)$ we need to evaluate the operator A of (1.5), resulting in, in region a,

$$A = \frac{1}{\sin^3\theta}\frac{\partial}{\partial\theta}\left(\sin^3\theta\frac{\partial}{\partial\theta}\right) - \frac{4\mathbf{J}^2}{\sin^2\theta} - \frac{2(1-\cos\theta)}{\sin^2\theta}[\mathbf{K}^2 - \mathbf{J}^2 - \mathbf{I}^2]$$
$$- \frac{(1-\cos\theta)(3+\cos\theta)}{\sin^2\theta}\mathbf{I}^2 \quad (i\mathbf{Y} = \mathbf{I}). \tag{6.4}$$

The details will be given in Appendix B. Since we have assumed that $X^{(a)}$ belongs to $(p,q)_5$, the eigenvalue of A is, by Theorem 1, $-\frac{1}{2}p^2 - \frac{1}{2}q^2 - 2p - q$. Those of $\mathbf{J}^2$, $\mathbf{K}^2$, and $\mathbf{I}^2$ are $j(j+1)$, $k(k+1)$, and $I(I+1)$, respectively. Thus

$$(\tfrac{1}{2}p^2 + \tfrac{1}{2}q^2 + 2p + q)G$$
$$= -s^{-3}d_\theta(s^3 d_\theta G) + [4j(j+1) + 2(1-c)[k(k+1) - j(j+1) - I(I+1)] + (1-c)(3+c)I(I+1)]Gs^{-2}, \tag{6.5}$$

where $c = \cos\theta$, $s = \sin\theta$. Putting

$$G = H(\sin\theta)^{-1}, \tag{6.6}$$

one obtains

$$\gamma H = \frac{-1}{\sin\theta}\,\frac{d}{d\theta}\left(\sin\theta\,\frac{dH}{d\theta}\right) + \frac{[j-k+(j+k+1)\cos\theta]^2}{\sin^2\theta}\,H, \tag{6.7}$$

where

$$-\gamma = (j+k+1)^2 - 2 + I(I+1) - \tfrac{1}{2}p^2 - \tfrac{1}{2}q^2 - 2p - q. \tag{6.8}$$

Equation (6.7) is of the form of Eq. (22) of Ref. 1. It has no allowable solution for $0 \leq \theta \leq \pi$ unless

$$\gamma \geq j+k+1, \tag{6.9}$$

which follows from the usual indicial equation–polynomial expansion treatment. Now we concentrate on the leading state of $(p,q)_5$ so that $p=2j$, $q=2k$. This state must exist if $(p,q)_5$ exists. Equations (6.8) and (6.9) then become

$$I(I+1) \leq [\tfrac{1}{2}(p-q)][\tfrac{1}{2}(p-q)+1].$$

Thus $I \leq \frac{1}{2}(p-q)$.

Combining with (6.3) we obtain $I=\frac{1}{2}(p-q)$. Thus we have

Theorem 7: The only SU_2 monopole harmonics are those for which $I=\frac{1}{2}(p-q)$.

We notice that for $I=0$ this reduces to what was already known for orbital harmonics: $p=q$.

Putting $p-q=2I$ into (6.8), (6.7) becomes identical to Eq. (22) of Ref. 1 with $l=I+q+1$. Thus we can read off the solution from Eq. (28) of that paper,

$$H = (1-\cos\theta)^{\alpha/2}(1+\cos\theta)^{\beta/2}P_n^{\alpha,\beta}(\cos\theta), \tag{6.10}$$

where $P_n^{\alpha,\beta}$ is the Jacobi polynomial and

$$\alpha = 2j+1, \quad \beta = -2k-1, \text{ and } n = I+q+1+k-j \tag{6.11}$$

are all integers (n, $n+\alpha$, $n+\beta$, $n+\alpha+\beta$ are all ≥ 0).

We have thus proved

Theorem 8: The SU_2 monopole harmonics are

$$X_{I,a,j,k,m_j,m_k} = (\sin\theta)^{a-1}(1-\cos\theta)^{\alpha/2}(1+\cos\theta)^{\beta/2} \times P_n^{\alpha,\beta}(\cos\theta)\,U_{j,k,m_j,m_k}, \tag{6.12}$$

which belongs to the representation $(p,q)_5$ where $p=q+2I$. The integers α,β,n are defined by (6.11). Equation (6.12) is valid in region a. In region b, $X^{(b)}$ is obtained from (6.12) by operating on it with the representation τ of the transition function. [Compare (5.10).] Since τ operates only on U, the θ part of (6.12) is unchanged. Equation (6.12) has not been normalized.

The condition $p=q+2I$ means that all SU_2 monopole harmonics belong to irreducible representations $(q+2I,q)_5$ which in Fig. 1 consist of $(j,k)_4$'s lying along $2I+1$ parallel lines running from the lower left corner to the upper right. The smallest such representation is $(2I,0)_5$.

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APPENDIX A

To prove (5.9) we observe that by (4.1)

$$\tau^{-1}(\overset{o}{L}_{12} - Y_3)\,\tau = \overset{o}{L}_{12} + \tau^{-1}\left[\xi_1\frac{\partial\tau}{\partial\xi_2} - \xi_2\frac{\partial\tau}{\partial\xi_1}\right] - \tau^{-1}Y_3\tau. \tag{A1}$$

For the case of $I=\frac{1}{2}$, by Eq. (24β) of Ref. 3,

$$\tau = (1+\xi^2)^{-2}[1-\xi^2 - 2i\xi\cdot\sigma]. \tag{A2}$$

Using this we can evaluate explicitly the righthand side of (A1) obtaining

$$\tau^{-1}(\overset{o}{L}_{12} - Y_3)\,\tau = \overset{o}{L}_{12} - Y_3. \tag{A3}$$

Now the second and third terms on the rhs of (A1) for the general case (i.e., any I) must each be linear homogeneous in Y_i, because τ is the representation of the gauge group with $\mathbf{Y}$ as the infinitesimal operators. Thus the validity of (A3) for one case, the case of $I=\frac{1}{2}$, is enough to show that it is valid in general.

Similarly we can prove

$$\tau^{-1}(\overset{o}{L}_{i4} + Y_i)\,\tau = \overset{o}{L}_{i4} - Y_i.$$

Equation (5.9) then follows easily.

APPENDIX B

To prove (6.4) we first evaluate $\frac{1}{2}\sum_1^5 L_{\mu\nu}^2$ by separating out the terms of degrees 0, 1 and 2 in $f_{\mu\nu}$. The degree 1 terms vanish because of $f_{\mu\nu}^i x_\mu = 0$. The degree 0 term can be further separated according to the powers of b_μ. We thus obtain

$$A = r^2[\partial_\nu^2 + (b_\nu Y)^2 + 2b_\nu Y\partial_\nu + b_{\nu,\nu}Y] - (r\partial_r)^2 - 3r\partial_r + \tfrac{1}{2}r^4\sum(f_{\mu\nu}Y)^2, \tag{B1}$$

where we have suppressed all i indices. For example, $b_\nu Y = b_\nu^i Y_i$.

Now we use the explicit expressions (34'β) and (37β) of Ref. 3 for b_μ and $f_{\mu\nu}$ to evaluate (B1), resulting in, in region a,

$$A = \frac{1}{\sin^3\theta}\,\frac{\partial}{\partial\theta}\left(\sin^3\frac{\partial}{\partial\theta}\right) + \frac{(1+\xi^2)^3}{4\sin^2\theta}\,\frac{\partial}{\partial\xi^i}\left(\frac{1}{1+\xi^2}\,\frac{\partial}{\partial\xi^i}\right) - \frac{2(1-\cos\theta)}{\sin^2\theta}\left(\beta_i^k Y_k\,\frac{\partial}{\partial\xi_i}\right) + \frac{4(1-\cos\theta)(3+\cos\theta)}{(1+\xi^2)^2\sin^2\theta}(\beta_i^k Y_k)^2,$$

where

$$\beta_j^i \equiv (1+\xi^2)^2 f_{\theta j}^i/(4\sin\theta) = \xi_i\xi_j + \tfrac{1}{2}(1-\xi^2)\,\delta_{ij} - \epsilon_{ijk}\xi_k \tag{B3}$$

and $f_{\theta j}^i$ is $f_{\theta\xi_j}^i$ as defined in Ref. 3. Now (B3) and (4.1) lead to

$$\beta_i^3\,\frac{\partial}{\partial\xi_i} = \overset{o}{L}_{12} - \overset{o}{L}_{34}.$$

Hence

$$\beta_i^k Y_k \frac{\partial}{\partial \xi i} = 2i(\overset{o}{\mathbf{K}} \cdot \mathbf{Y}) = \mathbf{K}^2 - \mathbf{J}^2 + \mathbf{Y}^2, \tag{B4}$$

where

$$\mathbf{K}^2 = \overset{o}{\mathbf{K}}{}^2 + 2i\overset{o}{\mathbf{K}} \cdot \mathbf{Y} - \mathbf{Y}^2 = \mathbf{J}^2 + 2i\overset{o}{\mathbf{K}} \circ \mathbf{Y} - \mathbf{Y}^2, \tag{B5}$$

which follows from (5.7) and (3.1). Furthermore

$$(\beta_i^k Y_k)^2 = \beta_i^k Y_k \beta_i^j Y_j = -\tfrac{1}{4}(1+\xi^2)^2 \mathbf{I}^2. \tag{B6}$$

Now (3.1) and (5.7) show that (4.3) is equal to $-4\overset{o}{\mathbf{J}}{}^2 = -4\mathbf{J}^2$. Using this fact and (B4), (B6) we obtain (6.4).

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Neutron stars: Analytical continuation of the ingoing gravitational wave amplitudes and asymptotic eigenfrequencies distribution for even modes

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With reference to a hot perfect fluid neutron star with an equation of state whose behavior is polytropic near the surface and in the framework of an arbitrary multipole of even order $l \geq 2$, the "ingoing" gravitational wave amplitude of frequency ω is analytically continued to the region $\mathrm{Im}\omega < 0$. This is performed by suitable rotations of the integration paths in the multiple integrals expressing the successive iterations for such amplitude. The analytical continuation allows us to successively obtain the asymptotic eigenfrequency distribution for $\omega \to \infty$. This differs in some cases from that obtained in a previous paper on the basis of a conjecture regarding the analytical continuation of the ingoing amplitude, although it maintains the same qualitative features.

I. INTRODUCTION

In a previous paper,[1] hereafter denoted by I, with reference to an even mode of given frequency ω, belonging to a multipole of order $l \geq 2$ and in the framework of general relativity, we constructed systems of integral equations for amplitudes describing coupled sound and gravitational waves in a hot perfect fluid neutron star with an equation of state whose behavior is polytropic near the surface. This was achieved, among other things, in view of obtaining the eigenfrequency distribution for $\omega \to \infty$.

This, in its turn, may be useful to establish the completeness (if any) of eigenmodes with respect to a small arbitrary perturbation of the star and of the surrounding gravitational field.

If $W(\omega)$ denotes the Wronskian constructed with the physical internal amplitude and the ingoing one for a given ω, any eigenfrequency ω_n is a solution of the equation $W(-\omega) = 0$ and vice versa.

Now, for $\mathrm{Im}\omega < 0$ and $\omega \to \infty$ the above equation is never satisfied, as can be deduced from Sec. 7 of Ref. 2, hereafter denoted by II.

On the other hand, the analytical continuation of the ingoing solution $u_-(-\omega)$ for $\mathrm{Im}\omega > 0$ is necessary for the determination of the eigenfrequencies in this region. Equivalently, one has to continue $u_-(\omega)$ to the region $\mathrm{Im}\omega < 0$.

Indeed in such a case, the multiple integrals expressing the successive iterations for the ingoing amplitude diverge.

In the present context suitable rotations of the integration paths in the Gauss plane for the integration variables are performed; by means of them, new integral representations are obtained for the iterative terms, which hold both for $\mathrm{Im}\omega > 0$ and $\mathrm{Im}\omega < 0$.

We observe that in Paper II we obtained an asymptotic expression for $W(-\omega)$ holding for $\mathrm{Im}\omega < 0$; the same expression was used also for $\mathrm{Im}\omega > 0$ on the basis of two assumptions on the analytical continuation of the ingoing amplitude to the region $\mathrm{Im}\omega < 0$.

Such assumptions, however, turn out to be verified only for distances larger than the star radius and for particular values of the polytropic index.

The correct eigenfrequency distribution obtained in this context differs in some cases from that obtained in Paper II, even if it maintains in any case the same qualitative features.

The plan of this paper is the following.

In Sec. 2 the analytical continuation of the ingoing amplitude is performed.

In Sec. 3 the general asymptotic eigenfrequency distribution is determined.

In Sec. 4 we compare such distribution with that obtained in Paper II.

2. ANALYTICAL CONTINUATION OF u_-

For the symbols appearing in this context reference is made to Paper I; moreover, as in Papers I and II, in the following C, C_0, C_1, $C_2, \cdots$ will denote positive ω independent constants.

As seen from (I. 5. 3) the $(n+1)$th iteration for u_- reads

$$u_-^{(n+1)}(r;\omega) = \int_\infty^r g_1(r, r_1;\omega)\, V_{11}(r_1;\omega)\, dr \int_\infty^{r_1} g_1(r_1, r_2;\omega) \times V_{11}(r_2;\omega)\, dr_2 \cdots \int_\infty^{r_n} g_1(r_n, r_{n+1};\omega)\, V_{11}(r_{n+1};\omega) \times u_-^{(0)}(r_{n+1};\omega)\, dr_{n+1}, \tag{2.1}$$

where, for the moment, r_i are real nonnegative variables and $u_-^{(0)}$ is given by (I. 5. 3), (I. 3. 20). As stated in Sec. 1, the above expression does not define $u_-^{(n+1)}$ for $\mathrm{Im}\omega < 0$, since the integral over r_{n+1} diverges.

 0022-2488/78/1912-2628$1.00

Therefore, the analytical continuation of $u_-^{(n+1)}$ for $\mathrm{Im}\omega < 0$ is required and this will be achieved by means of a new integral representation of $u_-^{(n+1)}$, which is equivalent to the above one for $\mathrm{Im}\omega \geq 0$. In order to obtain it, we first choose the integration variables to be $W_i = W_g(r_i)$ instead of r_i, W_g being defined by (I. 3. 6), and then we perform suitable rotations of the integrations paths in the W_i complex planes. The convenience of such new representation lies in the fact that the integrals involved in it are convergent also for $\mathrm{Im}\omega < 0$.

In order to carry out the above program, an inductive procedure will be adopted by means of the expression

$$u_-^{(n+1)}(W_g; \omega) = \int_\infty^{W_g} g_1(W_g, W_1; \omega)[V_{11} u_-^{(n)} \exp[(\nu - \lambda)/2]]_{W_1;\omega}\, dW_1, \tag{2.2}$$

which is equivalent to (2. 1).

Consider the region D in the W_g complex plane consisting of the real interval Δ defined by $0 \leq W_g \leq W_g(r_0)$ plus the domain D_0 defined by $0 \leq \arg(W_g - W_g(r_0)) \leq \pi/2$, r_0 being the star radius.

For $r > r_0$ the function $W_g(r)$, as obtained from (I. 5. 18), reads

$$W_g(r) = W_{\mathrm{ext}}(r) = W_g(r_0) + r - r_0 + 2M \ln\left(\frac{r - 2M}{r_0 - 2M}\right), \tag{2.3}$$

where M is the star mass.

In the following we allow r to assume complex values, and it is understood that the logarithmic function appearing in the above expression is defined by

$$\ln z = \ln|z| + i \arg z, \quad -\pi \leq \arg z \leq \pi. \tag{2.4}$$

Equation (2. 3) defines an implicit function $r = f(W_g)$ in the W_g complex plane, which may be many valued; when r spans its complex plane completely, the whole W_g complex plane is correspondingly mapped. Indeed, suppose that this is not the case. Then some boundary lines should exist dividing the mapped and unmapped regions. Consider then a point $\bar{r}$ different from $2M$ such that $W_{\mathrm{ext}}(\bar{r})$ belongs to a boundary line. In a small neighborhood δ of $\bar{r}$ we can write from (2. 3)

$$W_g(r) - W_g(\bar{r}) = r - \bar{r} + 2M \ln\left(\frac{r - 2M}{\bar{r} - 2M}\right) \simeq (r - \bar{r})\left(1 + \frac{2M}{\bar{r} - 2M}\right) \tag{2.5}$$

So, when r varies on the boundary of δ in such a way that

$$0 \leq \arg(r - \bar{r}) \leq 2\pi, \tag{2.6}$$

correspondingly, also the nonvanishing vector $W_g(r) - W_g(\bar{r})$ makes a rotation of 2π in its complex plane. But this fact contradicts the assumption that $W_{\mathrm{ext}}(\bar{r})$ is a point of a boundary line.

For $W_g = \infty$ we have $r = \infty$ and $r = 2M$. More generally, there is no one-to-one correspondence between r and W_g; this implies that some regions of the W_g complex plane may be mapped more than once. Clearly, for $W_g \neq \infty$, r is finite and $\neq 2M$.

Moreover, from (2. 3) we obtain

$$\frac{dr}{dW_g} = \left(\frac{dW_{\mathrm{ext}}}{dr}\right)^{-1} = \frac{r}{r - 2M}. \tag{2.7}$$

Now, on the real axis for $W_g \geq W_g(r_0)$ a one-to-one correspondence can be established between W_g and r since $W_{\mathrm{ext}}(r)$ is monotonic.

Then we choose the determinations of $r = f(W_g)$ to satisfy such correspondence together with the condition $f(\infty) = \infty$ in D_0.

The rhs of the above differential equation is an analytic function of r in such region since $r \neq 2M$; so its solution is univocally determined and analytic in D_0 for $|W_g| < \infty$.[3]

As seen from (2. 5), the correspondence $f(\infty) = \infty$ implies

$$\lim_{W_g \to \infty} \frac{r}{W_g} = 1. \tag{2.8}$$

Now we observe that in the region D_0 $f(W_g)$ never vanishes. Indeed, for $r = 0$ Eq. (2. 3) furnishes

$$\frac{W_{\mathrm{ext}}(0) - W_g(r_0)}{2M} = -\left[\frac{r_0}{2M} + \ln\left(1 - \frac{r_0}{2M}\right)\right]; \tag{2.9}$$

on the other hand, for all the reasonable models of neutron stars which have been proposed, the real part of the rhs of the above equality can be verified to be negative.

By summarizing the results, we can state that

(i) $f(W_g)$ is analytic in D_0 for $|W_g| < \infty$;

(ii) $f(W_g)$ never vanishes in D_0;

(iii) it obeys (2. 8).

We complete the one-to-one correspondence between r and W_g in D, as regards the real interval $0 \leq W_g \leq W_g(r_0)$ by means of the monotonic $W_g(r)$ given by (I. 3. 6), where ν, λ are determined by the equilibrium equations for the star.

Let us go back to Eq. (2. 2), where the functions $V_{11} \exp(\nu - \lambda)$, g_1, $u_-^{(n)}$ are involved in the integrand. From (i)–(iii) and (I. 5. 6)–(I. 5. 10) one deduces that $\exp(\nu - \lambda)\, V_{11}$ is completely analytical in D_0.

Moreover, for $|\omega|$ large enough, in D_0 it obeys the inequality

$$|\exp(\nu - \lambda)\, V_{11}| < C |W_g|^2; \tag{2.10}$$

for $0 \leq W_g \leq W_g(r_0)$ we observe that V_{11}, given by (I. 3. 10) together with (I. 3. 9) and (I. 18) of Ref. 4 is proportional to terms containing ν''' or λ'', which, in their turn, are proportional to ρ' [see Eqs. (1. 2)–(1. 4) of Ref. 4].

For stars whose behavior near the surface is polytropic, we have $\rho \sim_{r_0} (r_0 - r)^N$. Then for noninteger values of N, we have

$$\frac{d^m}{dr^m}\left[\exp((\nu-\lambda)\,V_{11})\right]_{r\to r_0} \simeq k_m(r_0-r)^{N-1-m}+\text{const}\quad (m\geq 0), \tag{2.11}$$

$$\left|\frac{d^m}{dr^m}\exp((\nu-\lambda)\,V_{11})\right| < C\,|r_0-r|^{N-1-m}+C_1. \tag{2.12}$$

The kernel g_1 deserves particular attention. For $0\leq W_g\leq W_1\leq W_g(r_0)$ it satisfies [see (I. 3. 17), (I. 3. 20), (I. 3. 23), (I. 3. 28) and (3. 10) of Ref. 5]

$$\left|\frac{\phi_g(W_1)}{\phi_g(W_g)}\,g_1\right| < \frac{\bar{C}}{|\omega|}\exp\left[|\mathrm{Im}\omega|\,(W_1-W_g)\right]\frac{(L(|\omega W_1|))^{l+1}}{(L(|\omega W_g|))^{l}},$$

$$L(z)=\frac{z}{1+z}. \tag{2.13}$$

When both W_g and W_1 belong to D_0, it is suitable to express g_1 in terms of $\bar{h}_l^{(\pm)}(z)$, given by (I. 3. 22), according to (I. 5. 4) which is reported for convenience:

$$g_1(W_g,W_1;\omega)=\frac{1}{2i\omega}\,(\exp(\nu-\lambda)/2)_{W_1}\,\frac{\phi_g(W_g;\omega)}{\phi_g(W_1;\omega)} \times[\bar{h}_l^{(+)}(\omega W_g)\,\bar{h}_l^{(-)}(\omega W_1)-\bar{h}_l^{(-)}(\omega W_g)\,\bar{h}_l^{(+)}(\omega W_1)], \tag{2.14}$$

where ϕ_g is defined by (I. 3. 20), (I. 5. 6), (I. 5. 7), (I. 5. 10) whereas $\bar{h}_l^{(\pm)}(z)$ can be written as

$$\bar{h}_l^{(\pm)}(z)=P_l^{(\pm)}(1/z)\exp(\pm iz), \tag{2.15}$$

$P_l^{(\pm)}(1/z)$ being polynomials in $1/z$. As verified by inspection, for $|\omega|$ large enough $P_l^{(\pm)}$ in D_0 are majorized and minorized by a constant C. Then defining

$$\frac{\phi_g(W_g;\omega)}{\phi_g(W_1;\omega)}\,G=\exp(\nu-\lambda)\,V_{11}\exp[i\omega(W_1-W_g)], \tag{2.16}$$

we have

$$|G| < (C_1/|W_1|^2)\{1+|\exp[2i\omega(W_1-W_g)]|\}. \tag{2.17}$$

We observe that for $\mathrm{Im}\omega\geq 0$, W_g fixed in D_0 and W_1 varying in D_1 (belonging to D_0) defined by $0\leq\arg(W_1-W_g)\leq\pi/2$, we have

$$|\exp[2i\omega(W_1-W_g)]| = \exp[-2|\omega|\,|W_1-W_g|\sin(\vartheta_\omega+\vartheta_1)]\leq 1, \tag{2.18}$$

where $\vartheta_\omega=\arg\omega$, $\vartheta_1=\arg(W_1-W_g)$.

Suppose $u_-^{(n)}$ is defined in D_0 and analytical in such a region and that for $-\pi/2\leq\vartheta_\omega\leq\pi/2$ it can be written as

$$u_-^{(n)}=\frac{1}{\omega^n}\exp(i\omega W_g)\,\phi_g F^{(n)}(W_g;\omega), \tag{2.19}$$

where

$$|F^{(n)}| < C_0[\pi C_1/|W_g(r_0)|]^n, \tag{2.20}$$

C_1 being the constant appearing in (2.17).

Then we want to prove that $u_-^{(n+1)}$ can also be defined in D_0 and has properties quite analogous to those of $u_-^{(n)}$.

For the moment let us fix ω in the region $0\leq\vartheta_\omega\leq\pi/2$; so we can define $u_-^{(n+1)}(W_g,\omega)$, as given by (2.2), also for complex values of W_g in D_0 by assigning the integration path for W_1. Indeed, let us allow W_1 to go from W_g to infinity along any line belonging to D_1; the integral converges and is independent of the choice of such line, since the integrand I is completely analytical in D_1 and vanishes for $W_1\to\infty$ in such a way that $|I| < C/|W_1|^2$, owing to (2.17)—(2.20). Then as an integration path we choose the line $\arg(W_1-W_g)=\pi/2$; this allows us to extend the definition of $u_-^{(n+1)}$ in D_0 also for $\mathrm{Im}\omega < 0$.

Indeed, with the above choice, for any ω such that $-\pi/2 < \vartheta_\omega < \pi/2$ the inequality (2.18) holds altogether.

Then for any W_g in D_0 the integral in (2.2) converges also for $-\pi/2\leq\vartheta_\omega < 0$ and $|\omega|$ large enough. In addition, $u_-^{(n+1)}(W_g;\omega)$ is analytical in D_0, owing to the fact that the integrand is analytical for W_g and W_1 in the same domain.

Now from (2.2), (2.16), (2.19) we can write

$$u_-^{(n+1)}=\frac{\exp(i\omega W_g)}{\omega^{n+1}}\,\phi_g F^{(n+1)}(W_g;\omega), \tag{2.21}$$

$$F^{(n+1)}(W_g;\omega)=\int_\infty^{W_g} G(W_g,W_1;\omega)\,F^{(n)}(W_1;\omega)\,dW_1. \tag{2.22}$$

Then from (2.17)—(2.20) we get

$$\begin{aligned}|F^{(n+1)}| &< C_0\left(\frac{\pi C_1}{|W_g(r_0)|}\right)^n 2C_1\int_0^\infty \frac{|d(W_1-W_g)|}{|W_1|^2}\\ &= C_0\left(\frac{\pi C_1}{|W_g(r_0)|}\right)^n 2C_1 \times\int_0^\infty \frac{d|W_1-W_g|}{|W_1-W_g|^2+|W_g|^2+2\,\mathrm{Re}[(W_1-W_g)^*W_g]}\\ &< C_0\left(\frac{\pi C_1}{|W_g(r_0)|}\right)^n 2C_1\int_0^\infty \frac{d|W_1-W_g|}{|W_1-W_g|^2+|W_g|^2}\\ &\leq C_0\left(\frac{\pi C_1}{|W_g(r_0)|}\right)^{n+1};\end{aligned} \tag{2.23}$$

the third step proceeds from the fact that $\mathrm{Re}[(W_1-W_g)^*W_g]\geq 0$.

We note that (2.21) and (2.23) are completely analogous to (2.19), (2.20).

In order to treat the case $0\leq W_g < W_g(r_0)$, we assume that in such interval

$$u_-^{(n)}=\frac{\exp(i\omega W_g)}{\omega^n}\,\phi_g F_1^{(n)}(W_g;\omega)\quad(\mathrm{Im}\omega\geq 0), \tag{2.24}$$

$$u_-^{(n)}=\frac{\exp[i\omega[2W_g(r_0)-W_g]]}{\omega^n}\,\phi_g F_2^{(n)}(W_g;\omega)\quad(\mathrm{Im}\omega < 0), \tag{2.25}$$

where

$$|F_i^{(n)}| < C_0C_2^n[L(|\omega W_g|)]^{-l}, \tag{2.26}$$

C_2 being a constant which majorizes the expression

$$\bar{C}[|V_{11}\exp(\nu-\lambda)|]_{\Delta} W_g(r_0)\frac{\pi C_1}{W_g(r_0)}+\left[\tfrac{1}{2}|W_1|^2 \times (|V_{11}\exp(\nu-\lambda)|)_{W_1} [L(|\omega W_g|)]^l \left\{\left|P_l^{(+)}\left(\frac{1}{\omega W_g}\right)\cdot P_l^{(-)}\left(\frac{1}{\omega W_1}\right)\right| + \left|P_l^{(+)}\left(\frac{1}{\omega W_1}\right) P_l^{(-)}\left(\frac{1}{\omega W_g}\right)\right|\right\}\right]_{D_0}, \tag{2.27}$$

where $\bar{C}$ appears in (2.13) while the notations Δ, D_0 mean that W_1 belongs to the respective domains.

We want to prove that quite analogous properties hold for $u_-^{(n+1)}$, which is defined by choosing the integration path in (2.2) to coincide with the interval $W_g \leq W_1 \leq W_g(r_0)$ plus the boundary line of D_0 for which $\arg(W_1 - W_g(r_0)) = \pi/2$.

Then let us write (2.2) as a sum of two parts A, B:

$$A = \int_{W_g}^{W_g(r_0)} I(W_g, W_1)\, dW_1, \quad B = \int_{W_g(r_0)}^{\infty} I(W_g, W_1)\, dW_1 . \tag{2.28}$$

As regards the first part we take W_1 to be real, so that (2.13) can be applied together with the relation $|V_{11}\exp(\nu-\lambda)| < C$. Then in the case $\mathrm{Im}\omega < 0$, for example, by making use of (2.25) we obtain

$$|A| < \left|\frac{\exp\{i\omega[2W_g(r_0) - W_g]\}}{\omega^{n+1}}\right| |\phi_g| C_0 C_2^n C_3 [L(|\omega W_g|)]^{-l}, \tag{2.29}$$

where C_3 is a constant which majorizes the first term of (2.27).

As regards the second part, taking into account (2.14), (2.15), and (2.19), we can write the integrand in the form

$$I(W_g, W_1) = \frac{1}{\omega^{n+1}}\{\alpha(W_g, W_1)\exp(i\omega W_g) + \beta(W_g, W_1)\exp[i\omega(2W_1 - W_g)]\}, \tag{2.30}$$

where α and β do not contain exponentials. For $\mathrm{Im}\omega < 0$ $I(W_g, W_1)$ is analytical for W_1 in D_0 and for $W_1 \to \infty$ along any line in the same domain.

Then we shall choose the line $\arg(W_1 - W_g(r_0)) = \pi/2$ as integration path. In this way $u_-^{(n+1)}$ can be analytically continued to the region $\mathrm{Im}\omega < 0$. In this case indeed we can write

$$I = \frac{\exp\{i\omega[2W_g(r_0) - W_g]\}}{\omega^{n+1}}(\alpha\exp\{2i\omega[W_g - W_g(r_0)]\} + \beta\exp\{2i\omega[W_1 - W_g(r_0)]\}), \tag{2.31}$$

where the exponentials involved in the curly brackets are majorized by unity. Furthermore, taking into account (2.10), (2.19), (2.20), we get

$$|B| \leq \left|\frac{\exp\{i\omega[2W_g(r_0) - W_g]\}}{\omega^{n+1}}\right| \times |\phi_g| C_0 \left(\frac{\pi C_1}{W_g(r_0)}\right)^n C_4 [L(|\omega W_g|)]^{-l}, \tag{2.32}$$

where C_4 majorizes the last two terms in (2.27). Observing that $C_2 \geq C_1/W_g(r_0)$ and $C_2 \geq C_3 + C_4$, we obtain

$$|A+B| \leq |A| + |B| \leq \left|\frac{\exp\{i\omega[2W_g(r_0) - W_g]\}}{\omega^{n+1}}\right| |\phi_g| C_0 C_2^{n+1} [L(|\omega W_g|)]^{-l}, \tag{2.33}$$

so that our statement is proved.

3. ANALYTICAL CONTINUATION AND ASYMPTOTIC EVALUATION FOR $|\omega| \to \infty$ OF THE WRONSKIAN $W(u, u_-)$

We want now to obtain the continuation to the region $\mathrm{Im}\omega < 0$ of the Wronskian $W(u, u_-)$ where u is the physical internal solution. This is given by (II.7.1), (II.7.2), (II.7.3), (II.7.5). Introducing (II.7.5) in (II.7.3), one can write for $\mathrm{Im}\omega \geq 0$

$$\Gamma(\omega) = \sum_{n=0}^{\infty}\left(\int_0^{W_g(r_0)} \exp(\nu-\lambda)\bar{j}_l(\omega W_g) V_{11}\frac{u_-^{(n)}}{\phi_g}\, dW_g - \frac{1}{2i}\int_{W_g(r_0)}^{\infty} \exp(\nu-\lambda)\bar{h}_l^{(-)}(\omega W_g)\frac{u_-^{(n)}}{\phi_g} V_{11}\, dW_g + \frac{1}{2i}\exp[2i\omega W_g(r_0)]\int_{W_g(r_0)}^{\infty}[\exp(\nu-\lambda)]\bar{h}_l^{(+)}(\omega W_g) \times \frac{u_-^{(n)}}{\phi_g}\{\exp[-2i\omega W_g(r_0)]\} V_{11}\, dW_g\right). \tag{3.1}$$

An alternative definition of $\Gamma(\omega)$ for $\mathrm{Im}\omega \geq 0$ is obtained by rotating the integration path for the third integral just in the same way as that used for $u_-^{(n+1)}$ in the previous section, in the case $W_g = W_g(r_0)$. The proof is quite similar to that given for $u_-^{(n+1)}$ and will be omitted here. The new integration path lies in D_0, where it is specified by the condition $\arg(W_g - W_g(r_0)) = \pi/2$. With such a choice also the third integral in (3.1) converges for $\mathrm{Im}\omega < 0$. As regards the second integral, we note that, since $|\bar{h}_l^{(-)} u_-^{(n)}| < C/|\omega|^n$, the above path rotation can be performed altogether. In this way we obtain

$$\Gamma(\omega) = \sum_{n=0}^{\infty}\left[\int_0^{W_g(r_0)} F^{(n)}(W_g;\omega)\, dW_g + \int_{W_g(r_0)}^{W_g(r_0)+i\infty} F^{(n)}(W_g;\omega)\, dW_g\right],$$

$$F^{(n)} = \exp(\nu-\lambda)\bar{j}_l V_{11} u_-/\phi_g . \tag{3.2}$$

This provides the desired analytical continuation of $\Gamma(\omega)$.

We want now to obtain a majorization for the remainder $R^{(m)}$ of $\Gamma(\omega)$, defined by an expression similar to the above one, where n runs from m to infinity.

To this aim we recall that

(i) $|P_l^{(\pm)}|$, which appear in (2.13), are majorized by C;

(ii) $\sum_{n=m}^{\infty} x^n = x^m/1 - x$ $(|x| < 1)$.

Then let us introduce in the first integral Eq. (2.22)

or (2.23) according to the case and (2.17) in the other two integrals; taking into account (2.24) together with the relation $|V_{11}\exp(\nu-\lambda)|<C$, (2.18) together with (2.10) and recalling the points (i) and (ii) with $x=C_2/\omega$ or $x=\pi C_1/[\omega W_g(r_0)]$ according to the case, we obtain straightforwardly

$$|R^{(m)}|<\frac{C^{m+1}}{\omega^m}\exp(-2\,\mathrm{Im}\omega W_g(r_0)). \tag{3.3}$$

As specified in Sec. 1, in order to obtain the eigenfrequency distribution it is necessary to evaluate $\Gamma(-\omega)$. In order to do this, consider the first term in (3.2) [where $u_-^{(0)}=\phi_g\bar{h}_l^{(+)}(\omega,W_g)$]

$$\Gamma^{(0)}=\Gamma_{\mathrm{int}}^{(0)}+\Gamma_{\mathrm{ext}}^{(0)},\quad \Gamma_{\mathrm{int}}^{0}=\int_0^{W_g(r_0)}\exp(\nu-\lambda)\,V_{11}\bar{j}_l\bar{h}_l^{(+)}\,dW_g,$$

$$\Gamma_{\mathrm{ext}}^{(0)}=\int_{W_g(r_0)}^{W_g(r_0)+i\infty}\exp(\nu-\lambda)\,V_{11}\bar{j}_l\bar{h}_l^{(+)}\,dW_g\,; \tag{3.4}$$

the evaluation of $\Gamma_{\mathrm{ext}}^{(0)}$ can be performed by means of the integration techniques given in Paper II. These allow us to develop it into the successive approximations for $\omega\to\infty$ according to (II.A7); the mth approximation reads

$$\Gamma_{\mathrm{ext}}^{(0)}=\sum_{n=0}^{m}\left[a_{\mathrm{ext}}^{(n)}\bar{j}_l\bar{h}_l^{(+)}+b_{\mathrm{ext}}^{(n)}\bar{j}_{l+1}\bar{h}_l^{(+)}+c_{\mathrm{ext}}^{(n)}\bar{j}_l\bar{h}_{l+1}^{(+)}\right.$$
$$\left.+d_{\mathrm{ext}}^{(n)}\bar{j}_{l+1}\bar{h}_{l+1}^{(+)}\right]_{W_g(r_0)}^{W_g(r_0)+i\infty}+R_{\mathrm{ext}}^{(m)}, \tag{3.5}$$

where $R_{\mathrm{ext}}^{(m)}$ is the remainder expressed by

$$R_{\mathrm{ext}}^{(m)}=\int_{W_g(r_0)}^{W_g(r_0)+i\infty}B^{(m+1)}(\bar{j}_{l+1}\bar{h}_l^{(+)}+\bar{j}_l\bar{h}_{l+1})\,dW_g, \tag{3.6}$$

$$B^{(m+1)}=\frac{-1}{4\omega}\frac{d}{dW_g}\left[f^{(m)}-\frac{2l+2}{W_g}\int_0^{W_g}f^{(m)}\,dW_g^1\right], \tag{3.7}$$

$$f^{(m)}=\delta_{m,0}\exp(\nu-\lambda)\,V_{11}+(1-\delta_{m,0})\left[\frac{2l+2}{\omega W_g}+\frac{1}{\omega}\frac{d}{dW_g}\right]B^{(m)}; \tag{3.8}$$

$R_{\mathrm{ext}}^{(m)}$ factorizes at least $1/\omega^m$ as can be seen by inspection.

The above approximation method cannot be used up to calculate $\Gamma_{\mathrm{int}}^{(0)}$ when the polytropic index N, appearing in (2.11) is in the interval $0<N<1$. The reason lies in the fact that, in such case, for $r\to r_0$, V_{11} behaves as $\sim(r_0-r)^{N-1}$, so that the remainder $R_{\mathrm{int}}^{(0)}$ analogous to that appearing in (3.5), would diverge.

For $0<N<1$, $\Gamma_{\mathrm{int}}^{(0)}(\omega)$ is calculated according to the method developed in the Appendix. The result is

$$\Gamma_{\mathrm{int}}^{(0)}(-\omega)\simeq\frac{(-1)^l}{2i}k_0\exp[-2i\omega W_g(r_0)]\,\frac{\Gamma(N)}{(-2i\omega)^N}, \tag{3.9}$$

where k_0 is defined by (2.11) and $\Gamma(N)$ is the Euler function.

Furthermore, the explicit asymptotic evaluation of $\Gamma_{\mathrm{ext}}^{(0)}$ with $m=0$ together with a straightforward majorization of $R_{\mathrm{ext}}^{(0)}$ shows that $\Gamma_{\mathrm{ext}}^{(0)}\ll\Gamma_{\mathrm{int}}^{(0)}$, so that

$$\Gamma^{(0)}(-\omega)\simeq\Gamma_{\mathrm{int}}^{(0)}(-\omega)\quad(0<N<1). \tag{3.10}$$

In the case $N>1$, $\Gamma_{\mathrm{int}}^{(0)}$ may be calculated in the same way as $\Gamma_{\mathrm{ext}}^{(0)}$

$$\Gamma_{\mathrm{int}}^{(0)}=\sum_{n=0}^{m}\left[a^{(n)}\bar{j}_l\bar{h}_l^{(+)}+b^{(n)}\bar{j}_{l+1}\bar{h}_l^{(+)}+c^{(n)}\bar{j}_l\bar{h}_l^{(+)}\right.$$
$$\left.+d^{(n)}\bar{j}_{l+1}\bar{h}_{l+1}^{(+)}\right]_0^{W_g(r_0)}+R_{\mathrm{int}}^{(m)}, \tag{3.11}$$

$$R_{\mathrm{int}}^{(m)}=\int_0^{W_g(r_0)}B^{(m+1)}(\bar{j}_l\bar{h}_{l+1}^{(+)}+\bar{j}_{l+1}\bar{h}_l^{(+)})\,dW_g\,; \tag{3.12}$$

however, the approximation procedure can be applied only up to the largest $m=\bar{m}$ such that

$$0<N-1-\bar{m}<1; \tag{3.13}$$

indeed, owing to (2.11), (3.7), and (3.8),

$$B^{(\bar{m}+1)}\underset{r\to r_0}{\simeq}(r_0-r)^{N-1-(2\bar{m}+1)}$$

so that the integrand in $R_{\mathrm{int}}^{(\bar{m})}$ diverges. However, $R_{\mathrm{int}}^{(\bar{m})}$ can be asymptotically evaluated with the method already used for $\Gamma_{\mathrm{int}}^{(0)}$ in the case $0<N<1$. So we obtain

$$R_{\mathrm{int}}^{(\bar{m})}(-\omega)\underset{\omega\to\infty}{\simeq}\frac{(-1)^{l+1}}{2i}\,k_0\exp[-2i\omega W_g(r_0)]\,\frac{\Gamma(N)}{(-2i\omega)^N}. \tag{3.14}$$

Note that the above expression is independent of $\bar{m}$. We are now in position to calculate $\Gamma^{(0)}(\omega)$ in the case $N>1$. We observe that the upper limit of the summation appearing in (3.11) cancels the corresponding one in (3.5) since the coefficients are continuous in r_0 up to the order $\bar{m}$. On the other hand, no contribution arises from the limits $W_g=0$ and $W_g=W_g(r_0)+i\infty$.

In this way we are left with the remainders only, so that

$$\Gamma^{(0)}(-\omega)\underset{\omega\to\infty}{\simeq}R_{\mathrm{ext}}^{(\bar{m})}(-\omega)+R_{\mathrm{int}}^{(\bar{m})}(-\omega). \tag{3.15}$$

With a straightforward procedure similar to that which leads to the inequality $\Gamma_{\mathrm{ext}}^{(0)}\ll\Gamma_{\mathrm{int}}^{(0)}$ in the case $0<N<1$ one can show that $R_{\mathrm{ext}}^{(\bar{m})}(-\omega)\ll R_{\mathrm{int}}^{(\bar{m})}(-\omega)$; so we have

$$\Gamma^{(0)}(-\omega)\underset{\omega\to\infty}{\simeq}R_{\mathrm{int}}^{(\bar{m})}(-\omega). \tag{3.16}$$

Moreover, let us denote with T_k the contribution of the kth iteration $u_-^{(k)}$ to the second term T in the rhs of (II.7.1).

In Paper II, on the basis of the assumption (II.7.4), in the limit $\omega\to\infty$, we could deduce that

$$\left|\sum_{k=1}^{\infty}T_k\right|\ll|T_0|; \tag{3.17}$$

so the asymptotic contribution to T arises from the lowest order iteration $u_-^{(0)}$. On the other hand in the present context, a direct analytical continuation of $u_-^{(k)}$ has been achieved and the above assumption is avoided. However, making use of (2.25) and (2.26) (with a procedure quite similar to that followed in Sec. 7 of Paper II) one can see that the inequality (3.17) for $r=r_0$ holds altogether. So the contribution to the Wronskian arising from T, for $r=r_0$, is asymptotically the same as in Paper II. Collecting the results, for $W(-\omega)$ we have [see (II.7.1), (II.7.2), (II.7.5)]

$$[W(-\omega)]_{r_0}\simeq\omega[\phi_g^2\exp((\nu-\lambda)/2)]_{r_0}$$
$$\times\left[1-\frac{\Gamma(-\omega)}{\omega}+\exp[-2i\omega W_g(r_0)]\,\frac{\alpha}{i\omega^{11}},\right]$$

$$\frac{\Gamma(-\omega)}{\omega} = \epsilon(N-1)(-1)^{l+1} k_0 \times \exp[-2i\omega W_g(r_0)]\ \Gamma(N)/(-2i\omega)^{N+1}, \qquad (3.18)$$

where α is given by (II.7.13), N is noninteger, $\Gamma(N)$ and $\epsilon(x)$ are respectively the Euler and the sign function.

4. FINAL REMARKS

The equation $W(-\omega)=0$ which gives the eigenfrequencies, in the present context has an additional term in comparison with (II.7.12). As seen from (3.18), the results of Paper II remain valid if $N \gtrsim 10$.

If $N < 10$ the second term in (3.18) is the leading one; so in this case the asymptotic eigenfrequency distribution depends on the self-coupling term V_{11} of the gravitational field [see (2.11)] rather than on the coupling terms V_{12} and V_{21} between the matter and the gravitational field [which are contained in the constant α]. However, such distribution is qualitatively the same as in the case $N < 10$.

$$\mathrm{Re}\omega_n \simeq \frac{(2n+\frac{1}{2})\pi + \arg\bar{\alpha}}{2W_g(r_0)}, \qquad (4.1)$$

$$\mathrm{Im}\omega_n \simeq \frac{(N+1)\ln|\mathrm{Re}\omega_n| - \ln|\bar{\alpha}|}{2W_g(r_0)}, \qquad (4.2)$$

$$\bar{\alpha} = \tfrac{1}{2}\epsilon(N-1)\ \frac{(-1)^{l+1}}{(-2i)^N}\ k_0\Gamma(N); \qquad (4.3)$$

in particular we note that the zeroes of $W(-\omega)$ are in any case simple.

Finally, we want to point out that the above method to obtain the analytical continuation of the external solution to the lower half ω plane is probably extensible to the Kerr metric.

APPENDIX

A simple majorization of $\Gamma(-\omega)/\omega$, of the same type as those already used in Papers I and II, shows that

$$\left|\frac{\Gamma(-\omega)}{\omega}\right| < C\ \frac{\exp[2\,\mathrm{Im}\omega W_g(r_0)]}{|\omega|} \quad (\mathrm{Im}\omega > 0). \qquad (A1)$$

So the second term in the rhs of (3.18) may be significant for $\omega \to \infty$ only if

$$\mathrm{Im}\omega \gtrsim \frac{1}{2W_g(r_0)}\ \ln|\omega|. \qquad (A2)$$

Since we are interested in a possible modification of the eigenfrequencies distribution obtained on the basis of (II.7.12), we will consider values of ω for which the above inequality is verified.

In order to evaluate $\Gamma(-\omega)$, for $\omega \to \infty$ and $N < 1$, let us split the first integral in (3.4) as follows:

$$\int_0^{W_g(r_0)} I\,dW_g = \int_0^{\lambda} I\,dW_g + \int_{\lambda}^{W_g(r_0)} I\,dW_g, \qquad (A3)$$

$$W_g(r_0) - \lambda = \Delta = \frac{W_g(r_0)}{\ln|\omega|}. \qquad (A4)$$

Since Δ vanishes in the limit $\omega \to \infty$, in the second integral on rhs of (A3) we can replace for the integrand I its asymptotic expression I_0 for $r \to r_0$ and $\omega \to \infty$. So, retaining the exponential terms only in the product $\bar{j}_l \bar{h}_l^{(+)}$, we have

$$I \simeq I_0 = \frac{k_0 \exp(-2i\omega W_g)}{[W_g(r_0) - W_g]^{1-N}}, \qquad (A5)$$

k_0 being defined by (2.11); then

$$\int_{\lambda}^{W_g(r_0)} I\,dW_g \simeq \int^{W_g(r_0)} I_0\,dW_g; \qquad (A6)$$

moreover, we have

$$\frac{\exp(2i\omega W_g(r_0))}{k_0}\int_{\lambda}^{W_g(r_0)} I_0\,dW_g = \int_{\lambda}^{W_g(r_0)} \frac{\exp\{2i\omega[W_g(r_0) - W_g]\}}{[W_g(r_0) - W_g]^{1-N}}\,dW_g = \frac{1}{(-2i\omega)^N}\int_0^{-2i\omega\Delta} \exp(-l)\,l^{N-1}\,dl = \frac{1}{(-2i\omega)^N}\,\gamma(N, -2i\omega\Delta) \underset{\omega\to\infty}{\simeq} \frac{1}{(-2i\omega)^N}\,\Gamma(N), \qquad (A7)$$

$\gamma(x, y)$ being the incomplete gamma function; the last step is justified by the fact that $\omega\Delta \gg 1$, owing to (A4).

As regards the first integral of rhs of (A3), we can use up (II.A22) since in the integrand, in the interval $(0, \lambda)$, the coefficient of Bessel functions is finite, together with its derivative with respect to W_g. By straightforward majorizations one can see that, for $\omega \to \infty$, such an integral can be written as

$$\int_0^{\lambda} I\,dW_g = \exp[-2i\omega W_g(r_0)]\sum_k A_k, \qquad (A8)$$

where

$$|A_k| < \frac{C}{|\omega|^N(\ln|\omega|)^{1-N}}. \qquad (A9)$$

So the leading contribution, for $\omega \to \infty$ to the given integral (A3) arises from the interval $(\lambda, W_g(r_0))$ as seen by comparing (A8) and (A9) with (A6) and (A7).

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Stochastic systems and integral inequalities [a)]

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A stochastic control system of the form

$dx = F(t,x)dt + G(t,x)d\beta(t) + \zeta_1(t)dt + \zeta_2(t)d\beta(t)$,

$t \in R_+ \equiv (0,\infty)$, $x, F, \zeta_1 \in R^n$,

G and ζ_2 are $n \times p$ matrix-valued functions, and $\beta(t)$ is a p-dimensional Brownian motion process, is investigated. Utilizing stochastic Lyapunov functions and the theory of stochastic integral inequalities, conditions are stated under which the above stochastic control is *integrally stable in the mean* and *asymptotically integrally stable in the mean*. Conditions are also developed for the stochastic differential system in finite time to be *mean stable, uniformly stable in mean, quasiexpansively stable in the mean,* and *quasicontractively stable in the mean*.

I. INTRODUCTION

The object of the present study is to consider the stochastic control system of the form

$$dz = F(t,z)dt + G(t,z)d\beta(t) + \zeta_1(t)dt + \zeta_2(t)d\beta(t), \quad (1.1)$$

where

(i) $t \in R_+ \equiv [0,\infty]$,

(ii) $z, F, \zeta_1 \in R^n$,

(iii) G and ζ_2 are $n \times p$ matrix valued functions,

(iv) $\beta(t)$ is a standard p-dimensional Brownian motion process.

The function $\zeta_1(t)$ can be construed as a control variable and $\zeta_2(t)d\beta(t)$ a stochastic noise. The aim of the present investigation is to obtain sufficient conditions under which the system is stable in a probabilistic setting. These type of problems have been considered in a deterministic setting by Bellman,[1] Barbasin,[2] Liberman,[3] Kayande and Muley,[4] Lakshmikantham and Tsokos,[5] among others. Our results are natural extensions to the systems in their probabilistic behavior.

The necessary preliminary mathematical assumptions will be stated along with the definitions of the types of stabilities to be investigated in Sec. 2. In particular we will consider criteria for the stochastic differential control system to be *integrally stable in the mean* and *asymptotically integrally stable in the mean* in Sec. 3. In Sec. 4 we will present criteria for the stochastic differential system to be *finite time mean stable, uniformly stable in mean, quasiexpansively stable in the mean,* and *quasicontractively stable in the mean*.

2. PRELIMINARIES

We shall consider the stochastic control system (1.1) subject to the following conditions:

(a) There exists a probability measure space (Ω, A, P) with sample points ω and a set of σ-algebras $\{A_t\}$ in A such that:

(i) $A_s \subset A_t$ for $s < t$,

(ii) $\beta(t;\omega)$ is measurable with respect to A_t and $[\beta(t+h;\omega) - \beta(t;\omega)]$ $(h > 0)$ is independent of A_t.

(b) $F(t,x)$ and $G(t,x)$, ζ_1 and ζ_2 are continuous and $\|F(t,x) - F(t,y)\| + \|G(t,x) - G(t,y)\| \leq K\|x - y\|$ for some constant $K > 0$; here $\|\cdot\|$ denotes the Euclidean norm of a vector or a matrix.

Under the above conditions, it is known[6] that the system (1.1) has a unique random solution which is a separable second-order random process and that the random solution is almost surely continuous.

Corresponding to the stochastic differential system (1.1), we shall have need to consider the comparison scalar differential equation of the form

$$u'(t) = g(t, u + \xi(t)), \quad u(t_0) = u_0. \quad (2.1)$$

We shall assume that Eq. (2.1) has global solutions and $g(t,0) \equiv 0$.

The function $g(t,u) \in C[R_+ \times R, R]$ is said to belong to the class Γ if, for each $t \in R_+$, g is monotone increasing and concave in u.

We shall utilize the following stochastic stability definitions in presenting our main results.

Definition 2.1: The stochastic differential control system (1.1) is *integrally stable in the mean* if for any $\alpha > 0$, $t_0 \in R_+$, $T > 0$ there is $\beta = \beta(\alpha) > 0$ such that, for any solution $z(t)$ with control ζ_1 of the stochastic control system (1.1), the inequality

$$E\|z(t)\| < \alpha$$

holds for $t \in [t_0, t_0 + T)$, whenever

$$\|z_0\| < \beta \quad \text{and} \quad \int_{t_0}^{t_0+T} (\|\zeta_1(s)\| + \|\zeta_2(s)\|^2)\,ds < \beta.$$

Definition 2.2: The stochastic differential control system (1.1) is *asymptotically integrally stable in the mean* if it is integrally stable in the mean and if for every solution $z(t)$ with controls ζ_1 and for every $\epsilon > 0$, $t_0 \in R_+$, there exists two numbers $T = T(\alpha,\epsilon)$ and $\lambda = \lambda(\alpha,\epsilon)$ such that the inequality

$$E\|z(t)\| < \epsilon$$

holds for $t \geq t_0 + T$, provided

$$\|z_0\| < \alpha \quad \text{and} \quad \int_{t_0}^{\infty} (\|\zeta_1(s)\| + \|\zeta_2(s)\| + \|\zeta^2(s)\|)\,ds < \lambda.$$

We now introduce the following functions. Let V be

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a map from $R_+ \times R^n$ into R_+. Define

$$D^* E_{t,z}[V(t,z)] \equiv \limsup_{h \to 0^+} (1/h) E\{[V(t+h, z + hF(t,z) + G(t,z)(\beta(t+h) - \beta(t))] - V(t,z) \mid z\}, \tag{2.2}$$

subject to the condition that there exist constants K_1 and K_2, positive, such that

$$V(t,z) \leq K_1 \|z\| + K_2 \|z\|^2.$$

In what follows we shall use the notation that $F = \{t \in R_+ : t \in [t_0, t_0 + T) \text{ and } T > 0\}$, and we shall denote $\tilde{F} = \{t \in R_+ : t \in [t_0, t_0 + T] \text{ and } T > 0\}$. We shall further use the following notation:

$$B(a) = \{z(\omega) : E\|z(\omega)\| < a\}, \quad \bar{B}(a) = \{z(\omega) : E\|z(\omega)\| \leq a\}.$$

A function V is said to belong to the class Λ if, for each $t \in \tilde{F}$, $V = V(t,z) : C[\tilde{F} \times R^n, R]$ is continuously differentiable in z such that

$$V(t,z_1) - V(t,z_2) \leq \frac{\partial V}{\partial z}(t,z_2)(z_1 - z_2) + \phi(t)\|z_1 - z_2\|^2,$$

where $\phi(t) \in C[\tilde{F}, R]$ and $z_1, z_2 \in B(\beta) - B(\alpha)$ $(0 \leq \alpha < \beta)$.

We shall also let

$$V_m^{\alpha}(t) = \inf_{\{z(t;\omega) : E\|z\| = \alpha\}} E[V(t,z)],$$

$$V_M^{\alpha}(t) = \sup_{\{z(t;\omega) : E\|z\| = \alpha\}} E[V(t,z)],$$

$$V^{\alpha}(t) = \sup_{\{z(t;\omega) : E\|z\| < \alpha\}} E[V(t,z)],$$

$$V_{\delta}^{\alpha}(t) = \sup_{z \in \bar{B}(\alpha) - B(\delta)} E[V(t,z)],$$

with $\delta < \alpha$.

The following definitions will be needed when we consider stability properties in finite time for the random differential system (1.1).

Definition 2.3: The stochastic differential control system (1.1) is said to be *mean stable* if, for $\gamma > 0$, $t_0 \in R_+$, $T > 0$, there exists α and ζ_1 where $0 < \alpha \leq \gamma$ and $\zeta_1(t) \in C[F, R^n]$ such that

$$\|z(t_0)\| < \alpha$$

implies

$$E\|z(t)\| < \gamma \quad \text{for all } t \geq t_0,\ t \in F,$$

for every solution $z(t)$ with control $\zeta_1(t)$.

Definition 2.4. The stochastic differential control system (1.1) is said to be *uniformly stable in mean* if for $\gamma > 0$, $t_0 \in R_+$, $T > 0$, there exist α and ζ_1 where $0 < \alpha \leq \gamma$ and $\zeta_1(t) \in C[F, R^n]$ such that

$$\|z(t_1)\| < \alpha$$

implies

$$E\|z(t)\| < \gamma \quad \text{for all } t \geq t_1,\ t, t_1 \in F,$$

for every solution $z(t)$ of the stochastic control system (1.1) with control $\zeta_1(t)$.

Definition 2.5: The stachastic differential control system (1.1) is said to be *quasiexpensively stable in mean* if for $\beta > 0$, $t_0 \in R_+$, $T > 0$, there exist α, t_1, and ζ_1, where $0 < \alpha \leq \beta$ and $\zeta_1(t) \in C[F, R^n]$ such that

$$\|z(t_0)\| < \alpha$$

implies

$$E\|z(t)\| < \beta \quad \text{for } t \in (t_1, t_0 + T)$$

for every solution $z(t)$ of the stochastic control system (1.1) with control $\zeta_1(t)$.

Definition 2.6: The stachastic differential control system (1.1) is said to be *expansively stable in mean* if for $\beta > 0$, $\gamma > 0$, $t_0 \in R_+$, $T > 0$, where $\beta < \gamma$, it is mean stable and quasiexpansively stable in mean with $\alpha \leq \beta < \gamma$.

Definition 2.7: The stochastic differential control system (1.1) is said to be *quasicontractively stable in mean* if for $\beta > 0$, $t_0 \in R_+$, $T > 0$ there exists α, t_1, ζ_1, where $\alpha > \beta$ and $\zeta_1(t) \in C[F, R^n]$ such that

$$\|z(t_0)\| < \alpha$$

implies

$$E\|z(t)\| < \beta \quad \text{for } t \in (t_1, t_0 + T),$$

for every solution $z(t)$ of the stochastic control system (1.1) with control ζ_1.

Definition 2.8: The stochastic differential control system is said to be *contractively stable in mean* if for $\beta > 0$, $\gamma > 0$, $t_0 \in R_+$, $T > 0$, where $\beta < \gamma$, it is mean stable and quasicontractively stable in mean with $\beta < \alpha \leq \gamma$.

The following notation will be used when we consider the finite time stabilities. The function $g(t,u) \in C[\tilde{F} \times R, R]$ is said to belong to the class Γ' if, for each $t \in \tilde{F}$, g is monotone increasing and concave in u, and it is smooth enough to insure a maximal solution of the scalar differential equation (2.1), where $\xi(t)$ is a continuous function over $\tilde{F}$.

We shall now state a lemma which will be used in presenting our results.

Lemma 2.1: If

$$u(t) \leq \xi(t) + \int_{t_0}^{t} g(s, u(s))ds + u(t_0), \tag{2.3}$$

where $g \in \Gamma$, $u(t)$ and $\xi(t)$ are continuous for $t \in R_+$, then

$$u(t) \leq \xi(t) + r(t, t_0, u_0), \tag{2.4}$$

where $r(t, t_0, u_0)$ is the maximal solution of (2.1) through $(t_0, u(t_0))$.

The proof of the Lemma 2.1 can be found in Ref. 7.

3. STABILITY PROPERTIES OF THE STOCHASTIC DIFFERENTIAL SYSTEM

We shall now present a theorem concerning the integral stability in the mean and the asymptotic integral stability in the mean of the stochastic system (1.1).

Theorem 3.1: Suppose that there exists functions g, V, a, and b satisfying the following conditions:

(i) $g(t,u)\in C[R_+\times R, R]$ and g is concave in u for each t.

(ii) $V(t,z)\in C[R_+\times R^n, R_+]$ continuously differentiable in z for each t such that

$$V(t,z_1)-V(t,z_2)\leq \frac{\partial V}{\partial z}(t,z_2)(z_1-z_2)+M_1\|z_1-z_2\|^2,$$

where M_1 is a positive constant.

(iii) Let $\partial V/\partial z\equiv W(t,z)$. Then

$$\limsup_{h\to 0^+}(1/h)\times\{E\|W(t,z+hF(t,z)+G(t,z)\times(\beta(t+h)-\beta(t))-W(t,z)\|^2\,|\,z\}<\infty.$$

(iv) For $t\in R_+$, $\|z(t;w)\|<\rho$,

$$\limsup_{h\to 0^+}(1/h)\times E[W(t,z(t)+hF(t,z(t))+G(t,z(t))(\beta(t+h)-\beta(t)))\|\|(\beta(t+h)-\beta(t)\|z(t)]\leq M_2,$$

where M_2 is a positive constant and

$$\sup_{\|z\|<\rho}\|W(t,z)\|\leq M_3,\quad \text{where } M_3>0$$

and for $\|z\|\geq\rho$ there exists $K_1,K_2>0$ such that

$$V(t,z)\leq K_1\|z\|+K_2\|z\|^2.$$

(v) Let $\xi(t)$ in Eq. (2.1) be such that

$$\xi(t)=M(\|\zeta_1(t)\|+\|\zeta_2(t)\|+\|\zeta_2(t)\|^2)$$

with

$$M=\max(M_1,M_2,M_3).$$

(vi) $D^+E_{t,z}\{V(t,z)\}\leq g(t,V(t,z))-\xi(t)$.

(vii) There exists functions a and $b\in K$ such that

$$b(\|z\|)\leq V(t,z)\leq a(\|z\|).$$

(viii) $V(t_0,z_0)=u(t_0)$.

Then

(1) the uniform-integral stability of (2.1)[5] implies the integral stability in the mean of (1.1);

(2) the quasiasymptotic uniform integral stability of (2.1)[5] implies the asymptotic integral stability in the mean of (1.1).

Remark: It has been shown[6] that if V is twice continuously differentiable such that

$$|V|+|V_t|+\|z\|\,\|V_z\|+\|z\|^2\|V_{zz}\|\leq K(1+\|z\|^2)$$

where $V_z=\partial V/\partial z$, $V_t=\partial V/\partial t$, and $V_{zz}=\partial^2 V/\partial z^2$, then

$$D^+E_{t,z}(V)=\sum_i F_i\frac{\partial V_i}{\partial z_i}+\tfrac{1}{2}\sum_{i,j}(GG^T)_{i,j}\frac{\partial^2 V}{\partial z_i\partial z_j}+\frac{\partial V}{\partial t}.$$

In this case it can be shown that V, V_t, and V_z satisfy the condition of the theorem.

Proof: we shall first prove (1). For notational convenience denote

$$d\beta(t)\equiv\beta(t+h;\omega)-\beta(t;\omega).$$

Let $z(t)$ be any solution of the differential system (1.1). Then using the assumption (ii), we have

$$\begin{aligned}V(t+h,z(t)+hF(t,z(t))+G(t,z(t))d\beta(t)+h\zeta_1(t)&\\+\zeta_2(t)d\beta(t))-V(t+h,z(t)+hF(t,z(t))+G(t,z(t))d\beta(t))&\\\leq W(t+h,z(t)+hF(t,z(t))+G(t,z(t))d\beta(t))(h\zeta_1(t)&\\+\zeta_2(t)d\beta(t))+M_1\|h\zeta_1(t)+\zeta_2(t)d\beta(t)\|^2.&\qquad(3.1)\end{aligned}$$

In view of our assumption (iv) we obtain

$$\begin{aligned}\limsup_{h\to 0^+}(1/h)E[V(t+h,z(t)+hF(t,z(t)&\\+G(t,z(t))d\beta(t)+h\zeta_1(t)+\zeta_2(t)d\beta(t))&\\-V(t+h,z(t)+hF(t,z(t))+G(t,z(t))d\beta(t))\,|\,z(t)]&\\\leq M_3\|\zeta_1(t)\|+(M_1\|\zeta_2(t)\|+M_2)\|\zeta_2(t)\|&\\\leq M[\|\zeta_1(t)\|+\|\zeta_2(t)\|\,\|\zeta_2(t)\|^2]=\xi(t).&\qquad(3.2)\end{aligned}$$

Hence

$$\begin{aligned}D^+E_{t,z}[V(t,z)]_{1,1}&\\\equiv\limsup_{h\to 0^+}(1/h)E[V(t+h,z(t)+hF(t,z(t))&\\+G(t,z(t))d\beta(t)+h\zeta_1(t)+\zeta_2(t)d\beta(t))-V(t,z(t))\,|\,z(t)]&\\=\limsup_{h\to 0^+}(1/h)E[V(t+h,z(t)+hF(t,z(t))&\\+G(t,z(t))d\beta(t)+h\zeta_1(t)+\zeta_2(t)d\beta(t))&\\-V(t+h,z(t)+hF(t,z(t))+G(t,z(t))d\beta(t))\,|\,z(t)]&\\+\limsup_{h\to 0^+}(1/h)E[V(t+h,z(t)+hF(t,z(t))&\\+G(t,z(t))d\beta(t))-V(t,z(t))\,|\,z(t)].&\end{aligned}$$

Now using Eqs. (2.2) and (3.2) above, we have

$$D^+E_{t,z}[V(t,z)]_{1,1}\leq\xi(t)+D^+E_{t,z}(V(t,z)),\qquad(3.3)$$

and, by condition (vi), (3.3) becomes

$$D^+E_{t,z}[V(t,z)]_{1,1}\leq g(t,V(t,z)).\qquad(3.4)$$

Hence from the inequality (3.4) we obtain the integral inequality

$$E_{t,z}[V(t,z)]-V(t_0,z_0)]\leq\int_{t_0}^t g(s,V(s,z))ds.$$

And since g is concave in u for each t by condition (i), we have, taking the expected value which exists by (iv),

$$\begin{aligned}E[V(t,z)]-V(t_0,z_0)&\leq E\int_{t_0}^t g(s,V(s,z))ds.\\&\leq\int_{t_0}^t g(s,E(V(s,z)))ds.\end{aligned}$$

Now by lemma (2.1) and by condition (viii) it follows that

$$E[V(t,z(t))]\leq r(t,t_0,u_0),\qquad(3.5)$$

where $r(t,t_0,u_0)$ is the maximal solution of (2.1) with $\xi(t)\equiv 0$ through $(t_0,u(t_0))$. Now by assumption (vii) of the theorem, the above inequality (3.5) implies

$$E(\|z(t)\|)\leq b^{-1}(r(t,t_0,u_0)).\qquad(3.6)$$

Let $\alpha > 0$ be given. Choose

$$\alpha_1 < b(\alpha). \tag{3.7}$$

Since the system (2.1) is uniformly-integrally stable, there exists a $\lambda_1 = \lambda_1(\alpha)$ such that for any $t_0 \in R_+$ and for any solution $r(t, t_0, u_0)$ of (2.1) the inequality

$$r(t, t_0, u_0) < \alpha_1 \quad (t \geq t_0) \tag{3.8}$$

holds, whenever

$$|u_0| < \lambda_1 \text{ and } \int_{t_0}^{t_0+T} \xi(s)ds < \lambda_1. \tag{3.9}$$

for each $T > 0$. By assumption (vii) there exists functions a and $b \in K$ such that

$$b(\|z_0\|) < V(t_0, z_0) < a(\|z_0\|). \tag{3.10}$$

If we are given the condition

$$u_0 < \lambda_1, \tag{3.11}$$

then it follows from condition (viii) and Eq. (3.10) that

$$\|z_0\| < b^{-1}(\lambda_1). \tag{3.12}$$

Hence, if $\beta = \max(b^{-1}(\lambda_1), \lambda_1/M)$, we can conclude that the first part of inequality (3.9) follows.

Also, if we let

$$\int_{t_0}^{t_0+T} (\|\xi_1(s)\| + \|\xi_2(s)\| + \|\xi_2(s)\|^2)\, ds < \lambda_1/M \tag{3.13}$$

then by directly using assumption (v) we have

$$\int_{t_0}^{t_0+T} \xi(s)ds < \beta. \tag{3.14}$$

Hence we have shown using (3.7) that the second part of inequality (3.9) follows from (3.13).

From Eqs. (3.5) and (3.8) we obtain the inequality

$$E(\|z(t)\|) < b^{-1}(\alpha_1) < \alpha, \tag{3.15}$$

provided

$$\|z_0\| < \beta \text{ and } \int_{t_0}^{t_0+T} \xi(s)ds < \beta.$$

We have thus shown that the uniform-integral stability of (2.1) implies the integral stability in the mean of (1.1).

To prove part (2) of the theorem, we let $\epsilon > 0$, $\alpha > 0$ be given and we set

$$\epsilon_1 = b(\epsilon). \tag{3.16}$$

Then the quasiasymptotic uniform stability of Eq. (2.1) implies that there exists a $\lambda_1 = \lambda_1(\alpha_1, \epsilon_1)$ and a $T_1 = T_1(\alpha_1, \epsilon_1)$ such that

$$r(t, t_0, u_0) < \epsilon_1 \quad (t \geq t_0 + T_1) \tag{3.17}$$

whenever

$$r_0 < \alpha_1 \text{ and } \int_{t_0}^{\infty} \xi(s)ds < \lambda_1. \tag{3.18}$$

If we let $\lambda > \lambda_1/M$, we have that

$$\int_{t_0}^{\infty} (\|\xi_1(s)\| + \|\xi_2(s)\| + \|\xi_2(s)\|^2)\, ds < \lambda \tag{3.19}$$

is implied, using condition (v) in the theorem that

$$\int_{t_0}^{\infty} \xi(s)ds < \lambda_1, \tag{3.20}$$

which is the right-hand side of (3.18).

In addition, if we consider the condition

$$u_0 < \lambda_1 \tag{3.21}$$

coupled with condition (vii) in the theorem, we have

$$b(\|z_0\|) < V(t_0, z_0) < a(\|z_0\|) \tag{3.22}$$

Using condition (viii) and Eq. (3.16), we have that (3.22) yields

$$\|z_0\| < b^{-1}(\lambda_1) < \lambda, \tag{3.23}$$

which is the left-hand side of inequality (3.18)

From inequalities (3.18) and (3.16) we have

$$E(\|z(t)\|) \leq b^{-1}(\epsilon_1) < \epsilon \tag{3.24}$$

provided

$$\|z_0\| < \alpha \text{ and } \int_{t_0}^{\infty} (\|\xi_1(s)\| + \|\xi_2(s)\| \|\xi_2(s)\|^2)\, ds < \lambda.$$

Thus the quasiasymptotic uniform integral stability of (2.1) implies the asymptotic integral stability in the mean of (1.1).

4. STABILITY PROPERTIES IN FINITE TIME OF A STOCHASTIC DIFFERENTIAL SYSTEM

We shall consider various types of stability for the stochastic differential system (1.1) over a finite time interval and employ the concept of stochastic Lyapunov like functions and the theory of integral inequalities to study the problem in a unified manner by characterizing the controls in different ways.

With respect to the aims of this section, we first state the following lemma.

Lemma 4.1: Let there exist function $V \in \Lambda$, $g \in \Gamma'$, and $\xi_1(t)$ defined by (1.1) such that:

(i) For all $t \in F$ and $z \in \bar{B}(\beta) - B(\alpha)$ we have

$$D^+ E_{t,z}[V(t,z)] \leq g(t, V(t,z)). \tag{4.1}$$

(ii) Let $\xi_2(t)$ defined by (1.1) and choose the function $U(t)$ so that

$$U(t) = M \int_{t_0}^{t} (\|\xi_1(s)\| + \|\xi_2(s)\| \|\xi_2(s)\|^2)\, ds, \quad t \in \tilde{F}, \tag{4.2}$$

where

$$M = \max(M_1, M_2, M_3). \tag{4.3}$$

(iii) For $\|z\| \leq \rho$, let

(a) $$\sup_{\|z\| \leq \rho} \left\| \frac{\partial V}{\partial z}(t,z) \right\| \leq M_1, \text{ where } M_1 > 0, \tag{4.4}$$

(b) $$\phi(t) \leq M_2, \tag{4.5}$$

and

(c) $$\limsup_{h \to 0^+} (1/h) E \left[\left\| \frac{\partial V}{\partial z}(t, z(t) + hF(t, z(t)) + G(t, z(t)) d\beta(t)) \right\| \| d\beta(t) \| z(t) \right] \leq M_3. \tag{4.6}$$

Then letting $z_1 \in B(\beta) - B(\alpha)$, $z(t, t_1, z_1)$ any solution of the stochastic differential system (1.1), and

$$u_1 = V_M^{\|z_1\|}(t_1) - U(t_1), \tag{4.7}$$

we have

$$E[V(t, z(t, t_1, z_1))] \leq r(t, t_1, U_1) + U(t) \tag{4.8}$$

for $t \geq t_1$ as long as $z(t, t_1, z_1) \in \bar{B}(\beta) - B(\alpha)$, where $r(t, t_1, u_1)$ denotes the maximal solution of the scalar differential equation

$$u' = g(t, u + U(t)) \tag{4.9}$$

through (t_1, u_1).

Proof: Let $z_1 \in B(\beta) - B(\alpha)$ and $z(t, t_1, z_1) \in B(\beta) - B(\alpha)$, then for sufficiently small $h > 0$, $z(t+h, t_1, z_1) \in \bar{B}(\beta) - B(\alpha)$. Denoting $z(t, t_1, z_1)$ by $z(t)$ and $m(t) = E_{t,z} \times [V(t, z(t))]$ [(1.1)], we have

$$\begin{aligned} m(t+h) - m(t) &= E[V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t) \\ &\quad + h\zeta_1(t) + \zeta_2(t)d\beta(t)) - V(t, z(t)) \,|\, z(t)] \\ &= E[V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t) \\ &\quad + h\zeta_1(t) + \zeta_2(t)d\beta(t)) \\ &\quad - V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t)) \\ &\quad + V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t)) \\ &\quad - V(t, z(t)) \,|\, z(t)]. \end{aligned} \tag{4.10}$$

Thus,

$$\begin{aligned} &\limsup_{h \to 0^+} \frac{m(t+h) - m(t)}{h} \\ &= \limsup_{h \to 0^+} E[V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t) \\ &\quad + h\zeta_1(t) + \zeta_2(t)d\beta(t)) \\ &\quad - V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t)) \,|\, z(t)] \\ &\quad + \limsup_{h \to 0^+} E[V(t+h, z(t) + hF(t, z(t)) + G(t, z(t))d\beta(t)) \\ &\quad - V(t, z(t)) \,|\, z(t)]. \end{aligned} \tag{4.11}$$

Using (2.2) and the fact that $V \in \Lambda$, we obtain

$$\begin{aligned} &\limsup_{h \to 0^+} \frac{m(t+h) - m(t)}{h} \\ &\leq \limsup_{h \to 0^+} \times E\left[\left\| \frac{\partial V}{\partial v}(t+h, z(t) + hF(t, z(t)) \right.\right. \\ &\quad \left.\left. + G(t, z(t))d\beta(t)) \right\| h\zeta_1(t) + \zeta_2(t)d\beta(t)\| + \phi(t)\|h\zeta_1(t) \right. \\ &\quad \left. + \zeta_2(t)d\beta(t)\|^2\right] + D^+ E_{t,z}[V(t,z)]. \end{aligned} \tag{4.12}$$

As a result of Eq. (4.3) and condition (iii) of the theorem we have

$$\begin{aligned} \limsup_{h \to 0^+} \frac{m(t+h) - m(t)}{h} &\leq D^+ E_{t,z}[V(t,z)] + M(\|\zeta_1(t)\| \\ &\quad + \|\zeta_2(t)\| \|\zeta_2(t)\|^2). \end{aligned} \tag{4.13}$$

Using condition (i) from the lemma, we have

$$\begin{aligned} \limsup_{h \to 0^+} \frac{m(t+h) - m(t)}{h} &\leq g(t, V(t,z)) + M(\|\zeta_1(t)\| + \|\zeta_2(t)\| \\ &\quad \times \|\zeta_2(t)\|^2). \end{aligned} \tag{4.14}$$

Now inequality (4.14) can be integrated to yield results in

$$\begin{aligned} m(t) &\leq m(t_1) - U(t_1) + U(t) + \int_{t_1}^t g(s, V(s,z))ds \\ Em(t) &\leq U(t) + \int_{t_1}^t g(s, EV(s,z))\,ds + V_M^{\|z_1\|}(t_1) - U(t_1). \end{aligned} \tag{4.15}$$

Now by applying Lemma 2.1 we obtain the desired result.

Theorem 4.1: The solution of the stochastic differential control system (1.1) is mean stable if there exist functions $V \in \Lambda$, $g \in \Gamma'$, and $\zeta_1(t)$ such that

(i) for $t \in F$, $z \in \bar{B}(\gamma)$, $-B(\alpha)$, conditions (i), (ii), and (iii) of Lemma 4.1 hold, and

(ii) the maximal solution $r(t, t_0, u(t_0))$ of (4.9) with

$$u(t_0) = V^\alpha(t_0) - U(t_0)$$

satisfies the condition

$$r(t, t_0, u(t_0)) < V_m^\gamma(t) - U(t), \quad \alpha < r \leq \beta, \tag{4.16}$$

for all $t \geq t_0$.

Proof. Assume the solution of the stochastic control system (1.1) is not mean stable. That is, for some solution $z(t)$ of the stochastic control system (1.1) and some $\zeta_2(t)$, there exists a $\beta \geq r \geq \alpha$, $t_0 \in R_+$, and $T > 0$ where for all α, ζ_1 such that

$$\|z(t_0)\| < \alpha; \tag{4.17}$$

then

$$E\|z(t)\| = \gamma \tag{4.18}$$

for some $t > t_0$, $t \in F$. That is, for $t > t_0$ the solution of the stochastic system (1.1) reaches the boundary γ. However, by hypothesis (i) and Lemma 4.1 we have

$$E[V(t, z(t))] \leq r(t, t_0, u(t_0)) + U(t) \tag{4.19}$$

for all $t \geq t_0$. Now in view of inequalities (4.16) and (4.19) it follows that

$$E[V(t, z(t))] < V_m^\gamma(t) \tag{4.20}$$

for all $t > t_0$.

This is impossible because we have shown in (4.18) that

$$E[V(t, z(t))] \geq V_m^\gamma(t) \tag{4.21}$$

for all $t > t_0$. This contradiction completes the proof of the theorem.

Theorem 4.2: The solution of the stochastic differential control system (1.1) is uniformly stable in mean if there exist function $V \in \Lambda$, $g \in \Gamma'$, and $\zeta_1(t)$ such that such that

(i) for all $t \in F$ and $z \in \bar{B}(\gamma) - B(\alpha)$, conditions (i), (ii), and (iii) of Lemma 4.1 hold, and

(ii) the maximal solution $r(t, t_1, u(t_1))$ of (4.9) with initial condition

$$u(t_1) = V_m^\gamma(t_1) - U(t_1), \qquad \alpha < r \leq \beta$$

at any $t_1 \in F$ satisfies the condition

$$r(t, t_1, u(t_1)) < V_m^\gamma(t) - U(t) \tag{4.22}$$

for all $t > t_1$, $t \in F$.

Proof: Assume that the solution of the stochastic differential control system is not uniformly stable in mean. Then there exists some $\gamma > 0$, $t_0 \in R_+$ for all α and controls ζ_1 such that when $0 < \alpha \leq \gamma$ the condition

$$\|z(t_1)\| < \alpha \tag{4.23}$$

implies

$$E\|z(t)\| \geq \gamma \tag{4.24}$$

for all $t \geq t_1$, $t, t_1 \in F$. That is, for every control ζ_1 and time $t > t_1$ for this solution of the stochastic control system, $z(t)$ will reach the boundary. However, by hypothesis (i) and Lemma 4.1 have

$$E[(t, z(t))] \leq r(t, t_1, u(t_1)) + U(t) \tag{4.25}$$

for all $t \in F$. Hence, by assumption (ii) for all $t > t_1$, $t \in F$ we have

$$E[V(t, z(t))] < V_m^{\gamma}(t), \tag{4.26}$$

where $V_m^{\gamma}(t)$ is the smallest expected value over all z when z reaches the boundary γ. That is,

$$V_m^{\gamma}(t) \leq E[V(t, z(t))] < V_m^{\gamma}(t) \tag{4.27}$$

for all $t \geq t_1$, which is clearly a contradiction.

Theorem 4.3: The solution of the stochastic differential control system (1.1) is uniformly stable in mean if there exist functions $V \in \Lambda$, $g \in \Gamma'$, $\zeta_1(t)$ and positive numbers α, δ, where $\delta < \alpha$ such that

(i) for all $t \in F$, $z \in \bar{B}(\alpha) - B(\delta)$, conditions (i), (ii), and (iii) of Lemma 4.1 hold, and

(ii) the maximal solution $r(t, t_1, u(t_1))$ of (4.9) with initial condition

$$u(t_1) = V_{\delta}^{\alpha}(t_1) - U(t_1)$$

at any $t_1 \in F$, satisfies the condition

$$r(t, t_1, u(t_1)) < V_m^{\alpha}(t) - U(t) \tag{4.28}$$

for all $t \in F$, $t > t_1$.

Proof: Assume that the solution of the stochastic differential control system is not uniformly stable in mean. Then there exists for some solution $z(t)$ of the stochastic control system (1.1), a $\gamma > 0$, $t_0 \in R_+$ for all α and controls $\zeta_1(t)$ such that when $0 < \alpha \leq \gamma$, the condition

$$E\|z(t)\| \geq \gamma \tag{4.29}$$

is implied by

$$\|z(t_1)\| < \alpha \tag{4.30}$$

for some $t \geq t_1$, $t, t_1 \in F$ and some $\zeta_2(t)$. However, by hypothesis (i) and Lemma 4.1 we have

$$E[V(t, z(t))] \leq r(t, t_1, u(t_1)) + U(t) \tag{4.31}$$

for all $t \in F$. Now it follows from assumption (ii) that

$$E[V(t, z(t))] < V_m^{\alpha}(t) \tag{4.32}$$

for all $t \in F$, $t > t_1$. Clearly from inequalities (4.29) and (4.32) it follows that

$$V_m^{\alpha}(t) < V_m^{\alpha}(t)$$

for all $t \in F$, $t > t_1$. Hence a contradiction.

Theorem 4.4: The solution of the stochastic differential control system (1.1) is quasiexpansively stable in mean if there exist functions $V \in \Lambda$, $g \in \Gamma'$, $\zeta_1(t)$, and a positive number β' such that

(i) for all $t \in F$, $z \notin \bar{B}(\beta)$, $-B(\beta')$ conditions (i), (ii), and (iii) of Lemma 4.1 hold, and

(ii) the maximal solution $r(t, t_1, u(t_1))$ of (4.9) with initial condition

$$u(t_1) = V_m^{\beta'}(t_1) - U(t_1) \tag{4.33}$$

at any $t_1 \in F$, satisfies the condition

$$r(t, t_1, u(t_1)) < V_m^{\beta'}(t) - U(t) \tag{4.34}$$

for $t \in (t_1, t_0 + T)$.

Proof: Assume that the solution of the stochastic differential control system (1.1) is not quasiexpansively stable in the mean. That is, for some solution $z(t)$ of the stochastic control system (4.6) and some $\zeta_2(t)$ there exists $\beta' > 0$, $t_0 \in R_+$, and $T > 0$ such that for all α, t_1, and $\zeta_1(t)$, where $0 < \alpha \leq \beta$ such that

$$\|z_0\| < \alpha; \tag{4.35}$$

then this implies

$$E\|z(t)\| \geq \beta' \tag{4.36}$$

for some $t \in (t_1, t_0 + T)$. This implies by the definition of $V_m^{\beta}(t)$ that

$$V_m^{\beta'}(t) \leq E[V(t, z(t))] \tag{4.37}$$

for the $t \in (t_1, t_0 + T)$. However, by Lemma 4.1 and condition (i) of the theorem we have

$$E[V(t, z(t))] \leq r(t, t_1, u(t_1)) + U(t) \tag{4.38}$$

for all $t \in (t_1, t_0 + T)$. Therefore, from (4.33) and (4.34) we obtain

$$V_m^{\beta'}(t) \leq E[V(t, z(t))] \leq r(t, t_1, u(t_1)) + U(t) < V_m^{\beta'}(t) \tag{4.39}$$

for the $t \in (t_1, t_0 + T)$, which is a contradiction.

Theorem 4.5: The solution of the stochastic differential control system (1.1) is quasicontractively stable in the mean if there exist functions $V \in \Lambda$, $g \in \Gamma'$, and $\zeta_1(t)$ such that

(i) for all $t \in F$ and $z \notin B(\beta')$, conditions (i), (ii), and (iii) of Lemma (4.1) hold, and

(ii) the maximal solution $r(t, t_1, u(t_1))$ of (4.9) with initial condition

$$u(t_1) = V_m^{\beta'}(t_1) - U(t_1) \tag{4.40}$$

at any $t_1 \in F$ satisfies the condition

$$r(t, t_1, u(t_1)) < V_m^{\beta'}(t) - U(t) \tag{4.41}$$

for all $t \in (t_1, t_0 + T)$.

Proof: The solution of the stochastic differential control system (1.1) will fail to be quasicontractively stable in the mean if there is some solution $z(t)$ and some $\zeta_2(t)$ such that for some $\beta' > 0$, $t_0 \in R_+$, and $T > 0$, then for all $\alpha, t_1, \zeta_1(t)$, where $\alpha > \beta$ and $\zeta_1(t) \in C[(t_0, t_0 + T), R^n]$ such that if

$$\|z_0\| < \alpha, \tag{4.42}$$

then

$$E\|z(t)\| \geq \beta' \tag{4.43}$$

for some $t \in (t_1, t_0 + T)$. Using condition (i) of the theorem and Lemma 4.1 in conjunction with (4.42) and condition (ii), we have

$$V_m^{\beta'}(t) < V_m^{\beta'}(t)$$

for all $t \in (t_1, t_0 + T)$, which is a contradiction.

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Direct-inverse problems in transport theory, the inverse albedo problem for a finite medium[a)]

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In this paper we deal with the inverse problem in radiative transfer, which is equally applicable to the neutron transport, for a finite homogeneous medium. We give a method for computing the scattering function and the albedo for single scattering. The solution is given in terms of Legendre expansion of the scattering function. A decomposition of the equation of transfer is also given in which the relation between the direct and the inverse problem is exhibited via the principles of invariance. A relation of this work with Case's method of approach is outlined. This work should be of practical value to the problems associated with remote sensing of the terrestrial atmosphere and the neutron piles.

1. INTRODUCTION

In an earlier paper by Kanal and Moses,[1] an inverse problem in neutron (or radiative) transport theory was solved for an infinite medium containing a plane source emitting neutrons (or photons) in a direction whose angle's cosine was fixed arbitrarily at $\mu = \mu_0$. The objective was to reconstruct the scattering kernel $f(\mu' \to \mu)$ (or the phase function) from the information obtained from the experiment which measured the neutron (or photon) column density for all angles; which is the zeroth moment of the angular density (or the specific intensity of the radiation field). In contrast the object of the usual direct problem is to find the distribution function (angular density of neutrons or the specific intensity of radiation) for a given scattering function. In this paper we wish to treat the inverse-albedo problem of radiative transfer in an atmosphere which is finite in the total optical depth scale. The direct-albedo problem for a finite atmosphere is defined as follows: We are given an incident radiation field at $x=0$, where x is the optical depth. Also given are the phase function, the albedo for single scattering and the reflection boundary condition at $x=x_b$, where x_b is the total optical thickness of the atmosphere. The problem is to determine the radiation field everywhere and, in consequence, the reflected component at $x=0$ and the transmitted component at $x=x_b$. In contrast, the inverse-albedo problem for the finite atmosphere involves the construction of the phase function and the albedo for single scattering from the results of an experiment which measures a certain minimum set of suitable quantities. We discuss the nature of measurements that are required for the present treatment below.

In an earlier paper, Case[2] gives an elegant solution of an inverse problem for an infinite medium containing an isotropic plane neutron source and constructs the scattering function from the spectral data of the transport operator. He requires measurements of the neutron density for all relaxation lengths, and relates the density to the spectral function. He then proceeds to show by different routes (including the discretized version of the Gel'fand–Levitan equation) how one may construct the coefficients in the Legendre polynomial expansion of the scattering function. In our treatment of the albedo-inverse problem, which physically differs from the infinite medium problem, the measurements that we require are different from the ones required by Case. In parallel with the infinite medium problem,[1] we require the measurements to give information on the finite integral of the specific intensity, i.e., we require knowing

$$\int_{x_1}^{x_2} dx\, I(x,\mu)$$

and $I(x_1,\mu)$, $I(x_2,\mu)$, where x_1 and x_2 are two arbitrary points in the optical depth scale. We shall then see how that quantity is related to the infinite medium problem via the principles of invariance.[3] We shall also demonstrate how one may actually construct the spectral data for the Case model from our experiment and in consequence generate Case eigenfunctions from that experiment.

A final remark is due here. In our previous problem,[1] we used two different bases for the expansion of the phase function. One was the Legendre polynomia and the second was the complete set of Case's eigenfunctions[1] of the transport operator for the *isotropic* scattering medium. Both expansions have their inherent advantages. In the Legendre polynomial expansion, the inverse problem is exactly soluble and is particularly useful when the medium is not too anisotropically scattering. On the other hand, if the medium is highly anisotropically scattering, then the eigenfunction expansion is particularly suitable. For in that case we have a maximum variational principle which can be used (and in fact we have used[1]) to obtain a bounded estimate of the expansion coefficients. However, the primary aim of this paper is to relate the infinite medium solution to the inverse-albedo problem for a finite atmosphere by an alternate formulation of the principles of invariance. We shall address the albedo problem in radiative transfer.

2. INVERSE-ALBEDO PROBLEM FOR A FINITE ATMOSPHERE

Consider a finite medium optically bounded between $x=0$ and $x=x_b$ as shown in Fig. 1. For the one-dimensional, rotationally invariant case, the standard equa-

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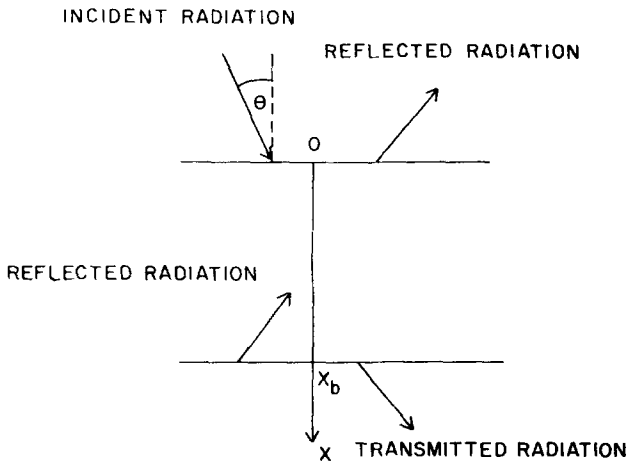

FIG. 1. Configuration for the inverse-albedo problem.

tion of radiative transfer is,[3]

$$\mu \frac{\partial I(x,\mu)}{\partial x} + I(x,\mu) = \frac{c}{2}\int_{-1}^{1} d\mu' f(\mu' \to \mu) I(x,\mu'), \quad (2.1)$$

where μ is the cosine of the angle corresponding to the unit vector pointing in the direction of propagation of radiation, x is the optical depth, $I(x,\mu)$ is the specific intensity of the radiation field, c is the albedo for single scattering and $f(\mu' \to \mu)$ is the phase function. The phase function is normalized to unity so that

$$\tfrac{1}{2}\int_{-1}^{1} d\mu' f(\mu' \to \mu) = 1. \quad (2.2)$$

Now imagine the finite medium, under consideration, imbedded in an infinite medium with the same scattering properties. Further, imagine a plane source of radiation at $x = x_0$ in the infinite medium emitting photons in a direction $\mu = \mu_0$. The equation of transfer for that case is

$$\mu \frac{\partial \Psi(x, \mu \to x_0, \mu_0)}{\partial x} + \Psi = \frac{c}{2}\int_{-1}^{1} d\mu' f(\mu' \to \mu)\Psi(x, \mu' \to x_0, \mu_0) + \delta(x - x_0)\delta(\mu - \mu_0). \quad (2.3)$$

Let us consider the column density of the radiation field for the infinite medium so that,

$$M_0(\mu, \mu_0) = \int_{-\infty}^{\infty} dx\, \Psi(x, \mu \to x_0, \mu_0). \quad (2.4)$$

Also, let us define the total emission term by

$$S_0(\mu, \mu_0) = \int_{-1}^{1} d\mu' f(\mu' \to \mu) M_0(\mu', \mu_0). \quad (2.5)$$

With the appropriate boundary conditions at $x = \pm\infty$,

$$\Psi(\pm\infty, \mu \to x_0, \mu_0) = 0, \quad (2.6)$$

we find from Eq. (2.3) that

$$M_0(\mu, \mu_0) = \delta(\mu - \mu_0) + \frac{c}{2} S_0(\mu, \mu_0). \quad (2.7)$$

By multiplying Eq. (2.7) on both sides with $f(\mu \to \mu_0)$ and integrating with respect to μ, we find that the total emission term $S_0(\mu, \mu_0)$ satisfies the integral equation of the Fredholm type,

$$S_0(\mu, \mu_0) = f(\mu \to \mu_0) + \frac{c}{2}\int_{-1}^{1} d\mu' f(\mu' \to \mu) S_0(\mu', \mu_0). \quad (2.8)$$

This is an integral equation for $S_0(\mu, \mu_0)$ for the infinite medium whose solutions are discussed in Ref. 1. In the same manner as above, consider the measurement of the column density for the finite medium between any two points x_1, x_2,

$$M_f(\mu, \mu_1 | x_1, x_2) = \int_{x_1}^{x_2} dx\, I(x, \mu), \quad (2.9)$$

where μ_1 refers to the cosine direction of the incidence beam at $x = 0$. Integrating Eq. (2.1) from x_1 to x_2, we obtain

$$M_f(\mu, \mu_1 | x_1, x_2) = \mu I(x_1, \mu) - \mu I(x_2, \mu) + \frac{c}{2} S_f(\mu, \mu_1 | x_1, x_2), \quad (2.10)$$

where

$$S_f(\mu, \mu_1 | x_1, x_2) = \int_{-1}^{1} d\mu' f(\mu' \to \mu) M_f(\mu' \mu_1 | x_1, x_2) \quad (2.11)$$

is the emission term for a slab of the atmosphere between $x = x_1$ and $x = x_2$. The question we ask is, what is the relation between the total emission term $S_0(\mu, \mu_0)$ and the emission term $S_f(\mu, \mu_1 | x_1, x_2)$ for the slab, if we know the specific intensity $I(x, \mu)$ of radiation at the two points $x = x_1$ and $x = x_2$? And from that knowledge, how do we construe the scattering properties of the finite medium? Answers to these questions are readily provided by the principles of invariance,[3] stated as follows: "The law of scattering by a finite homogeneous atmosphere must be invariant to the addition (or subtraction) of layers of arbitrary thickness to (or from) the homogeneous atmosphere."

Let us see how we may apply this principle to solve the inverse albedo problem. Consider Eq. (2.10) and multiply it by $f(\mu \to \mu_2)$ on both sides. An integration with respect to μ then yields

$$S_f(\mu, \mu_1 | x_1, x_2) = \int_{-1}^{1} d\mu' \mu' f(\mu' \to \mu)[I(x_1, \mu') - I(x_2, \mu')] + \frac{c}{2}\int_{-1}^{1} d\mu' f(\mu' \to \mu) S_f(\mu', \mu_1 | x_1, x_2), \quad (2.12)$$

where we have renamed the variables. As an intermediate step, expand $f(\mu' \to \mu)$ in terms of Legendre polynomia,

$$f(\mu' \to \mu) = \sum_{n=0}^{\infty} (2n+1) f_n P_n(\mu') P_n(\mu). \quad (2.13)$$

Insert (2.13) in (2.12) and use the orthogonality property of $P_n(\mu)$ to obtain,

$$f_n = \frac{\int_{-1}^{1} d\mu\, P_n(\mu) S_f(\mu, \mu_1 | x_1, x_2)}{\int_{-1}^{1} d\mu\, P_n(\mu)[2\mu(I(x_1, \mu) - I(x_2, \mu)) + c S_f(\mu, \mu_1 | x_1, x_2)]}. \quad (2.14)$$

Now in Ref. 1 [see Eq. (18) of that Ref.], we obtained the following relation for an infinite atmosphere:

$$f_n = \frac{q_n(\mu_0)}{2P_n(\mu_0) + c q_n(\mu_0)}, \quad (2.15)$$

where

$$q_n(\mu_0)=\int_{-1}^{1}d\mu' P_n(\mu)S_0(\mu,\mu_0), \tag{2.16}$$

so that

$$S_0(\mu,\mu_0)=\sum_{n=0}^{\infty}\frac{2n+1}{2}q_n(\mu_0)P_n(\mu). \tag{2.17}$$

Now we apply the principles of invariance by equating the right-hand sides of Eqs. (2.14) and (2.15). Transposing the denominator terms to the corresponding sides we obtain

$$\begin{aligned}\int_{-1}^{1}d\mu P_n(\mu)S_f(\mu,\mu_1|x_1,x_2)[2P_n(\mu_0)+cq_n(\mu_0)]\\ =\int_{-1}^{1}d\mu q_n(\mu_0)P_n(\mu)[2\mu(I(x_1,\mu)-I(x_2,\mu))\\ +cS_f(\mu,\mu_1|x_1,x_2)].\end{aligned} \tag{2.18}$$

Note that the second term in the bracket on the left-hand side cancels the last term in the bracket on the right-hand side. Now multiply Eq. (2.18) by $(2n+1)/2$ and sum over n. Noting the completeness relation for the Legendre polynomia

$$\sum_{n=0}^{\infty}\frac{2n+1}{2}P_n(\mu)P_n(\mu_0)=\delta(\mu-\mu_0), \tag{2.19}$$

and the definition (2.17) of $S_0(\mu,\mu_0)$, we get

$$S_f(\mu_0,\mu_1|x_1,x_2)=\int_{-1}^{1}d\mu\,\mu S_0(\mu,\mu_0)[I(x_1,\mu)-I(x_2,\mu)]. \tag{2.20}$$

Equation (2.20) represents a mathematical form of the principles of invariance relating the emission term for a finite slab embedded in an infinite atmosphere to its total emission term $S_0(\mu,\mu_0)$. Thus S_0 plays the role of a kind of Green's function. The symbol μ_1 is reserved for the direction of the incident beam at $x=0$ for the finite atmosphere.

From Eqs. (2.14) and (2.10) we readily see that the expansion coefficients f_n can be obtained from the measurement $M_f(\mu,\mu_1|x_1,x_2)$ of the column density between x_1,x_2. Thus, we have

$$f_n=\frac{1}{c}\left(1-\frac{\int_{-1}^{1}d\mu\,P_n(\mu)\mu(I(x_1,\mu)-I(x_2,\mu))}{\int_{-1}^{1}d\mu\,P_n(\mu)M_f(\mu,\mu_1|x_1,x_2)}\right). \tag{2.21}$$

For later purposes we introduce the quantity

$$g_n=1-cf_n, \tag{2.22}$$

where

$$g_n=\frac{\int_{-1}^{1}d\mu\,P_n(\mu)\mu(I(x_1,\mu)-I(x_2,\mu))}{\int_{-1}^{1}d\mu\,P_n(\mu)M_f(\mu,\mu_1|x_1,x_2)}. \tag{2.23}$$

For $n=0$, $f_0=1$, we obtain the value of the albedo for single scattering c,

$$c=1-\frac{\int_{-1}^{1}d\mu\,\mu(I(x_1,\mu)-I(x_2,\mu))}{\int_{-1}^{1}d\mu\,M_f(\mu,\mu_1|x_1,x_2)}. \tag{2.24}$$

Principles of invariance, represented by Eq. (2.20) give rise to an interesting decomposition of the equation of transfer (2.1). For in the limit $x_1\to x_2$ $(x_2=x)$, Eq. (2.20) becomes

$$\lim_{x_1\to x}\frac{S_f(\mu_0,\mu_1|x_1,x)}{x-x_1}=-\int_{-1}^{1}d\mu\,\mu S_0(\mu,\mu_0)\frac{\partial I(x,\mu)}{\partial x}, \tag{2.25}$$

while from Eqs. (2.10) and (2.9) we obtain,

$$\frac{2}{c}\left(I(x,\mu_0)+\mu_0\frac{\partial I(x,\mu_0)}{\partial x}\right)=\lim_{x_1\to x}\frac{S_f(\mu_0,\mu_1|x_1,x)}{x-x_1}. \tag{2.26}$$

Hence from (2.25) and (2.26) we get

$$\mu\frac{\partial I(x,\mu)}{\partial x}+I(x,\mu)=-\frac{c}{2}\int_{-1}^{1}d\mu' S_0(\mu',\mu')\mu'\frac{\partial I(x,\mu')}{\partial x}. \tag{2.27}$$

Equating the right-hand side of this equation with the right-hand side of Eq. (2.1) we also obtain the relation

$$\int_{-1}^{1}d\mu' S_0(\mu',\mu)\mu'\frac{\partial I(x,\mu')}{\partial x}+\int_{-1}^{1}d\mu' f(\mu'\to\mu)I(x,\mu')=0. \tag{2.28}$$

It is clear that Eqs. (2.27) and (2.28) are completely equivalent to the original equation (2.1) of radiative transfer. However, we remark that Eq. (2.28) is strictly a relation between the direct and the inverse problems. Of course, one would desire a converse relation to Eq. (2.20) in which the infinite medium measurement is related to the finite medium. Such a relation is readily obtained from Eq. (2.18), which gives the expansion coefficients $q_n(\mu_0)$ of $S_0(\mu,\mu_0)$ [see Eq. (2.17)]. Thus

$$q_n(\mu_0)=\frac{P_n(\mu_0)\int_{-1}^{1}d\mu\,P_n(\mu)S_f(\mu,\mu_1|x_1,x_2)}{\int_{-1}^{1}d\mu\,P_n(\mu)\mu(I(x_1,\mu)-I(x_2,\mu))} \tag{2.29}$$

or, in terms of M_f,

$$q_n(\mu_0)=\frac{2}{c}P_n(\mu_0)\times\left(\frac{\int_{-1}^{1}d\mu\,P_n(\mu)M_f(\mu,\mu_1|x_1,x_2)}{\int_{-1}^{1}d\mu\,P_n(\mu)\mu(I(x_1,\mu)-I(x_2,\mu))}-1\right). \tag{2.30}$$

Comparing (2.30) with (2.21) we find that

$$q_n(\mu_0)=P_n(\mu_0)\frac{2f_n}{1-cf_n}. \tag{2.31}$$

From this and Eq. (2.17) it clearly follows that

$$S_0(\mu,\mu_0)=\sum_{n=0}^{\infty}(2n+1)\frac{f_n}{1-cf_n}P_n(\mu)P_n(\mu_0), \tag{2.32}$$

where f_ns are obtained from the measurements as per Eq. (2.21). Thus, relations (2.20) and (2.32) represent a reciprocity between the measurements of a finite medium relating to the measurements of the infinite medium.

Next we shall consider the relationship between our process of measurement and the one considered by Case[2] and actually see how one may generate Case eigenfunctions from the *measurements* and also see how that leads to the construction of the spectral data.

3. RELATION OF INVERSE-ALBEDO PROBLEM TO CASE'S MODEL

For the sake of clarification some repetition of Case's work is essential here. In his model one has an infinite

medium with a plane neutron source emitting neutrons isotropically at $x=0$. The homogeneous equation of transfer is, then,

$$\mu\frac{\partial\psi}{\partial x}+\psi=c\sum_{l=0}^{\infty}\frac{2l+1}{2}f_lP_l(\mu)\int_{-1}^{1}d\mu'\,P_l(\mu')\psi(\mu'), \quad (3.1C)$$

where the scattering kernel has been expanded in terms of Legendre polynomia and we have suffixed the equations with C to acknowledge Case's work. Looking for infinite medium solutions of this equation in the form $\phi_\nu(\mu)\exp(-x/\nu)$ one finds

$$(\nu-\mu)\phi_\nu(\mu)=\frac{c\nu}{2}M(\mu,\nu), \quad (3.2C)$$

where

$$M(\mu,\nu)=\sum_{l=0}^{\infty}(2l+1)f_lP_l(\mu)h_l(\nu), \quad (3.3C)$$

with

$$h_l(\nu)=\int_{-1}^{1}d\mu\,\phi_\nu(\mu)P_l(\mu) \quad (3.4C)$$

and

$$h_0=1.$$

It has been shown that a complete set of eigenfunctions are

$$\phi_\nu(\mu)=\tfrac{1}{2}c\nu P[M(\mu,\nu)/(\nu-\mu)]+\lambda\delta(\nu-\mu) \quad (3.5C)$$

and

$$\phi_{\nu i}(\mu)=\tfrac{1}{2}c\nu_i[M(\mu,\nu_i)/(\nu_i-\mu)], \quad (3.6C)$$

where

$$\lambda(\nu)=\tfrac{1}{2}[\Lambda^+(\nu)+\Lambda^-(\nu)], \quad (3.7C)$$

$$\Lambda(\nu)=1-\tfrac{1}{2}c\nu\int_{-1}^{1}d\mu\frac{M(\mu,\nu)}{\nu-\mu}. \quad (3.8C)$$

$\Lambda(\nu_i)=0$, and $+(-)$ represents the boundary value of Λ as the branch cut is approached from the top (bottom). Under the given assumptions, there are only a finite number of real, simple ν_i with $|\nu_i|>1$. They occur in equal but opposite pairs.

These functions are orthogonal in the sense that

$$\int_{-1}^{1}d\mu\mu\,\phi_\nu(\mu)\phi_{\nu'}(\mu)=N(\nu)\delta(\nu-\nu'), \quad (3.9C)$$

$$\int_{-1}^{1}d\mu\,\mu\,\phi_i(\mu)\phi_j(\mu)=N_i\delta(i,j). \quad (3.10C)$$

As an application of the orthogonality and completeness properties one can calculate total density corresponding to a unit plane source at $x=0$. This is the solution of Eq. (3.1C) when the inhomogeneous term $\delta(x)/2\pi$ is added on the right. The result is

$$\Phi(x)=2\pi\int_{-\infty}^{\infty}\frac{d\rho(\nu)}{\nu}\exp(-|x/\nu|), \quad (3.11C)$$

where

$$\frac{d\rho(\nu)}{\nu}=\frac{d\nu}{N(\nu)}, \quad -1\le\nu\le1 \quad (3.12C)$$

$$=\sum_i\frac{\delta(\nu-\nu_i)d\nu}{N_i}, \quad |\nu|>1. \quad (3.13C)$$

Then Case states that, given measurements of $\Phi(x)$, one knows quite a bit about the spectral function $\rho(\nu)$.

The functions $h_l(\nu)$ obey a three-terms pure-recurrence relation

$$(l+1)h_{l+1}(\nu)+lh_{l-1}(\nu)=(2l+1)(1-cf_l)\nu h_l(\nu). \quad (3.14C)$$

Case's version of the inverse problem is thus reduced to the following: Given the information about $d\rho(\nu)$ which Eq. (3.11C) provides, what is $g(n)=1-cf_n$?

Now, Case has shown[4] that the normalization coefficients $N(\nu)$ and N_i in Eqs. (3.9C) and (3.10C) are related to the dispersion function $\Lambda(\nu)$ by

$$N(\nu)=\nu\Lambda^+(\nu)\Lambda^-(\nu) \quad (3.15C)$$

and

$$N_{i\pm}=\pm\frac{c}{2}\nu_i^2M(\nu_i,\nu_i)\frac{\partial\Lambda}{\partial\nu}\Big|_{\nu=\nu_i} \quad (3.16C)$$

respectively. Clearly therefore, the knowledge of the dispersion function is all one needs to generate $N(\nu)$, N_i and in consequence the spectral function, given by Eqs. (3.12C) and (3.13C) and all eigenfunctions. From Eq. (3.11C) it is not obvious as to how one may in practice actually obtain the information about the spectral function from the knowledge of $\Phi(x)$. However, in principle that is possible. Our main interest here is that from the solution of the inverse-albedo problem we have presented in the earlier section, the values of f_l are readily obtained from Eq. (2.21). Then, it is quite clear that all quantities in Case's model which involve f_l's are explicitly calculable. In particular, the inverse-albedo problem provides a method for constructing Case's eigenfunctions *from an experiment*. Further, it provides an experimental test of the discretized version of the Gel'fand–Levitan[5] equation, and all equations given by Case which involve f_l, become indentities.

It would be of pedagogical value to find a relation between the direct-inverse problems which are analogous to Eq. (2.28) and involve Case's eigenfunctions.

We make the ansatz in Eq. (2.28), $I(x,\mu)=e^{-x/\nu}\phi_\nu(\mu)$ and obtain

$$\int_{-1}^{1}d\mu'\,S_0(\mu',\mu)\mu'\phi_\nu(\mu')=\nu\int_{-1}^{1}d\mu'\,f(\mu'\to\mu)\phi_\nu(\mu') \quad (3.17)$$

for all values of ν. But these are nothing but the expansion coefficients of $S_0(\mu',\mu)$ and $f(\mu'\to\mu)$ in Case's eigenfunction base. More importantly, however, the invariance principles give this particular relation from which one can solve for $f(\mu'\to\mu)$, for a given $S_0(\mu',\mu)$ and vice versa by use of the completeness relation of the eigenfunctions.

It appears to us that Case's eigenfunctions may have a natural interpretation. In other words, could these eigenfunctions correspond to some pure state such that given a pure normal mode of radiation (or neutrons),

is there a scattering law which conserves this mode without dispersion? If so then one could construct a medium which will pass only one normal mode and not the others. In a sense that would be a filter.

We close this paper with a remark that the inverse-albedo problem for a finite homogeneous medium provides a very simple method of determining the scattering properties of the medium, which appears to be practical for both laboratory and space experiments.

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A system theoretic representation of mechanical systems. I. Decomposition of a mechanical system into a hierarchy of orthogonal stationary linear dynamical systems[a)]

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A system theoretic representation of mechanical systems is proposed. It is shown that mechanical systems, classical or quantal, described by the Liouville equation, can be realized as a stationary linear input–output system. This state space representation of mechanical systems is then extended to decompose a mechanical system into a hierarchy of orthogonal stationary linear dynamical systems.

I. INTRODUCTION

Mathematical system theory is a highly developed sophisticated branch of mathematics which has seen applications in a variety of fields. But as far as physics is concerned, not much effort has been made to use this powerful tool in problems of theoretical physics. With the belief that mathematical system theory can play a vital role in theoretical physics, we propose here, as a first step in this direction, a system theoretic representation of mechanical systems.

In this paper, the first of a series, we will present the formulation of the theory that *a mechanical system, classical or quantal, can be realized as a stationary linear dynamical system* and extend it to establish *a decomposition of the equation of motion of a mechanical system into a hierarchy of orthogonal stationary linear dynamical systems*. We will assume that the original dynamics of the mechanical system is formulated in the appropriate Liouville space $\mathbb{L}$, the time evolution of the dynamical variables $a(\cdot) \in \mathbb{L}$ being given by the Liouville equation. To avoid any undue loss of generality, we will write the Liouville equation as an abstract Cauchy problem of the first order and then decompose the Liouville space $\mathbb{L}$ as the direct sum of the orthogonal subspaces $\mathbb{K}$ and $\mathbb{K}^{\perp}$, using an appropriate projection operator, such that $\mathbb{K}$ contains the *slow* part of the mechanical motion, while $\mathbb{K}^{\perp}$ contains a rapidly fluctuating part that resembles a random motion. Considering this decomposed equation of motion to be the input–output map of a causal dynamical system we then show that the mechanical system can be represented as a stationary linear dynamical system whose input is the fluctuating part of the decomposed motion and whose output is the set of dynamical variables whose time evolution describes the mechanical system. We call it the *state space representation* of the mechanical system.

This procedure can be iterated and the motion in $\mathbb{K}^{\perp}$ can once again be decomposed into a relatively systematic part and a fluctuating part and a state space representation of the motion in $\mathbb{K}^{\perp}$ can be obtained in the same fashion. Following such an iterative process, we establish in the last section of the paper a decomposition of the mechanical system into a hierarchy of orthogonal stationary linear dynamical systems.

In the following paper we will present a stochastic interpretation of the theory. In the third paper of the series we will apply the theory to a many-body system and discuss some of the interesting consequences.

II. LIOUVILLE EQUATION AS AN ABSTRACT CAUCHY PROBLEM

We will assume that the original dynamics of the mechanical system is formulated in an appropriate Liouville space $\mathbb{L}$, the dynamical variables $a^{\alpha}(\cdot) \in \mathbb{L}$, $\alpha = 1, 2, \ldots, m$, satisfying the Liouville equation of motion. To avoid any undue loss of generality, we will write the Liouville equation as an abstract Cauchy problem of the first order

$$\frac{d}{dt} a^{\alpha}(t) = L a^{\alpha}(t), \tag{1}$$

where the *Liouvillian* L is a *skew adjoint* (not necessarily bounded) *linear* operator

$$L = -(L)^{*} \tag{2}$$

acting on a complex *separable* Hilbert space $\mathbb{L}$ called the *Liouville space*.[1] Accordingly, the dynamical variables $a^{\alpha}(\cdot)$ are $\mathbb{L}$-valued functions. Because of (2), the Cauchy problem is correctly set, that is, for any initial value $a^{\alpha}(0)$ belonging to the domain $\mathbb{D}(L)$ of the Liouvillian L Eq. (1) has an unique solution $a^{\alpha}(t)$,

$$a^{\alpha}(t) = \exp(tL)\, a^{\alpha}(0) \in \mathbb{D}(L), \quad 0 \leq t < \infty, \tag{3}$$

which depends continuously on the initial data.[2] The boundedness of all solutions of (1) permits the application of a Laplace transformation

$$\hat{a}^{\alpha}(z) \overset{\text{def}}{=} \int_0^{\infty} dt \exp(-tz)\, a^{\alpha}(t), \quad \mathrm{Re}(z) > 0, \tag{4}$$

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which is holomorphic in the half-plane $\mathrm{Re}(z) > 0$ and converges absolutely. The integral

$$\int_0^\infty dt \exp(-tz) \exp(t\mathcal{L})\, g \stackrel{\text{def}}{=} \mathcal{R}(z)\, g, \quad g \in \mathbb{L}, \quad \mathrm{Re}(z) > 0 \tag{5}$$

exists as an element of $\mathbb{L}$ in the complex half-plane $\mathrm{Re}(z) > 0$ for all $g \in \mathbb{L}$. The resolvent $\mathcal{R}(z)$ of the Liouvillian $\mathcal{L}$,

$$\mathcal{R}(z) = \int_0^\infty dt \exp(-tz) \exp(t\mathcal{L}) \stackrel{\text{def}}{=} (z - \mathcal{L})^{-1}, \quad \mathrm{Re}(z) > 0 \tag{6}$$

is a closed operator with range $\mathbb{D}(\mathcal{L})$ and satisfies the equations

$$(z - \mathcal{L})\mathcal{R}(z)\, g = g, \quad g \in \mathbb{L}, \tag{7a}$$

$$\mathcal{R}(z)(z - \mathcal{L})\, g = g, \quad g \in \mathbb{D}(\mathcal{L}), \tag{7b}$$

and commutes with $\exp(t\mathcal{L})$ for $t \geq 0$. With this, the Laplace transform solution of (1) is given by

$$\hat{a}^\alpha(z) = \mathcal{R}(z)\, a^\alpha(0) \in \mathbb{D}(\mathcal{L}), \quad \mathrm{Re}(z) > 0. \tag{8}$$

III. TIME EVOLUTION OF A SUBSPACE

Let $\mathbb{K}$ be a r-dimensional subspace of the Liouville space $\mathbb{L}$ such that the Liouvillian $\mathcal{L}$ is defined on $\mathbb{K}$,[3]

$$\mathbb{K} \subset \mathbb{D}(\mathcal{L}) \subset \mathbb{L}, \tag{9a}$$

$$\dim(\mathbb{K}) = r, \tag{9b}$$

and we denote by $\mathbb{K}^\perp$ the orthogonal complement of $\mathbb{K}$,

$$\mathbb{L} = \mathbb{K} \oplus \mathbb{K}^\perp. \tag{10}$$

Let $\mathcal{P}$ and $\mathcal{P}^\perp$ be the orthogonal projection operators onto $\mathbb{K}$ and $\mathbb{K}^\perp$, respectively,

$$\mathcal{P}\,\mathbb{L} = \mathbb{K}, \quad \mathcal{P}^\perp \mathbb{L} = \mathbb{K}^\perp, \tag{11a}$$

$$\mathcal{P} = (\mathcal{P})^* = (\mathcal{P})^2, \quad \mathcal{P}^\perp = (\mathcal{P}^\perp)^* = (\mathcal{P}^\perp)^2, \tag{11b}$$

$$\mathcal{P}\mathcal{P}^\perp = \mathcal{P}^\perp\mathcal{P} = 0, \quad \mathcal{P} + \mathcal{P}^\perp = 1. \tag{11c}$$

With a proper choice of the projection operators $\mathcal{P}$ and $\mathcal{P}^\perp$, and therefore the subspaces $\mathbb{K}$ and $\mathbb{K}^\perp$, one can separate the dynamical variables into classes whose characteristic time constants are entirely different. We assume that the dynamical variables $a(\cdot)$ and the projectors $\mathcal{P}$ and $\mathcal{P}^\perp$ have been chosen in such a way that the motion projected on $\mathbb{K}$ exhibits a slowly varying gross behavior while the complement $\mathbb{K}^\perp$ contains a rapidly fluctuating motion that resembles a random motion.

With these projection operators we decompose the Liouvillian $\mathcal{L}$ as

$$\mathcal{L} = \mathcal{L}^{\shortparallel} + \mathcal{L}^\perp + \mathcal{V}, \tag{12a}$$

$$\mathcal{L}^{\shortparallel} \stackrel{\text{def}}{=} \mathcal{P}\mathcal{L}\mathcal{P}, \tag{12b}$$

$$\mathcal{L}^\perp \stackrel{\text{def}}{=} \mathcal{P}^\perp\mathcal{L}\mathcal{P}^\perp, \tag{12c}$$

$$\mathcal{V} \stackrel{\text{def}}{=} \mathcal{P}\mathcal{L}\mathcal{P}^\perp + \mathcal{P}^\perp\mathcal{L}\mathcal{P}, \tag{12d}$$

and the relation $\mathbb{K} \subset \mathbb{D}(\mathcal{L})$ implies that both $\mathcal{L}^{\shortparallel}$ and $\mathcal{L}^\perp$ are skew-adjoint,[4]

$$\mathcal{L}^{\shortparallel} = -(\mathcal{L}^{\shortparallel})^*, \tag{13a}$$

$$\mathcal{L}^\perp = -(\mathcal{L}^\perp)^*. \tag{13b}$$

Evidently, $(\mathcal{L}^{\shortparallel} + \mathcal{L}^\perp)$ equals the maximal skew-adjoint part of $\mathcal{L}$ under which the subspace $\mathbb{K}$ is stable.

Furthermore, the range of the "perturbation" is a subspace whose dimension does not exceed $2r$. Hence $\mathcal{V}$ is an operator of finite rank

$$\mathrm{rank}(\mathcal{V}) \leq 2r. \tag{14}$$

Let $k^1, k^2, \ldots, k^r$, be an orthonormal basis of the subspace $\mathbb{K}$,

$$k^\alpha \in \mathbb{K}, \quad \alpha = 1, 2, \ldots, r, \tag{15a}$$

$$\langle k^\alpha \,|\, k^\beta \rangle = \delta^{\alpha\beta} \quad \alpha, \beta = 1, 2, \ldots, r, \tag{15b}$$

and we consider the time evolution of these elements

$$y^\alpha(t) \stackrel{\text{def}}{=} \exp(t\mathcal{L})\, k^\alpha, \quad \alpha = 1, 2, \ldots, r. \tag{16}$$

Let $\mathcal{R}$, $\mathcal{R}_0$, and $\mathcal{R}^\perp$ be the resolvents of the operators $\mathcal{L}$, $(\mathcal{L}^{\shortparallel} + \mathcal{L}^\perp)$, and $\mathcal{L}^\perp$, respectively, that is,

$$\mathcal{R}(z) \stackrel{\text{def}}{=} (z - \mathcal{L})^{-1} \quad \text{for } z \in \rho(\mathcal{L}), \tag{17a}$$

$$\mathcal{R}_0(z) \stackrel{\text{def}}{=} (z - \mathcal{L}^{\shortparallel} - \mathcal{L}^\perp)^{-1} \quad \text{for } z \in \rho(\mathcal{L}^{\shortparallel} + \mathcal{L}^\perp), \tag{17b}$$

$$\mathcal{R}^\perp(z) \stackrel{\text{def}}{=} (z - \mathcal{L}^\perp)^{-1} \quad \text{for } z \in \rho(\mathcal{L}^\perp), \tag{17c}$$

where ρ denotes the resolvent set. Furthermore, we define a generalized resolvent $\mathcal{G}$ by

$$\mathcal{G}(z) \stackrel{\text{def}}{=} \mathcal{P}\mathcal{R}(z)\mathcal{P} \quad \text{for } z \in \rho(\mathcal{L}). \tag{18}$$

The Laplace transform $\hat{y}^\alpha(z)$ of (16) is then given by

$$\hat{y}^\alpha(z) = \mathcal{R}(z)\, k^\alpha = \mathcal{R}(z)\mathcal{P}k^\alpha, \tag{19}$$

and using the relationship

$$\mathcal{R}(z)\mathcal{P} = \mathcal{G}(z) + \mathcal{R}^\perp(z)\mathcal{P}^\perp\mathcal{V}\mathcal{G}(z), \tag{20}$$

which has been proven in Appendix A, we get

$$\hat{y}^\alpha(z) = \mathcal{G}(z)\, k^\alpha + \mathcal{R}^\perp(z)\mathcal{P}^\perp\mathcal{V}\mathcal{G}(z)\, k^\alpha. \tag{21}$$

On introducing the $(r \times r)$-matrix $\mathbf{G}(t) = \{G^{\alpha\beta}(t)\}$ and its Laplace transform $\hat{\mathbf{G}}(z) = \{\hat{G}^{\alpha\beta}(z)\}$ by

$$\hat{G}^{\alpha\beta}(z) \stackrel{\text{def}}{=} \langle k^\beta \,|\, \mathcal{G}(z) \,|\, k^\alpha \rangle = \langle k^\beta \,|\, \mathcal{R}(z) \,|\, k^\alpha \rangle, \tag{22a}$$

$$G^{\alpha\beta}(t) = \langle k^\beta \,|\, \exp(t\mathcal{L}) \,|\, k^\alpha \rangle, \tag{22b}$$

we obtain the unique decomposition of motion[5]

$$\mathbf{y}(t) = \mathbf{y}^{\shortparallel}(t) + \mathbf{y}^\perp(t) \quad \in \mathbb{L}, \tag{23a}$$

$$\mathbf{y}^{\shortparallel}(t) = \mathbf{G}(t)\,\mathbf{k} \quad \in \mathbb{K}, \tag{23b}$$

$$\mathbf{y}^\perp(t) = \int_0^t dt'\, \mathbf{G}(t - t')\,\mathbf{u}(t') \quad \in \mathbb{K}^\perp, \tag{23c}$$

where

$$u^\alpha(t) \stackrel{\text{def}}{=} \exp(t\mathcal{L}^\perp)\, u^\alpha(0), \tag{24a}$$

$$u^\alpha(0) \stackrel{\text{def}}{=} \mathcal{P}^\perp\mathcal{V}k^\alpha = \mathcal{P}^\perp\mathcal{L}k^\alpha, \tag{24b}$$

and $\mathbf{y}$, $\mathbf{k}$, and $\mathbf{u}$ are r-dimensional vectors with elements y^α, k^α, and u^α, respectively, $\alpha = 1, 2, \ldots, r$.

IV. STRUCTURE OF THE GENERALIZED RESOLVENT

Let $\{\mathcal{E}(\lambda)\}$ be the spectral family associated to the skew-adjoint operator $\mathcal{L}$,

$$\mathcal{L} = i\int_{-\infty}^{\infty} \lambda\, d\mathcal{E}(\lambda), \tag{25}$$

where $\mathcal{E}(\lambda)$ are bounded operators on $\mathbb{L}$ satisfying

$$\mathcal{E}(\lambda) = (\mathcal{E}(\lambda))^*, \tag{26a}$$

$$\mathcal{E}(-\infty) = 0, \quad \mathcal{E}(+\infty) = 1, \tag{26b}$$

$$\mathcal{E}(\lambda+0)=\mathcal{E}(\lambda), \tag{26c}$$

$$\mathcal{E}(\lambda)\mathcal{E}(\mu)=\mathcal{E}(\lambda) \text{ if } \lambda\leq\mu. \tag{26d}$$

With these the resolvent $\mathcal{R}(z)$ is given by

$$\mathcal{R}(z)=\int_{-\infty}^{\infty}\frac{d\mathcal{E}(\lambda)}{z-i\lambda} \tag{27}$$

and the generalized resolvent $\mathcal{G}$ defined by (18) is given by

$$\mathcal{G}(z)=\int_{-\infty}^{\infty}\frac{d\mathcal{J}(\lambda)}{z-i\lambda}, \tag{28}$$

where $\mathcal{J}(\lambda)$ is the restriction of $P\mathcal{E}(\lambda)P$ to the subspace $\mathbb{K}=P\mathbb{L}$,

$$\mathcal{J}(\lambda)f \stackrel{\text{def}}{=} P\mathcal{E}(\lambda)Pf \text{ for all } f\in\mathbb{K}. \tag{29}$$

The *generalized resolution of the identity*[6] $\{\mathcal{J}(\lambda)\}$ is a normalized positive operator valued measure, that is, a one-parameter family of bounded operators $\{\mathcal{J}(\lambda)\}$ acting on the Hilbert space $\mathbb{K}$ and having properties

$$\mathcal{J}(\lambda)=(\mathcal{J}(\lambda))^*, \tag{30a}$$

$$\mathcal{J}(-\infty)=0, \quad \mathcal{J}(+\infty)=1, \tag{30b}$$

$$\mathcal{J}(\lambda+0)=\mathcal{J}(\lambda), \tag{30c}$$

$$\mathcal{J}(\lambda)\leq\mathcal{J}(\mu) \text{ if } \lambda<\mu, \tag{30d}$$

but in contrast to $\mathcal{E}(\lambda)$, the operators $\mathcal{J}(\lambda)$ are, in general, no longer orthogonal projections.

We will use the following characterizations of generalized resolvents in the later sections of this paper[7]: A family of operators $\mathcal{G}(z)$ on a Hilbert space is a generalized resolvent if and only if

$\mathcal{G}(z)$ is holomorphic in each half-plane $\mathrm{Re}(z)>0$ and

$$\mathrm{Re}(z)<0, \tag{31a}$$

$$\mathcal{G}(z^*)=-(\mathcal{G}(-z))^*, \quad \mathrm{Re}(z)\neq 0, \tag{31b}$$

$$\mathcal{G}(z)+(\mathcal{G}(z))^*\geq 0 \text{ for } \mathrm{Re}(z)>0, \tag{31c}$$

$$\text{w-}\lim_{x\to\infty} x\mathcal{G}(x)=1. \tag{31d}$$

It has been shown in Appendix B that the restriction of the generalized resolvent to the subspace $\mathbb{K}=P\mathbb{L}$ can be written as

$$\mathcal{G}(z)=\frac{1}{P(z-L^{\times})P-PVP\mathcal{R}^{\perp}(z)PVP} \tag{32}$$

and it is convenient to write this important relation[8] in the orthonormal basis $\{k^{\alpha}\}$. Introducing the skew-adjoint $(r\times r)$-matrix $\mathbf{L}=\{L^{\alpha\beta}\}$,

$$L^{\alpha\beta}=\langle k^{\beta}|L|k^{\alpha}\rangle, \tag{33}$$

we have from (32)

$$\hat{\mathbf{G}}(z)=(z\mathbf{1}-\mathbf{L}-\hat{\mathbf{F}}(z))^{-1}, \tag{34}$$

where $\mathbf{1}$ is the unit $(r\times r)$-matrix and $\mathbf{F}(z)=\{F^{\alpha\beta}(z)\}$ is defined by

$$\hat{F}^{\alpha\beta}(z)=\langle k^{\beta}|LP^{\perp}\mathcal{R}^{\perp}(z)P^{\perp}L|k^{\alpha}\rangle \tag{35a}$$

$$=\langle u^{\beta}|\mathcal{R}^{\perp}(z)|u^{\alpha}\rangle. \tag{35b}$$

The inverse Laplace transform of (34) then gives an integrodifferential equation for $\mathbf{G}(t)$,

$$\frac{d}{dt}\mathbf{G}(t)=\mathbf{L}\mathbf{G}(t)+\int_0^t dt'\,\mathbf{F}(t-t')\mathbf{G}(t') \tag{36}$$

with $\mathbf{F}(t)=\{F^{\alpha\beta}(t)\}$ defined by

$$F^{\alpha\beta}(t)=\langle k^{\beta}|LP^{\perp}\exp(tL^{\perp})P^{\perp}L|k^{\alpha}\rangle$$

$$=\langle u^{\beta}|\exp(tL^{\perp})|u^{\alpha}\rangle$$

$$=\langle u^{\beta}|u^{\alpha}(t)\rangle \tag{37}$$

We would like to point out here that with our choice $\mathbb{K}\subset\mathbb{D}(L)$, the matrix elements $L^{\alpha\beta}$ are all finite even when the Liouvillian L is an unbounded operator.

V. A REMARK ON THE MARKOV APPROXIMATION AND SEMIGROUP EVOLUTION

At this stage it is interesting to ask under what conditions the motion in the subspace $\mathbb{K}$ is governed by a *semigroup*. An often used heuristic argument proceeds as follows: *Suppose* that the orthogonal decomposition (23) is a decomposition into a slow collective motion $\mathbf{y}^{\parallel}(t)$ in $\mathbb{K}$ and a rapidly fluctuating part $\mathbf{u}(t)$ in $\mathbb{K}^{\perp}$, as was explained in Sec. III. We then expect that the autocorrelation matrix $\mathbf{G}(t)$ of the collective mode $\mathbf{y}^{\parallel}$,

$$G^{\alpha\beta}(t)=\langle y^{\parallel\beta}(0)|y^{\parallel\alpha}(t)\rangle,$$

is a slowly varying function of t relative to the autocorrelation matrix $\mathbf{F}(t)$ of the fluctuating part $\mathbf{u}$,

$$F^{\alpha\beta}(t)=\langle u^{\beta}(0)|u^{\alpha}(t)\rangle.$$

If we assume that $\mathbf{F}(t)$ decays to zero in a time which is short relative to the characteristic time constant T of the motion $\mathbf{y}^{\parallel}(t)$, then we can approximate the integral in (36) by

$$\int_0^t dt'\,\mathbf{F}(t-t')\mathbf{G}(t')\approx\int_0^t dt'\,\mathbf{F}(t')\mathbf{G}(t) \text{ for } t\gg T \tag{38}$$

which amounts to

$$\mathbf{F}(t)\approx F_0\delta(t), \tag{39a}$$

$$F_0\stackrel{\text{def}}{=}\int_0^{\infty}dt\,\mathbf{F}(t)=\hat{\mathbf{F}}(0). \tag{39b}$$

In this so-called *Markov approximation* the reduced motion in $\mathbb{K}$ is governed by the semigroup $\{\mathbf{G}_0(t);\,0\leq t<\infty\}$,

$$\mathbf{G}(t)\approx\mathbf{G}_0(t), \tag{39c}$$

$$\mathbf{G}_0(t)\stackrel{\text{def}}{=}\exp[t(\mathbf{L}+\mathbf{F}_0)], \tag{40a}$$

$$\mathbf{G}_0(t)\,\mathbf{G}_0(t')=\mathbf{G}_0(t+t'), \quad 0\leq t,t'<\infty. \tag{40b}$$

The question now is under what conditions is such an approximation valid. First of all, it is clear that $\mathbf{F}(t)$ cannot decay unless $L^{\perp}$ has a *purely continuous spectrum*. Furthermore, it is easy to show that our assumption (9a), that the subspace $\mathbb{K}$ is contained in the domain $\mathbb{D}(L)$ of L, is *not* compatible with the semigroup property of $\mathbf{G}(t)$.[9] This fact does not imply though that $\mathbf{G}(t)$ cannot be reasonably approximated by the semigroup $\mathbf{G}_0(t)$. However, if we require that in some limiting situation $\mathbf{G}(t)$ is approximated arbitrarily closely by $\mathbf{G}_0(t)$, then there must exist some element $k\in\mathbb{K}$ such that $\|Lk\|$ increases without limit,[10] that is,

if $\mathbf{G}(t) \to \mathbf{G}_0(t)$, then $\|\not\perp k\| \to \infty$ for some $k \in \mathbb{K}$. (41)

This result serves as an important guide in choosing the subspace $\mathbb{K}$ *if we want an approximate semigroup behavior of a collective mode.* However, we have to stress the fact that *the Markov approximation is inconsistent with our basic assumption* $\mathbb{K} \subset \mathbb{D}(\not\perp)$. This warning applies to all commonly used projection methods which are derived under the assumption (explicit or implicit) of differentiability at time $t = 0$, and use of such methods together with a Markov approximation may lead to severe mathematical inconsistencies.

VI. THE STATE SPACE REPRESENTATION

Let us now rewrite Eq. (23) as

$$y(t) = \mathbf{G}(t)\,\mathrm{k} + \int_0^t dt'\, \mathbf{G}(t - t')\,\mathrm{u}(t'), \quad 0 \le t < \infty. \tag{42}$$

It has proven to be fruitful to consider equations of the form (42) as the input–output map of a dynamical system and apply the powerful tools of mathematical system theory.[11] We therefore propose to regard Eq. (42) as a *causal linear time-invariant input–output system.* Following the jargon of mathematical system theory, we will call the r-dimensional vectors $\mathbf{u}(\cdot)$ the *input,* and $\mathbf{y}(\cdot)$ the *output.* The input–output relationship is fixed by the initial condition

$$\mathbf{y}(0) = \mathrm{k} \tag{43}$$

and the so-called *impulse response matrix* $\mathbf{G}(t)$, which in our case is a complex $(r \times r)$-matrix, fulfills, the condition

$$\mathbf{G}(0^+) = 1. \tag{44}$$

The Laplace transform $\hat{\mathbf{G}}(z)$ of the impulse response matrix $\mathbf{G}(t)$ is called the *transfer function matrix.* Following Abel's theorem, Eq. (44) implies

$$\lim_{x \to \infty} x\hat{\mathbf{G}}(x) = 1. \tag{45}$$

By a *state space representation* of a dynamical system we mean a triple $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ connecting the input vector $\mathbf{u}(\cdot)$, the output vector $\mathbf{y}(\cdot)$, and a *state vector* $\mathbf{x}(\cdot)$ by the following relations,

$$\frac{d}{dt}\,\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \tag{46a}$$

$$y(t) = \mathbf{C}\mathbf{x}(t), \qquad 0 \le t < \infty. \tag{46b}$$

The input, the output, and the state are elements of topological vector spaces called the *input space* $\mathbf{U}$, the the *output space* $\mathbf{Y}$ and the *state space* $\mathbf{X}$, respectively,

$$\mathbf{u} \in \mathbf{U}, \quad \mathbf{y} \in \mathbf{Y}, \quad \mathbf{x} \in \mathbf{X}.$$

In the context of the present work, the spaces $\mathbf{U}$, $\mathbf{Y}$, and $\mathbf{X}$ are Hilbert spaces with the input space $\mathbf{U}$ being equal to $\mathbb{K}^\perp$, the output space $\mathbf{Y}$ being equal to the Liouville space $\mathbb{L}$ which is a (proper or improper) subspace of the state space $\mathbf{X}$, that is,

$$\mathbf{U} = \mathbb{K}^\perp, \quad \mathbf{Y} = \mathbb{L}, \quad \mathbb{K}^\perp \subset \mathbb{L} \subset \mathbf{X}. \tag{47}$$

For the Cauchy problem (46a) to be well posed, the transformation $\mathbf{A} : \mathbf{X} \to \mathbf{X}$ has to be the infinitesimal generator of a strongly continuous one parameter semigroup of operators $\mathbf{T}(t)$,

$$\mathbf{T}(t) = \exp(t\mathbf{A}), \quad t \ge 0. \tag{48}$$

Furthermore, $\mathbf{B}$ is a bounded transformation from the input space $\mathbf{U}$ to the state space $\mathbf{X}$ and $\mathbf{C}$ is a bounded transformation from the state space $\mathbf{X}$ to the output space $\mathbf{Y}$. Accordingly, the motion of the state $\mathbf{x}(t)$ is given by

$$\mathbf{x}(t) = \mathbf{T}(t)\,\mathbf{x}(0) + \int_0^t dt'\, \mathbf{T}(t - t')\,\mathbf{B}\mathbf{u}(t'), \tag{49}$$

the impulse response matrix $\mathbf{G}(t)$ by

$$\mathbf{G}(t) = \mathbf{C}\mathbf{T}(t)\,\mathbf{B} = \mathbf{C}\exp(t\mathbf{A})\,\mathbf{B}, \tag{50}$$

and the transfer function matrix $\hat{\mathbf{G}}(z)$ by

$$\hat{\mathbf{G}}(z) = \mathbf{C}(z.\mathbf{1} - \mathbf{A})^{-1}\,\mathbf{B}. \tag{51}$$

The state vector x is an abstract quantity and has *a priori* no direct physical meaning. Intuitively, *the state of a system is the totality of information that is needed to predict the future response of the system to future inputs.* That is, the state $\mathbf{x}(0)$ at time $t = 0$ summarizes all the past effects such that the future behaviour of the system does not depend upon how the system was brought into the state $\mathbf{x}(0)$.

A crucial problem of mathematical system theory is the *realization problem* which is to deduce a state space model (46) from the input–output description (42). A given matrix $\mathbf{G}(\cdot)$ is said to be *realizable* as the impulse response matrix of a linear time-invariant dynamical system if there exists transformations $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ such that a state representation of the form (46) holds. The triple $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ is then called the realization of $\mathbf{G}(\cdot)$. Evidently, if a given matrix $\mathbf{G}(\cdot)$ has one realization, then it has many. Let $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ be a realization of $\mathbf{G}(\cdot)$ on the state space $\mathbf{X}$ and let $\mathbf{X}$ be any invertible bounded transformation, $\mathbf{X} : \mathbf{X} \to \tilde{\mathbf{X}}$ to another Hilbert space $\tilde{\mathbf{X}}$. Then the triple $\{\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}\}$ defined by

$$\tilde{\mathbf{A}} \stackrel{\text{def}}{=} \mathbf{X}^{-1}\mathbf{A}\mathbf{X}, \tag{52a}$$

$$\tilde{\mathbf{B}} \stackrel{\text{def}}{=} \mathbf{X}^{-1}\mathbf{B}, \tag{52b}$$

$$\tilde{\mathbf{C}} \stackrel{\text{def}}{=} \mathbf{C}\mathbf{X}, \tag{52c}$$

is also a realization of $\mathbf{G}(\cdot)$ on the state space $\tilde{\mathbf{X}}$. A system $\{\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}\}$ is said to be equivalent to the system $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ if there exists a bounded transformation $\mathbf{X} : \{\mathbf{A}, \mathbf{B}, \mathbf{C}\} \to \{\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}\}$ fulfilling Eq. (52).

Let $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ be a state space representation with the state space $\mathbf{X}$. Then two states $\mathbf{x} \in \mathbf{X}$ and $\mathbf{x}' \in \mathbf{X}$ are called indistinguishable if they generate the same input–output map, that is, whenever

$$\mathbf{C}\mathbf{T}(t)\,\mathbf{x}(0) + \int_0^t dt'\, \mathbf{T}(t - t')\,\mathbf{B}\mathbf{u}(t')$$

$$= \mathbf{C}\mathbf{T}(t)\,\mathbf{x}'(0) + \int_0^t dt'\, \mathbf{T}(t - t')\,\mathbf{B}\mathbf{u}(t')$$

for all inputs $\mathbf{u} \in \mathbf{U}$ and all $t \in [0, \infty)$. A state space representation $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ is called *irreducible* if no distinct states are indistinguishable in it. Any state space representation can be converted into an irreducible one by throwing away the superfluous states, that is, the original state space $\mathbf{X}$ has to be replaced by the quotient space of $\mathbf{X}$ under the equivalence relation induced by the notion of indistinguishability. Therewith, the following important result follows easily: If

a causal time-invariant linear input–output system has a state space representation (whereby the state space may be infinite-dimensional), then *there exists linear irreducible representations. All irreducible representations* of a given input–output system are equivalent and, furthermore, the state spaces of all irreducible representations are topologically equivalent.[12]

The state space $\mathbb{X}$ of an irreducible representation is *finite-dimensional* if and only if the transfer function matrix $\hat{\mathbf{G}}(z)$ is *rational*. A finite-dimensional dynamical system with a p-dimensional state space $\mathbb{X}$ is always equivalent to a matrix representation $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ where $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ represent time-independent complex matrices of dimensions $(p\times p)$, $(p\times r)$ and $(r\times p)$, respectively. A finite-dimensional realization of $\mathbf{G}(\cdot)$ is *minimal* if its state space has minimal dimension and if $\{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ is a minimal matrix realization then there is no other realization having a matrix $\mathbf{A}$ of minor size. *Any minimal realization is irreducible* and is unique within an equivalence class defined by Eq. (52) where $\mathbf{X}$ is now a $(p\times p)$-dimensional arbitrary nonsingular constant matrix. The dimension of the minimal realization of a rational transfer function matrix is given by

$$\text{minimum}(p) = \text{rank}\begin{vmatrix} \mathbf{G}(0) & \dot{\mathbf{G}}(0) & \ddot{\mathbf{G}}(0) & \cdots \\ \dot{\mathbf{G}}(0) & \ddot{\mathbf{G}}(0) & \dddot{\mathbf{G}}(0) & \cdots \\ \ddot{\mathbf{G}}(0) & \dddot{\mathbf{G}}(0) & \cdot & \cdots \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & & \\ \cdot & & & \end{vmatrix}. \tag{53}$$

All finite-dimensional nonminimal realizations are related to the minimal ones via Kalman's canonical structure theorem.[13]

It is to be noted here that the state $\mathbf{x}(t)$ is not uniquely determined by the input–output relationship. Equations (44) and (50) imply

$$\mathbf{CB} = \mathbf{1} \tag{54}$$

and therefore

$$\mathbf{CBC} = \mathbf{C}, \tag{55a}$$

$$\mathbf{BCB} = \mathbf{B}, \tag{55b}$$

$$(\mathbf{CB})^* = \mathbf{CB}, \tag{55c}$$

so that $\mathbf{B}$ is the generalized inverse of $\mathbf{C}$.[14] The general solution of the output map (46b) is then given by

$$\mathbf{x}(t) = \mathbf{B}\mathbf{y}(t) + (\mathbf{1} - \mathbf{BC})\,\mathbf{w}(t), \tag{56}$$

where $\mathbf{w}(t)$ is arbitrary and the $(p\times p)$ matrix $(\mathbf{1} - \mathbf{BC})$ is idempotent. Therewith the initial state is given by

$$\mathbf{x}(0) = \mathbf{Bk} + (\mathbf{1} - \mathbf{BC})\,\mathbf{w}(0). \tag{57}$$

This nonuniqueness of the state is quite convenient since it gives one enough freedom to define a *simple* fictitious mechanical system that mimics the input–output relationship. We plan to elaborate on this point in the third paper of this series.

We will call the homogeneous part of Eq. (46) the *free motion*,

$$\frac{d}{dt}\,\mathbf{x}_0(t) = \mathbf{A}\mathbf{x}_0(t), \tag{58a}$$

$$\mathbf{x}_0(0) = \mathbf{Bk} + (\mathbf{1} - \mathbf{BC})\,\mathbf{w}(0). \tag{58b}$$

We see then that the *free motion generates the projection of the true motion on the subspace* $\mathbb{K}$,

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}_0(t) \tag{59}$$

and the motion in the complimentary subspace $\mathbb{K}^\perp$ corresponds to the effect of the input $\mathbf{u}(t)$ on the system in the zero state

$$\mathbf{y}(t) = \mathbf{C}\int_0^t dt'\,\exp[(t-t')\,\mathbf{A}]\,\mathbf{B}\mathbf{u}(t'), \quad \mathbf{x}(0) = 0. \tag{60}$$

VII. RECURSIVE ORTHOGONAL DECOMPOSITION OF THE MECHANICAL MOTION

The orthogonal decomposition (23) can easily be iterated in such a way that the whole subspace reached by the motion of the m dynamical variables considered is completely decomposed into orthogonal subspaces of $\mathbb{L}$ of nonincreasing dimensions. In order to arrive at such a decomposition, we consider the time evolution of a set of m_j dynamical variables u_j^α, $\alpha = 1, 2, \ldots, m_j$, under the action of a skew-adjoint Liouvillian L_j,

$$u_j^\alpha(t) \overset{\text{def}}{=} \exp(tL_j)\,u_j^\alpha(0), \quad \alpha = 1, 2, \ldots, m_j, \tag{61}$$

$$L_j = -(L_j)^*. \tag{62}$$

We identify the original dynamical variables a^α with u_1^α and the original Liouvillian L with L_1,

$$u_1^\alpha(0) \overset{\text{def}}{=} a^\alpha(0), \quad \alpha = 1, 2, \ldots, m_0 \overset{\text{def}}{=} m, \tag{63a}$$

$$L_1 \overset{\text{def}}{=} L, \tag{63b}$$

and we assume, for simplicity, that the original dynamical variables $a^\alpha(0)$ are analytic vectors for the Liouvillian L.[15] The set $\mathbb{D}_{an}$ of all analytic elements of L is contained in the domain $\mathbb{D}(L)$ of L,

$$\mathbb{D}_{an} \subset \mathbb{D}(L) \subset \mathbb{L},$$

but is still dense in $\mathbb{L}$ and is invariant under L,

$$L\,\mathbb{D}_{an} = \mathbb{D}_{an}. \tag{64}$$

Let $\mathbb{K}_j$ be the smallest subspace of $\mathbb{L}$ that contains the elements $u_{j-1}^\alpha(0)$, $\alpha = 1, 2, \ldots, m_{j-1}$,

$$\mathbb{K}_j \overset{\text{def}}{=} \{f : f = \sum_{\nu=1}^{m_{j-1}} \lambda^\nu u_{j-1}^\nu(0),\ \lambda^\nu \in \mathbb{C}\}, \tag{65a}$$

$$\dim(\mathbb{K}_j) \overset{\text{def}}{=} m_j \leq m_{j-1}. \tag{65b}$$

We denote the orthogonal projection onto $\mathbb{K}_j$ by P_j,

$$P_j\,\mathbb{L} = \mathbb{K}_j \tag{66}$$

and define a projector $P_j^\perp$ by

$$P_j^\perp \overset{\text{def}}{=} P_{j-1}^\perp - P_j, \tag{67a}$$

$$P_0^\perp \overset{\text{def}}{=} 1. \tag{67b}$$

According to the lemma of Appendix C, there exists an orthonormal basis $\{k_j^\alpha\}$, $\alpha = 1, 2, \ldots, m_j$, of the subspace $\mathbb{K}_j$,

$$\langle k_j^\alpha | k_j^\beta \rangle = \delta^{\alpha\beta}, \quad k_j^\alpha \in \mathbb{K}_j, \quad \alpha = 1, 2, \ldots, m_j, \tag{68}$$

such that

$$\mathbf{k}_j = \mathbf{P}_j (\mathbf{S}_j^i)^{1/2} \mathbf{u}_j(0), \tag{69a}$$

$$\mathbf{u}_j(0) = (S_j)^{1/2} \mathbf{P}_j^* \mathbf{k}_j, \tag{69b}$$

where $\mathbf{k}_j$ is a m_j-dimensional vector with elements k_j^α and $\mathbf{u}_j$ is a m_{j-1}-dimensional vector with elements u_j^α. The $(m_{j-1}\times m_{j-1})$-dimensional Gram matrix $\mathbf{S}_j = \{S_j^{\alpha\beta}\}$ is defined by

$$S_j^{\alpha\beta} \overset{\text{def}}{=} \langle u_j^\beta | u_j^\alpha \rangle, \quad \alpha, \beta = 1, 2, \ldots, m_{j-1} \tag{70}$$

and $\mathbf{S}_j^i$ is its Moore-Penrose pseudoinverse.[16] The $(m_j \times m_{j-1})$-matrix $\mathbf{P}_j$ is a partial isometry[17] of rank $m_j \leq m_{j-1}$ and has properties

$$\mathbf{P}_j \mathbf{P}_j^* = \mathbf{1}_{m_j}, \tag{71a}$$

$$\mathbf{P}_j^* \mathbf{P}_j = \mathbf{S}_j \mathbf{S}_j^i = \mathbf{S}_j^i \mathbf{S}_j, \tag{71b}$$

$$\mathbf{P}_j = \mathbf{P}_j \mathbf{P}_j^* \mathbf{P}_j = \mathbf{P}_j (\mathbf{S}_j \mathbf{S}_j^i)^{1/2} = \mathbf{P}_j (\mathbf{S}_j^i \mathbf{S}_j)^{1/2}, \tag{71c}$$

with $\mathbf{1}_{m_j}$ representing the m_j-dimensional unit matrix. Using Eqs. (61) and (69b), the time evolution of u_j^α is given by

$$\mathbf{u}_j(t) = (\mathbf{S}_j)^{1/2} \mathbf{P}_j^* y_t(t), \tag{72}$$

where

$$y_j^\alpha(t) \overset{\text{def}}{=} \exp(t \mathcal{L}_j) k_j^\alpha. \tag{73}$$

If we now apply the orthogonal decomposition (23) to the motion of $\mathbf{y}_j$ with respect to the subspace $\mathbb{K}_j \subset \mathbb{D}_{an}$, we get

$$y_j(t) = \mathbf{G}_j(t) \mathbf{k}_j + \int_0^t dt' \, \mathbf{G}_j(t - t') \mathbf{u}_{j+1}(t'), \tag{74}$$

where we have introduced the $(m_j \times m_j)$-matrix $\mathbf{G}_j = \{G^{\alpha\beta}\}$,

$$G_j^{\alpha\beta}(t) \overset{\text{def}}{=} \langle k_j^\beta | \exp(t \mathcal{L}_j) | k_j^\alpha \rangle, \quad \alpha, \beta = 1, 2, \ldots, m_j, \tag{75}$$

a m_j-dimensional vector $\mathbf{u}_{j+1}$ with elements

$$u_{j+1}^\alpha(t) \overset{\text{def}}{=} \exp(t \mathcal{L}_{j+1}) u_{j+1}^\alpha(0), \tag{76a}$$

$$u_{j+1}^\alpha(0) \overset{\text{def}}{=} P_j^\perp \mathcal{L}_j k_j^\alpha, \tag{76b}$$

and a skew-adjoint operator $\mathcal{L}_{j+1}$ by

$$\mathcal{L}_{j+1} \overset{\text{def}}{=} \mathcal{L}_j^\perp \overset{\text{def}}{=} P_j^\perp \mathcal{L}_j P_j^\perp. \tag{77}$$

The skew-adjointness of the operator $\mathcal{L}_{j+1}$ follows iteratively from that of $\mathcal{L}$ [compare Eq. (13b)],

$$\mathcal{L}_{j+1} = -(\mathcal{L}_{j+1})^*, \quad j = 1, 2, \cdots \tag{78}$$

and it is to be noted that the domain of the operator $\mathcal{L}_j$ is contained in the domain of $\mathcal{L}$, that is, $\mathbb{D}(\mathcal{L}_j) \subset \mathbb{D}(\mathcal{L})$.

Evidently

$$y_j^\alpha(t) \in \mathbb{K}_{j-1}^\perp, \quad \mathbb{K}_0^\perp \overset{\text{def}}{=} \mathbb{L}, \tag{79a}$$

$$k_j^\alpha \in \mathbb{K}_j \tag{79b}$$

$$u_{j+1}^\alpha \in \mathbb{K}_j^\perp \overset{\text{def}}{=} \mathbb{K}_{j+1}, \tag{79c}$$

so that indeed we have achieved a complete orthogonal decomposition of motion

$$\mathbf{a}(t) = \sum_{j=1}^{\infty} \mathbf{b}_j(t), \tag{80}$$

with

$$\mathbf{b}_j(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{j-2}} dt_{j-1} \, \mathbf{H}_1(t - t_1) \times \mathbf{H}_2(t_1 - t_2) \cdots \mathbf{H}_j(t_{j-1}) \mathbf{k}_j, \tag{81a}$$

where

$$\mathbf{H}_j(t) \overset{\text{def}}{=} (\mathbf{S}_j)^{1/2} \mathbf{P}_j^* \mathbf{G}_j(t) \tag{81b}$$

and the mutually orthogonal elements k_j^α are given by

$$k_{j+1}^\alpha = \mathbf{P}_{j+1} (\mathbf{S}_{j+1}^i)^{1/2} P_j \mathcal{L}_j k_j^\alpha. \tag{81c}$$

The orthogonal expansion (80) corresponds to the orthogonal decomposition of the space $\mathbb{L} = \text{span}\{\exp(t\mathcal{L}) \mathbb{K}_1 : 0 \leq t < \infty\}$ spanned by the motion according to

$$\mathbb{L} = \mathbb{K}_1 \oplus \mathbb{K}_2 \oplus \mathbb{K}_3 \oplus \cdots, \tag{82}$$

with

$$b_j^\alpha(t) \in \mathbb{K}_j, \quad \alpha = 1, 2, \ldots, m_j, \quad 0 \leq t < \infty, \tag{83}$$

and the dimensions $m_1, m_2, m_3, \cdots$ of the mutually orthogonal subspaces $\mathbb{K}_1, \mathbb{K}_2, \mathbb{K}_3, \cdots$ are nonincreasing

$$m \geq m_1 \geq m_2 \geq m_3 \geq \cdots, \tag{84a}$$

$$m_j \overset{\text{def}}{=} \dim(\mathbb{K}_j). \tag{84b}$$

In analogy to Eq. (37c), we define a $(m_{j-1} \times m_{j-1})$-matrix $\mathbf{F}_j(t) = \{F_j^{\alpha\beta}(t)\}$ by

$$F_j^{\alpha\beta}(t) \overset{\text{def}}{=} \langle u_j^\beta(0) | u_j^\alpha(t) \rangle. \tag{85}$$

Then using Eqs. (61), (69b), and (75) we get

$$\mathbf{F}_j(t) = (\mathbf{S}_j)^{1/2} \mathbf{P}_j^* \mathbf{G}_j(t) \mathbf{P}_j (\mathbf{S}_j)^{1/2} \tag{86}$$

so that the integrodifferential Eq. (36) can be written as

$$\frac{d}{dt} \mathbf{G}_j(t) = \mathbf{G}_j(t) \mathbf{L}_j + \int_0^t dt' \, \mathbf{G}_j(t - t') (\mathbf{S}_{j+1})^{1/2} \times \mathbf{P}_{j+1}^* \mathbf{G}_{j+1}(t') \mathbf{P}_{j+1} (\mathbf{S}_{j+1})^{1/2} \tag{87}$$

with the skew-adjoint matrix $\mathbf{L}_j = \{L_j^{\alpha\beta}\}$ defined by

$$L_j^{\alpha\beta} \overset{\text{def}}{=} \frac{d}{dt} G_j^{\alpha\beta}(t) \Big|_{t=0} = \langle k_j^\beta | \mathcal{L}_j | k_j^\alpha \rangle. \tag{88}$$

Thus all matrices $\mathbf{G}_j(t)$ can be expressed in terms of the matrix $\mathbf{G}_1(t) = \mathbf{G}(t)$. In particular, the orthogonal components $\mathbf{b}_j(t)$ can be expressed in terms of the matrix $\mathbf{G}(t)$ and the constant matrices $\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_j$ and $\mathbf{P}_1, \mathbf{P}_2, \ldots, \mathbf{P}_j$. For example, using

$$\mathbf{G}_2(t) \mathbf{k}_2 = \mathbf{G}_2(t) \mathbf{P}_2 (\mathbf{S}_2^i)^{1/2} \mathbf{u}_2 = \mathbf{G}_2(t) \mathbf{P}_2 (\mathbf{S}_2)^{1/2} \mathbf{S}_2^i \mathbf{u}_2$$

and Eqs. (81) and (88), we get

$$\begin{aligned} \mathbf{b}_2(t) &= \int_0^t dt' (\mathbf{S}_1)^{1/2} \mathbf{P}_1^* \mathbf{G}_1(t - t') (\mathbf{S}_2)^{1/2} \\ &\quad \times \mathbf{P}_2^* \mathbf{G}_2(t') \mathbf{P}_2 (\mathbf{S}_2)^{1/2} \mathbf{S}_2^i \mathbf{u}_2 \\ &= (\mathbf{S}_1)^{1/2} \mathbf{P}_1^* \left(\frac{d}{dt} \mathbf{G}(t) - \mathbf{G}(t) \mathbf{L} \right) \mathbf{S}_2^i \mathbf{u}_2 \\ &= (\mathbf{S}_1)^{1/2} \mathbf{P}_1^* \left(\frac{d}{dt} \mathbf{G}(t) - \mathbf{G}(t) \mathbf{L} \right) (\mathbf{S}_2^i)^{1/2} \mathbf{P}_2^* \mathbf{k}_2. \end{aligned}$$

With the state space representation (50) of the matrix $\mathbf{G}(t)$,

$$\mathbf{G}(t) = \mathbf{C} \exp(t\mathbf{A}) \mathbf{B},$$

$$\mathbf{L} = \mathbf{CAB},$$

and noting that $(\mathbf{1} - \mathbf{BC})$ is idempotent and that $(\mathbf{1} - \mathbf{BC})\mathbf{B} = 0$, which follow from (54), we then have

$$\mathbf{b}_1(t) = (\mathbf{S}_1)^{1/2}\,\mathbf{P}_1^{*}\mathbf{C}\exp(t\mathbf{A})\,\mathbf{B}\mathbf{k}_1, \tag{89a}$$

$$\mathbf{b}_2(t) = (\mathbf{S}_1)^{1/2}\,\mathbf{P}_1^{*}\mathbf{C}\exp(t\mathbf{A})(\mathbf{1} - \mathbf{BC})\,\mathbf{AB}(\mathbf{S}_2^{i})^{1/2}\,\mathbf{P}_2^{*}\mathbf{k}_2, \tag{89b}$$

Following the discussions of the previous section, we propose to consider Eq. (74) as a causal linear time-invariant input–output system with input $\mathbf{u}_{j+1}(\cdot)$, output $\mathbf{y}_j(\cdot)$ and a transfer function matrix $\mathbf{G}_j(t)$. The input–output relationship of the system is fixed by the initial condition $\mathbf{y}_j(0) = \mathbf{k}_j$ [compare Eq. (73)]. If the triple $\{\mathbf{A}_j, \mathbf{B}_j, \mathbf{C}_j\}$ is a realization of the transfer function matrix $\mathbf{G}_j$,

$$\mathbf{G}_j(t) = \mathbf{C}_j \exp(t\mathbf{A}_j)\,\mathbf{B}_j, \tag{90}$$

then we have the state space representation

$$\frac{d}{dt}\,\mathbf{x}_j(t) = \mathbf{A}_j\mathbf{x}_j(t) + \mathbf{B}_j\mathbf{u}_{j+1}(t), \tag{91a}$$

$$\mathbf{y}_j(t) = \mathbf{C}_j\mathbf{x}_j(t), \tag{91b}$$

with the state $\mathbf{x}_j$ given by

$$\mathbf{x}_j(t) = \mathbf{B}_j\mathbf{y}_j(t) + (\mathbf{1} - \mathbf{B}_j\mathbf{C}_j)\,\mathbf{w}_j(t), \tag{91c}$$

where $\mathbf{w}_j(t)$ is arbitrary. Thus we have a decomposition of the mechanical motion into a hierarchy of *orthogonal* stationary linear dynamical systems.

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APPENDIX A: DERIVATION OF EQUATION (20)

From the definition (18) of the generalized resolvent $\mathcal{G}(z)$ and Eq. (11c), we have

$$R(z)P = \mathcal{G}(z) + P^{\perp}R(z)P \tag{A1}$$

which, with the second resolvent equation of Hille and Phillips,[18]

$$R(z) = R_0(z) + R_0(z)\,V R(z) \quad \text{for } z \in \rho(L) \cap \rho(L'' + L^{\perp}), \tag{A2}$$

gives

$$R(z)P = \mathcal{G}(z) + P^{\perp}R_0(z)P + P^{\perp}R_0(z)\,V R(z)P. \tag{A3}$$

Now with the definitions (12b) and (12c) of L'' and $L^{\perp}$ we see that

$$[P, L''] = 0, \quad [P, L^{\perp}] = 0, \tag{A4a}$$

$$[P^{\perp}, L''] = 0, \quad [P^{\perp}, L^{\perp}] = 0, \tag{A4b}$$

and therefore

$$[P, R_0(z)] = 0, \quad [P^{\perp}, R_0(z)] = 0, \tag{A5a}$$

$$[P, R^{\perp}(z)] = 0, \quad [P^{\perp}, R^{\perp}(z)] = 0, \tag{A5b}$$

from which we have

$$P^{\perp}R_0(z)P = 0, \tag{A6}$$

so that Eq. (A3) reduces to

$$R(z)P = \mathcal{G}(z) + P^{\perp}R_0(z)\,V R(z)P. \tag{A7}$$

Since $P^{\perp}L''P^{\perp} = 0$, it follows that $P^{\perp}R_0(z)P^{\perp} = P^{\perp}R^{\perp}(z)P^{\perp}$ and therefore with the definition (12d) of V and (A6) we get

$$\begin{aligned} P^{\perp}R_0(z)\,V &= P^{\perp}R_0(z)P^{\perp}LP \\ &= P^{\perp}R^{\perp}(z)P^{\perp}LP \\ &= P^{\perp}R^{\perp}(z)P^{\perp}VP, \end{aligned} \tag{A8}$$

where we have used $P^{\perp}LP = P^{\perp}VP$. Inserting (A8) into (A7) and using the definition of the generalized resolvent $\mathcal{G}(z)$ we then have

$$R(z)P = \mathcal{G}(z) + R^{\perp}(z)P^{\perp}V\mathcal{G}(z)$$

which is Eq. (20).

APPENDIX B: DERIVATION OF EQUATION (32)

On iterating the second resolvent equation (A2) of Hille and Phillips, we have

$$R(z) = R_0(z) + R_0(z)\,V[R_0(z) + R_0(z)\,VR(z)]$$

so that

$$\begin{aligned} PR(z)P = {} & PR_0(z)P + PR_0(z)\,VR_0(z)P \\ & + PR_0(z)PVR_0(z)\,VR(z)P. \end{aligned} \tag{B1}$$

Since $R_0(z)$ commutes with P and $PVP = 0$, the second term on the right side of (B1) vanishes. With $PV = PLP^{\perp} = PVP^{\perp}$ and the fact that $R_0(z)$ also commutes with $P^{\perp}$, we have

$$PVR_0(z) = PVP^{\perp}R_0(z) = PVR_0(z)P^{\perp}$$

and therefore

$$PVR_0(z)\,V = PVR_0(z)P^{\perp}V = PVR_0(z)P^{\perp}VP, \tag{B2}$$

where we have used $P^{\perp}V = P^{\perp}VP$. On inserting (B2) in the last term of the right side of (B1), we get

$$PR(z)P = PR_0(z)P + PR_0(z)PVR_0(z)P^{\perp}VPR(z)P \tag{B3}$$

or

$$\mathcal{G}(z) = PR_0(z)P + PR_0(z)\,VR^{\perp}(z)P^{\perp}VP\mathcal{G}(z), \tag{B4}$$

where we have used $R_0(z)P^{\perp} = R^{\perp}(z)$. Since $PL^{\perp}P = 0$, the first term on the right side of (B4) becomes

$$\begin{aligned} PR_0(z)P = PR_0(z) &= P(z - L'' - L^{\perp})^{-1} \\ &= P(z - L'')^{-1} = (z - L'')^{-1}P \end{aligned} \tag{B5}$$

and we get from (B4)

$$(z - L'')\mathcal{G}(z) = P + PVR^{\perp}(z)P^{\perp}VP\mathcal{G}(z)$$

so that

$$\mathcal{G}(z) = [P(z - L'')P - PVR^{\perp}(z)P^{\perp}VP]^{-1}$$

which is Eq. (32).

APPENDIX C: ORTHOGONALIZATION OF LINEARLY DEPENDENT VECTORS

Lemma: Let u^ν, $\nu = 1, 2, \ldots, m$, be the elements of a Hilbert space, with the inner product $\langle \circ | \circ \rangle$ defined, that span a r-dimensional subspace $\mathbb{K}$,

$$\mathbb{K} \overset{\text{def}}{=} \{v : v = \sum_{\nu=1}^{m} \lambda^\nu u^\nu, \quad \lambda^\nu \in \mathbb{C}\}, \tag{C1}$$

$$r \overset{\text{def}}{=} \dim(\mathbb{K}), \quad r \leq m \leq \infty. \tag{C2}$$

Then the r elements $k^\alpha \in \mathbb{K}$, $\alpha = 1, 2, \ldots, r$,

$$k^\alpha \overset{\text{def}}{=} \sum_{\nu=1}^{m} [\mathbf{P}(\mathbf{S}^i)^{1/2}]^{\alpha\nu} u^\nu \tag{C3}$$

form an orthonormal basis of $\mathbb{K}$,

$$\langle k^\alpha | k^\beta \rangle = \delta^{\alpha\beta}, \quad \alpha, \beta = 1, 2, \ldots, r, \tag{C4}$$

where the $(m \times m)$-matrix $\mathbf{S}$ is the Gram matrix of the elements u^ν,

$$\begin{aligned} &\mathbf{S} \overset{\text{def}}{=} \{S^{\nu\mu}\}, \quad S^{\nu\mu} \overset{\text{def}}{=} \langle u^\mu | u^\nu \rangle, \quad \mu, \nu = 1, 2, \ldots, m \\ &\mathbf{S} = \mathbf{S}^* > 0, \end{aligned} \tag{C5}$$

and $\mathbf{S}^i$ is its Moore–Penrose pseudoinverse.[16] The $(r \times m)$-dimensional matrix $\mathbf{P}$ is a partial isometry[17] having properties

$$\begin{aligned} &\mathbf{P}\mathbf{P}^* = \mathbf{1}_r, \\ &\mathbf{P}^*\mathbf{P} = \mathbf{S}\mathbf{S}^i = \mathbf{S}^i\mathbf{S}, \\ &\mathbf{P} = \mathbf{P}\mathbf{P}^*\mathbf{P} = \mathbf{P}\mathbf{S}\mathbf{S}^i = \mathbf{P}\mathbf{S}^i\mathbf{S} = \mathbf{P}(\mathbf{S}\mathbf{S}^i)^{1/2} = \mathbf{P}(\mathbf{S}^i\mathbf{S})^{1/2}, \\ &r = \operatorname{rank}(\mathbf{S}) = \operatorname{rank}(\mathbf{P}) = \operatorname{tr}(\mathbf{S}\mathbf{S}^i). \end{aligned} \tag{C6}$$

The original elements u^ν in this $\{k^\alpha\}$ basis are given by

$$u^\nu = \sum_{\alpha=1}^{r} [(\mathbf{S})^{1/2}\mathbf{P}^*]^{\nu\alpha} k^\alpha. \tag{C7}$$

Proof of the lemma: Let $\mathbf{U} = \{U^{\nu\mu}\}$ be a unitary $(m \times m)$-matrix that transforms $\mathbf{S}$ into the diagonal form,

$$\mathbf{U}\mathbf{S}\mathbf{U}^* = \mathbf{D}, \quad \mathbf{D} = \{\delta^{\nu\mu} s^\nu\}, \quad \mathbf{U}^* = \mathbf{U}^{-1}. \tag{C8}$$

If $\dim(\mathbb{K}) = r \leq m$, then the r eigenvalues s^ν are nonzero and we may arrange them in such a way that

$$\begin{aligned} &s^\nu > 0 \quad \text{for} \quad \nu = 1, 2, \ldots, r, \\ &s^\nu = 0 \quad \text{for} \quad \nu = r+1, r+2, \ldots, m. \end{aligned}$$

The r elements k^α defined by

$$k^\alpha = \frac{1}{s^\alpha} \sum_{\nu=1}^{m} U^{\alpha\nu} u^\nu, \quad \alpha = 1, 2, \ldots, r \tag{C9}$$

are orthogonal since

$$\langle k^\alpha | k^\beta \rangle = \frac{1}{[(s^\alpha s^\beta)]^{1/2}} (\mathbf{U}\mathbf{S}\mathbf{U}^*)^{\beta\alpha} = \delta^{\alpha\beta}. \tag{C10}$$

Let us define a $(r \times m)$-matrix $\mathbf{V} = \{V^{\alpha\nu}\}$ by

$$\begin{aligned} &V^{\alpha\nu} = 0, \quad \alpha \neq \nu, \\ &V^{\alpha\alpha} = 1, \quad \alpha = 1, 2, \ldots, r, \quad \nu = 1, 2, \ldots, m, \end{aligned} \tag{C11}$$

so that we can write

$$\mathbf{k} = \mathbf{V}(\mathbf{D}^i)^{1/2}\mathbf{U}\mathbf{u}, \tag{C12}$$

where $\mathbf{k}$ is the r-dimensional vector with elements k^α, $\mathbf{u}$ is the m-dimensional vector with elements u^ν, and $\mathbf{D}^i$ is the Moore–Penrose pseudoinverse of $\mathbf{D}$,

$$\begin{aligned} &(D^i)^{\nu\nu} = (s^\nu)^{-1} \quad \text{for } \nu = 1, 2, \ldots, r, \\ &(D^i)^{\nu\mu} = 0 \qquad \text{otherwise.} \end{aligned} \tag{C13}$$

Using the relation $\mathbf{U} f(\mathbf{S}^i) = f(\mathbf{D}^i)\mathbf{U}$ we can rephrase the last result as

$$\mathbf{k} = \mathbf{V}\mathbf{U}(\mathbf{S}^i)^{1/2}\mathbf{u}, \tag{C14}$$

and defining a partial isometry $\mathbf{P}$ by

$$\mathbf{P} \overset{\text{def}}{=} \mathbf{V}\mathbf{U}, \tag{C15}$$

we arrive at the polar decomposition

$$\mathbf{k} = \mathbf{P}(\mathbf{S}^i)^{1/2}\mathbf{u}, \tag{C16}$$

where we have used $\mathbf{P}\mathbf{P}^* = \mathbf{V}\mathbf{V}^* = \mathbf{1}_r$.

The inversion of the relation (C16) follows trivially from the expansion of the vector $\{u^\nu\}$ in the orthonormal basis $\{k^\alpha\}$,

$$u^\nu = \sum_{\alpha=1}^{r} \langle k^\alpha | u^\nu \rangle k^\alpha = \sum_{\alpha=1}^{r} [\mathbf{S}(\mathbf{S}^i)^{1/2}\mathbf{P}^*]^{\nu\alpha} k^\alpha,$$

and with the relation

$$(\mathbf{S}\mathbf{S}^i)^{1/2}\mathbf{P}^* = \mathbf{U}^*(\mathbf{D}\mathbf{D}^i)^{1/2}\mathbf{U}\mathbf{U}^*\mathbf{V}^* = \mathbf{U}^*(\mathbf{D}\mathbf{D}^i)^{1/2}\mathbf{V}^* = \mathbf{U}^*\mathbf{V}^* = \mathbf{P}^*,$$

we finally get the inverse polar decomposition

$$\mathbf{u} = (\mathbf{S})^{1/2}\mathbf{P}^*\mathbf{k}.$$

From the relations given, it follows at once that

$$\mathbf{P}\mathbf{P}^* = \mathbf{1}_r, \quad \mathbf{P}^*\mathbf{P} = \mathbf{S}\mathbf{S}^i = \mathbf{S}^i\mathbf{S},$$

and

$$\mathbf{P} = \mathbf{P}(\mathbf{S}\mathbf{S}^i)^{1/2}, \quad \mathbf{P}^* = (\mathbf{S}^i\mathbf{S})^{1/2}\mathbf{P}^*.$$

Remark: For the particular case $r = m$, we have $\mathbf{P} = \mathbf{1}_m$, and $k^1, k^2, \ldots, k^m$ equals the unique orthogonal basis that minimizes the sum of the squared distances between each u^ν and the corresponding basis elements k^ν,[19]

$$\sum_{\nu=1}^{m} \langle u^\nu - k^\nu | u^\nu - k^\nu \rangle = \text{minimum}.$$

Of course, in this case the Moore-Penrose pseudoinverse $\mathbf{S}^i$ equals the inverse $\mathbf{S}^{-1}$ and $\mathbf{S}^{-1/2}$ is to be understood, as the inverse of the unique positive definite Hermitian square root $\mathbf{S}^{1/2}$ of $\mathbf{S}$.

[1]Generalizations are possible, but can cause severe mathematical difficulties. Nevertheless, many of our considerations can be extended to the more general evolution equation $(d/dt)a(t) = \mathcal{L}\, a(t) + \mathcal{B}\, b(t)$, where $\mathcal{L}$ is the infinitesimal generator of a strongly continuous semigroup of operators in a complex Banach space $\mathbb{L}$ and $\mathcal{B}$ is a bounded operator from an input Banach space to $\mathbb{L}$.

[2]E. Hille and R. S. Phillips, *Functional Analysis and Semigroups* (American Mathematical Society, Providence, R.I., 1957); T. Kato, *Perturbation Theory for Linear Operators* (Springer, Berlin, 1957); S. G. Krein, *Linear Differential Equations in Banach Space* (American Mathematical Society, Providence, R.I., 1971).

[3]It is not too difficult to extend our discussions to the case where $\mathbb{K}$ is an infinite-dimensional subspace. The impulse response matrix $\mathbf{G}(t)$ then corresponds to a Hilbert port. [See A. H. Zemanian, *Realizability Theory of Continuous*

Linear Systems (Academic, New York, 1972).] However, the assumption that $\mathbb{K}$ is contained in the domain $\mathbb{D}(\underline{L})$ of the Liouvillian $\underline{L}$ has far reaching consequences. If $\underline{L}$ is an unbounded operator, then necessarily $\mathbb{D}(\underline{L}) \neq \mathbb{L}$. Nevertheless, the time evolution of a subspace *not* contained in $\mathbb{D}(\underline{L})$ is well defined and shows an interesting behavior which is of substantial physical interest. However, the analysis has to use different methods and is outside the scope intended by this paper.

[4]W. Stenger, "On the projection of a self-adjoint operator," Bull. Amer. Math. Soc. **74**, 369—372 (1968).

[5]A useful measure for the portion of the motion outside of the subspace $\mathbb{K}$ is given by the norm of the fluctuating part $u^{\alpha}(0)$ at the initial time and one easily finds that

$$\sum_{\alpha=1}^{r} \left|\left| u^{\alpha}(0) \right|\right|^2 = \langle (\underline{L} - \langle \underline{L} \rangle)^2 \rangle$$

with the definition of the mean value $\langle \cdot \rangle$ given by

$$\langle \underline{A} \rangle = \sum_{\alpha=1}^{r} \langle k^{\alpha} | \underline{A} | k^{\alpha} \rangle .$$

[6]N. I. Achiser and I. M. Glasmann, *Theorie der linearen Operatoren im Hilbert-Raum* (Akademie—Verlag, Berlin, 1968).

[7]J. A. Sohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, Providence, R.I., 1963); R. Shankwiler, "On the generalized resolvents and an integral representation of Neranlinna," J. Math. Anal. Appl. **40**, 723—734 (1972).

[8]This relation goes back to the paper by W. H. Heitler and S. T. Ma, "Quantum theory of radiation damping for discreet states," Proc. Roy. Irish Acad. **52A**, 109—125 (1949), and plays a crucial role in Mori's theory of time correlation functions and collective motion [See H. Mori, "On correlation theory of transport in non-uniform systems," Phys. Lett. **9**, 136—137 (1964); "Transport, collective motion and Brownian motion," Progr. Theor. Phys. **33**, 423—455 (1965), and "A continued fraction representation of the time-correlation functions," Progr. Theor. Phys. **34**, 399—416 (1965).] However, these pioneering investigations are formal only. Because the Liouvillian is in general an unbounded operator, formal mathematical calculations may be quite dangerous. An evident correctionto Mori's work is the replacement of his operator $\underline{P}^{\perp}\underline{L}$ (in our notation) by $\underline{P}^{\perp}\underline{L}\underline{P}^{\perp}$. Moreover, one has to show that $\underline{L}^{\perp}$ is essentially skew-adjoint (and not only skew-Hermitian) and one also has to care about the domains of the operators used.

[9]L. P. Horowitz and J. P. Marchand, "The decay-scattering systems," Rocky Mountain, J. Math. **1**, 225—53 (1977).

[10]As an example, choose as Liouville space $\mathbb{L}$ the Hilbert space of all square-integrable functions $\phi(x)$, $x \in \mathbb{R}$, and choose as the Liouvillian the essentially skew-adjoint multiplication operator $\underline{L} = -ix$. Let $\mathbb{K}$ be the one-dimensional subspace spanned by the function $k_{\nu}(x) = c(1+x^2)^{-1/2}e^{-\nu x}$, where c is a normalization constant such that $\| k_{\nu} \| = 1$. Now for all $\nu > 0$, $k_{\nu} \in \mathbb{L}$, but only for $\nu > 0$, $k_{\nu} \in \mathbb{D}(\underline{L})$. For $\nu = 0$, $k_0 \notin \mathbb{D}(\underline{L})$ and $G_{\nu=0}(t) = \langle k_0 | e^{t\underline{L}} | k_0 \rangle = c^2 \int_{-\infty}^{\infty} dx\, (1+x^2)^{-1} e^{-itx} = e^{-|t|}$ so that for $t > 0$, $G(t)$ is indeed a semigroup. However, for $\nu \neq 0$, $G_{\nu}(t) = \langle k_{\nu} | e^{t\underline{L}} | k_{\nu} \rangle$ is not a semigroup and for $\nu \to +0$ we have $G_{\nu} \to G_0$ and $\| \underline{L} k_{\nu} \| \to \infty$.

[11]R. E. Kalman, P. L. Falb, and M. A. Arbib, *Topics in Mathematical System Theory* (McGraw Hill, New York, 1969).

[12]V. Jurdjevic, "Causal dynamical systems: irreducible realizations," in *Geometric Methods in System Theory*, edited by D. Q. Mayne and R. W. Brockett (Reidel, Dordrecht, 1973).

[13]R. E. Kalman, "Canonical structures in linear dynamical systems," Proc. Natl. Acad. Sci. (USA) **48**, 596—600 (1962); "Mathematical description of linear dynamical systems," J. Soc. Indust. Appl. Math., Ser. A Control **1**, 152—92 (1963).

[14]C. R. Rao, *Linear Statistical Interference and its Applications* (Wiley, New York, 1973).

[15]An analytic vector f for an (unbounded) linear operator $\underline{L}$ on a Hilbert space $\mathbb{L}$ is an element $f \in \mathbb{L}$ such that $(\underline{L})^n f$ is defined for all n and $\sum_{n=0}^{\infty} (t^n/n!) \| (\underline{L})^n f \| < \infty$ for some $t > 0$. Any skew-adjoint operator has a dense set of analytic vectors. See E. Nelson, "Analytic vectors," Ann. Math. **70**, 572—615 (1959).

[16]E. H. Moore, "On the reciprocal of the general algebraic matrix," Bull. Amer. Math. Soc. **26**, 394—5 (1920). R. Penrose, "A generalized inverse for matrices," Proc. Cambridge Philos. Soc. **51**, 406—13 (1955). A. Albert, *Regression and Moore—Penrose Pseudoinverses* (Academic, New York, 1972).

[17]P. R. Halmos and J. E. McLaughlin, "Partial isometries," Pac. J. Math. **13**, 585—96 (1962).

[18]See Ref. 2, Theorem 5.10.3 of Hille and Phillips.

[19]B. C. Carlson and J. M. Keller, "Orthogonalization procedures and the localization of Wannier functions," Phys. Rev. **105**, 102—3 (1957).

A system theoretic representation of mechanical systems. II. Stochastic interpretation[a)]

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In a previous paper by the authors it was shown that mechanical systems, classical or quantal, can be realized as stationary linear dynamical systems. In this state space representation of mechanical systems, the input space, the output space, and the state space are Hilbert spaces and to make a connection with the language of a mathematical system theory, in which the corresponding spaces are topological vector spaces, it is shown here that the input, the output, and the state of the dynamical systems representing mechanical systems can be interpreted as second order stochastic processes. An orthogonal decomposition of mechanical motion into a deterministic and a purely nondeterministic motion, suggested by the stochastic interpretation, is discussed and it is pointed out that by iterating the decomposition procedure one can obtain a simple model which approximates the true mechanical motion.

I. INTRODUCTION

In a previous paper,[1] to be referred to here as I, we presented a system theoretic representation of mechanical systems. We considered a finite mechanical system whose original dynamics is formulated in an appropriate complex separable Hilbert space $\mathbb{L}$ called the Liouville space. Using suitable orthogonal projection operators P and $P^{\perp}$ we decomposed the Liouville space Liouville space $\mathbb{L}$ into orthogonal subspaces $\mathbb{K}$ and $\mathbb{K}^{\perp}$, $\mathbb{L}=\mathbb{K}\oplus\mathbb{K}^{\perp}$, such that $\mathbb{K}$ contains the "relevant" part of the original motion while the "irrelevant" part is contained in $\mathbb{K}^{\perp}$. It was shown then that the motion $v^{\alpha}(t)\in\mathbb{L}$,

$$v^{\alpha}(t)\stackrel{\text{def}}{=}\exp(tL)k^{\alpha},\quad \alpha=1,2,\ldots,r, \tag{1}$$

where k^{α}, $\alpha=1,2,\ldots,r$, is an orthonormal basis of the r-dimensional subspace $\mathbb{K}$ and the Liouvillian L is a skew-Hermitian (not necessarily bounded) linear operator acting on $\mathbb{L}$, can be uniquely decomposed as

$$\mathbf{y}(t)=\mathbf{G}(t)\,\mathbf{k}+\int_0^t dt'\,\mathbf{G}(t-t')\,\mathbf{u}(t')\in\mathbb{L}, \tag{2a}$$

$$\mathbf{G}(t)\,\mathbf{k}\in\mathbb{K},\quad \int_0^t dt'\,\mathbf{G}(t-t')\,\mathbf{u}(t')\in\mathbb{K}^{\perp}, \tag{2b}$$

where the above equations are to be read as matrix equations with $\mathbf{y}(t)$ and $\mathbf{k}$ being r-dimensional vectors with elements $v^{\alpha}(t)$ and k^{α}, $\mathbf{G}(t)$ is a $(r\times r)$-matrix with elements $G^{\alpha\beta}(t)$,

$$G^{\alpha\beta}(t)\stackrel{\text{def}}{=}\langle k^{\beta}\,|\exp(tL)\,|k^{\alpha}\rangle \tag{3}$$

and $\mathbf{u}(t)$ is also a r-dimensional vector with elements $u^{\alpha}(t)$ defined by

$$u^{\alpha}(t)\stackrel{\text{def}}{=}\exp(tP^{\perp}LP^{\perp})u^{\alpha}(0), \tag{4a}$$

$$u^{\alpha}(0)\stackrel{\text{def}}{=}P^{\perp}Lk^{\alpha}. \tag{4b}$$

Considering the decomposition (2a) of the mechanical motion to be an input–output map of a causal dynamical system, we had arrived at the state space representation of the mechanical system

$$\frac{d}{dt}\mathbf{x}(t)=\mathbf{A}\mathbf{x}(t)+\mathbf{B}\mathbf{u}(t), \tag{5a}$$

$$\mathbf{y}(t)=\mathbf{C}\mathbf{x}(t), \tag{5b}$$

establishing that a mechanical system can be realized as a stationary linear dynamical system with input vector $\mathbf{u}(t)$, output vector $\mathbf{y}(t)$ and state vector $\mathbf{x}(t)$,

$$\mathbf{x}(t)=\mathrm{B}v(t)+(\mathbf{1}-\mathrm{BC})\,\mathbf{w}(t),$$

where $\mathbf{w}(t)$ is arbitrary, and whose impulse response matrix $\mathrm{G}(t)$ is given by

$$\mathrm{G}(t)=\mathrm{C}\exp(t\mathrm{A})\mathrm{B}.$$

In this paper we will present a stochastic interpretation of this system theoretic representation of mechanical systems. In mathematical system theory, the input, output, and state vectors are elements of topological vector spaces called the input space, the output space, and the state space, respectively. In the context of the formulation presented in I, these spaces are Hilbert spaces so that the input, output, and the state are Hilbert space-valued functions. To make connection with the language of mathematical system theory, we propose to show that the input, output, and the state can be interpreted as *second order stochastic process* and that the state space description (5) of the mechanical motion $\mathbf{y}(t)$ represents a *stochastic dynamical system*. Since any stochastic process can be decomposed into a deterministic and a purely nondeterministic process, this stochastic interpretation suggests a decomposition of the mechanical motion into a deterministic motion and a purely nondeterministic motion. We discuss this decomposition in the last section of the paper and conclude that through such a decomposition one can arrive at a much simpler model of the mechanical system which approximates the true motion in an excellent manner.

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In a later paper we will present the application of the theory, developed in I and here, to a quantal many-body system.

II. STOCHASTIC INTERPRETATION

In the language of mathematical system theory, the input $\mathbf{u}(\cdot)$, the output $\mathbf{y}(\cdot)$, and the state $\mathbf{x}(\cdot)$ are elements of topological vector spaces called the *input space* $\mathbb{U}$, the *output space* $\mathbb{Y}$, and the *state space* $\mathbb{X}$, respectively,

$$\mathbf{u}\in\mathbb{U},\quad \mathbf{y}\in\mathbb{Y},\quad \mathbf{x}\in\mathbb{X}.$$

In the context of the system theoretic representation of mechanical systems presented in I, the input space, the output space, and the state space are complex separable Hilbert spaces with the input space $\mathbb{U}$ being equal to the subspace $\mathbb{K}^{\perp}$, the output space $\mathbb{Y}$ being equal to the Liouville space $\mathbb{L}$ which is a (proper or improper) subspace of the state space $\mathbb{X}$, that is, $\mathbb{U}=\mathbb{K}^{\perp}$, $\mathbb{Y}=\mathbb{L}$, $\mathbb{K}^{\perp}\subset\mathbb{L}\subset\mathbb{X}$, so that the input, the output, and the state are Hilbert space-valued functions. In order to make connection with the language of mathematical system theory, we propose to interprete $\mathbf{y}(\cdot)$, $\mathbf{u}(\cdot)$, and $\mathbf{x}(\cdot)$ as *stationary second order stochastic processes*.

Such a reinterpretation can be done without any loss of generality[2] because any second order stationary stochastic process can be considered as *a curve in an appropriate Hilbert space* and any curve in an abstract Hilbert space can be realized as a second order stochastic process.[3]

Consider a probability space (Ω, Σ, μ) where Ω is the sample space of elementary events ω and μ is a probability measure on the σ-algebra Σ,

$$\mu(\Omega)=1.$$

Let $s=s(\omega)$ be a complex-valued random variable relative to the probability space (Ω, Σ, μ),

$$s:\Omega\to\mathbb{C},$$

and let us denote the expectation value of a function $\phi(s)$ by $\epsilon\{\phi\}$,

$$\epsilon\{\phi\}\overset{\text{def}}{=}\int_{\Omega}d\mu(\omega)\,\phi\{s(\omega)\}.$$

We will restrict our attention to random variables with vanishing means and finite second order moments, that is,

$$\epsilon\{s\}=0,\quad \epsilon\{|s|^2\}<\infty,$$

and if any two random variables s_1 and s_2 are μ-equivalent,

$$\epsilon\{|s_1-s_2|^2\}=0,$$

we will regard them as identical.

Now any second order random variable can be considered as an element of the Hilbert space $L_2(\Omega, \mu)$ of complex-valued quadratically μ-integrable functions, endowed with the inner product

$$\langle s_1|s_2\rangle\overset{\text{def}}{=}\epsilon\{s_1^*s_2\}=\int_{\Omega}d\mu(\omega)\,s_1^*(\omega)\,s_2(\omega).$$

The convergence in the norm topology of $L_2(\Omega, \mu)$ coincides with the convergence in the quadratic mean in the sense of probability theory. A *stochastic process* $\{s(t)\}$ is a family of random variables $s(t)$ with t varying over the real axis, that is, $t\in\mathbb{R}$. For every fixed t, the random variable $s(t)$ corresponds to a point in $L_2(\Omega, \mu)$, and therefore the stochastic process $\{s(t),\ t\in\mathbb{R}\}$ describes a *curve* in $L_2(\Omega, \mu)$.

Given the abstract Liouville space $\mathbb{L}$ and the motion $\mathbf{y}(t)$, we can construct a Hilbert space $L_2(\Omega, \mu)$ of an appropriate probability space (Ω, Σ, μ). With the definitions (2), (16) and (22) of I, the elements of the impulse response matrix $\mathbf{G}(\cdot)$ can be written in the form

$$G^{\alpha\beta}(t-t')=\langle y^{\beta}(t')\,|\,y^{\alpha}(t)\rangle, \tag{6a}$$

$$G^{\alpha\beta}(t)=[G^{\beta\alpha}(-t)]^*,\quad \alpha,\beta=1,2,\ldots,r. \tag{6b}$$

The matrix $\mathbf{G}(\cdot)$ is positive definite in the sense of Bochner, that is, for all $(r\times r)$-matrices $\mathbf{R}_j$, $j=1,2,\ldots,m$ and all real numbers $t_1, t_2, \ldots, t_m$, the condition

$$\sum_{j=1}^{m}\sum_{l=1}^{m}\mathbf{R}_j\,\mathbf{G}(t_j-t_l)\,\mathbf{R}_l^{\dagger}\geq 0,\quad m=1,2,\cdots$$

holds. Using the spectral decomposition (25) or (28) of I, we get the representation

$$G^{\alpha\beta}(t)=\int_{-\infty}^{\infty}\exp(i\lambda t)\,dE^{\alpha\beta}(\lambda), \tag{7}$$

where

$$E^{\alpha\beta}(\lambda)\overset{\text{def}}{=}\langle k^{\beta}\,|\,\mathcal{E}(\lambda)\,|\,k^{\alpha}\rangle \tag{8a}$$

$$=\langle k^{\beta}\,|\,\mathcal{J}(\lambda)\,|\,k^{\alpha}\rangle \tag{8b}$$

are complex-valued functions of bounded variation and $E^{\alpha\alpha}(\lambda)$ are real nondecreasing functions. These results imply that $\mathbf{y}(\cdot)$ can be considered as a *second-order stationary stochastic vector process with zero mean value*

$$\epsilon\{y^{\alpha}(t)\}=0, \tag{9}$$

with the *covariance matrix* $\mathbf{G}(t)=\{G^{\alpha\beta}(t)\}$ given by

$$G^{\alpha\beta}(t-t')=\epsilon\{y^{\beta}(t')^*y^{\alpha}(t)\}=\langle y^{\beta}(t')\,|\,y^{\alpha}(t)\rangle. \tag{10}$$

The matrix $\mathbf{E}(\lambda)=\{E^{\alpha\beta}(\lambda)\}$ is called the *spectral distribution matrix* of $\mathbf{y}(t)$. Therewith, the *Cramer representation* of $\mathbf{y}(t)$ is given by

$$y^{\alpha}(t)=\int_{-\infty}^{\infty}\exp(i\lambda t)\,dz^{\alpha}(\lambda), \tag{11}$$

where $\mathbf{z}(\lambda)$ is a uniquely determined vector process with orthogonal increments,

$$z^{\alpha}(-\infty)=0, \tag{12a}$$

$$\epsilon\{z^{\alpha}(\lambda)\}=0, \tag{12b}$$

$$\epsilon\{[z^{\alpha}(t_4)-z^{\alpha}(t_3)]^*[z^{\beta}(t_2)-z^{\beta}(t_1)]\}=0\quad\text{for } t_4>t_3\geq t_2>t_1, \tag{12c}$$

$$\epsilon\{dz^{\alpha}(\lambda)^*\,dz^{\beta}(\lambda)\}=dE^{\alpha\beta}(\lambda). \tag{12d}$$

With these remarks it is clear that the state space description (5) of the mechanical motion $\mathbf{y}(t)$ represents a *stochastic dynamical system whose impulse response matrix* $\mathbf{G}(\cdot)$ *equals the covariance matrix of the second order stochastic vector process* $\mathbf{y}(t)$. This result is valid for quite general classical or quantal systems.

The essential prerequisties are that the original Liouville space is a Hilbert space, the Liouvillian is skew-adjoint, and that the initial conditions belong to the domain of the Liouvillian.

III. ORTHOGONAL DECOMPOSITION INTO A DETERMINISTIC AND A PURELY NONDETERMINISTIC MOTION

It is well known that any stochastic process can be decomposed into a deterministic process and a purely nondeterministic process.[4] Let us denote by $\mathbb{L}(\mathbf{y}, t)$ the closed subspace of $\mathbb{L}$ which is spanned by the random variables $y^1(t'), y^2(t'), \ldots, y^r(t')$, for all $t' \leq t$,

$$\mathbb{L}(\mathbf{y}, t) \stackrel{\text{def}}{=} \operatorname{clos}\{f : f = \sum_{\nu=1}^{r} \lambda^\nu y^\nu(t'), \quad \lambda^\nu \in \mathbb{C}, \quad t' \leq t\}. \tag{13}$$

Evidently, $\mathbb{L}(\mathbf{y}, t_1) \subset \mathbb{L}(\mathbf{y}, t_2)$ whenever $t_1 < t_2$, so that the limiting space $\mathbb{L}(\mathbf{y}, -\infty)$ exists. A stochastic process $\mathbf{s}(\cdot)$ with

$$\mathbb{L}(\mathbf{s}, -\infty) = \mathbb{L}(\mathbf{s}, +\infty) \tag{14}$$

is called a *deterministic process*. If

$$\mathbb{L}(\mathbf{s}, -\infty) \neq \mathbb{L}(\mathbf{s}, +\infty), \tag{15}$$

then $\mathbf{s}(\cdot)$ is called *nondeterministic* and if

$$\mathbb{L}(\mathbf{s}, -\infty) = 0, \tag{16}$$

then $\mathbf{s}(\cdot)$ is called *purely nondeterministic*. Any stochastic vector process can be decomposed uniquely into a sum of a deterministic process and a purely nondeterministic process by a projection. Let $P_{-\infty}$ be the projection operator onto the subspace $\mathbb{L}(\mathbf{y}, -\infty)$ of $\mathbb{L}$ and let us define for every t

$$y^\alpha_{\text{det}}(t) = P_{-\infty} y^\alpha(t) \in \mathbb{L}(y, t), \tag{17a}$$

$$y^\alpha_{\text{pnd}}(t) = (1 - P_{-\infty}) y^\alpha(t) \in \mathbb{L}(y, t), \qquad \alpha = 1, 2, \ldots, r. \tag{17b}$$

Evidently, $\mathbf{y}_{\text{det}}(\cdot)$ is a deterministic process and $\mathbf{y}_{\text{pnd}}(\cdot)$ is a purely nondeterministic process orthogonal to $y_{\text{det}}(\cdot)$,

$$\mathbf{y}(t) = \mathbf{y}_{\text{det}}(t) + \mathbf{y}_{\text{pnd}}(t), \tag{17c}$$

$$\mathbf{y}_{\text{det}}(t) \perp \mathbf{y}_{\text{pnd}}(t') \quad \text{for all } t, t' \in \mathbb{R}, \tag{18a}$$

or

$$\epsilon\{y^\alpha_{\text{det}}(t)^* \; y^\beta_{\text{pnd}}(t')\} = \langle y^\alpha_{\text{det}}(t) \mid y^\beta_{\text{pnd}}(t') \rangle = 0, \quad \text{for all } t, t' \in \mathbb{R}, \quad \alpha, \beta = 1, 2, \ldots, r. \tag{18b}$$

With this, the Hilbert space $\mathbb{L}(\mathbf{y}, t)$ can be decomposed as

$$\mathbb{L}(\mathbf{y}, t) = \mathbb{L}(\mathbf{y}_{\text{det}}, t) \oplus \mathbb{L}(\mathbf{y}_{\text{pnd}}, t). \tag{19}$$

A related decomposition of the motion $\mathbf{y}(\cdot)$ corresponds to the Lebesgue decomposition. The extension of Lebesgue's decomposition to matrix-valued functions is due to Cramer[5] which allows one to decompose the spectral distribution matrix $\mathbf{E}(\lambda)$ into a decrete $\mathbf{E}_d(\lambda)$, a singular $\mathbf{E}_s(\lambda)$, and an absolutely continuous $\mathbf{E}_a(\lambda)$ spectral distribution matrix,

$$\mathbf{E}(\lambda) = \mathbf{E}_d(\lambda) + \mathbf{E}_s(\lambda) + \mathbf{E}_a(\lambda). \tag{20}$$

Correspondingly, we can decompose the stochastic vector process $\mathbf{y}(t)$ into three independent stochastic vector processes $\mathbf{y}_d(t)$, $\mathbf{y}_s(t)$, and $\mathbf{y}_a(t)$,

$$\mathbf{y}(t) = \mathbf{y}_d(t) + \mathbf{y}_s(t) + \mathbf{y}_a(t), \tag{21}$$

having spectral distribution matrices $\mathbf{E}_d$, $\mathbf{E}_s$, and $\mathbf{E}_a$, respectively. The components $\mathbf{y}_d(\cdot)$ and $\mathbf{y}_s(\cdot)$ are always *deterministic*. If the absolutely continuous part $\mathbf{y}_a(\cdot)$ has maximal rank, it is *purely nondeterministic* if and only if

$$\int_{-\infty}^{\infty} \log[\det \mathbf{f}(\lambda)](1 + \lambda^2)^{-1} \, d\lambda \gg -\infty, \tag{22}$$

where $\mathbf{f} = \{f^{\alpha\beta}\}$ and $f^{\alpha\beta}(\lambda) = dE_a^{\alpha\beta}(\lambda)/d\lambda$.

The singular continuous component $\mathbf{y}_s(\cdot)$ is very pathological and has not been encountered in physics so far. It is evident then that if $\mathbf{G}(\cdot)$ possesses a finite-dimensional realization, then $\mathbf{y}(\cdot)$ is deterministic. The purely nondeterministic part is due to the continuous part of the spectrum of the Liouvillian L.

The stochastic state representation of a mechanical many-body system is a powerful tool for the development of consistent approximative methods. *Any consistent approximative model for the true mechanical motion can be rephrased in terms of a relevant motion characterized by a subspace of the Liouville space and a prediction problem for the stochastic input process* $\mathbf{u}(\cdot)$. In order to pursue this problem it is necessary to iterate the projection procedure, in the fashion described in the last section of I, until the new input is very erratic. The main question is what is to be understood by an "erratic" function. *We will call a stochastic process "erratic" if it has such a high computational complexity*[6] *that, within the problem under discussion, it is not feasible to distinguish it from a completely nondeterministic stochastic process.* Of course, the replacement of a deterministic but erratic stochastic process by a completely nondeterministic process amounts to making an approximation and it is our claim that every consistent approximation, that is, every approximation without intrinsic inconsistencies, is of this type. Consider a consistent model and let $\mathbf{s}(t)$ be the final input in its system theoretic representation. Then it is useful to consider $\mathbf{s}(\cdot)$ as a filtered white noise so that $\mathbf{s}(\cdot)$ has to be represented as the output of a causal and causally invertible linear filter with white noise input. The impulse response matrix $\mathbf{H}(t)$ of the filter involved fulfills the equation

$$\int_{-\infty}^{\infty} dt' \, \mathbf{H}(t - t') \, \mathbf{H}(t') = \mathbf{G}_s(t), \tag{23}$$

where $\mathbf{G}_s(\cdot)$ is the covariance matrix of the vector process $\mathbf{s}(\cdot)$.[7]

A very useful and consistent approximation can be obtained by changing the spectrum of the Liouvillian L. Let $f \in \mathbb{L}$ be a cyclic vector for the maximum Abelian Neumann algebra generated by the spectral family of the Liouvillian L described by Eq. (26) of I. We define a measure μ by

$$\mu(\lambda) \stackrel{\text{def}}{=} \langle f \mid \mathcal{E}(\lambda) \mid f \rangle, \tag{24}$$

so that $\mu(\cdot)$ is a distribution function in the sense of probability theory and it can be uniquely decomposed into a step function with a countable number of steps,

an absolutely continuous part μ_a, and a continuous singular function. Since the continuous singular part is always absent in practical problems, $\mu(\cdot)$ can be written as

$$\mu(\lambda) = \sum_{\nu=1}^{\infty} \mu_\nu \theta(\lambda - \lambda_\nu) + p_a \mu_a(\lambda), \tag{25a}$$

where

$$\sum_{\nu=1}^{\infty} \mu_\nu = p_d \leq 1, \quad \mu_\nu > 0 \tag{25b}$$

$$p_d + p_a = 1, \tag{25c}$$

and $\theta(\cdot)$ is a step function defined by $\theta(x) = 1$ for $x \geq 0$ and $\theta(x) = 0$ for $x < 0$. In many practical problems, the discrete spectrum $\{\lambda_1, \lambda_2, \cdots\}$ of the Liouvillian contains a part, say $\{\lambda_{p+1}, \lambda_{p+2}, \cdots\}$, which is extremely narrowly spaced. The characteristic function $\phi_{nd}(t)$ of the narrowly spaced discrete part μ_{nd} of the measure μ has an exorbitantly long recurrence time,

$$\mu_{nd}(\lambda) \stackrel{\text{def}}{=} p_{nd}^{-1} \sum_{\nu=p+1}^{\infty} \mu_\nu \theta(\lambda - \lambda_\nu), \tag{26a}$$

$$p_{nd} \stackrel{\text{def}}{=} \sum_{\nu=p+1}^{\infty} \mu_\nu, \tag{26b}$$

$$\phi_{nd}(t) \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} \exp(it\lambda)\, d\mu_{nd}(\lambda), \tag{26c}$$

and, typically, the characteristic function ϕ_{nd} fulfills an inequality of the type

$$\phi_{nd}(t) < \epsilon \quad \text{for } T_1 \leq t \leq T_2. \tag{27}$$

Now if $T_2 \gg T_1$ where T_2 is astronomically large and T_1 is of the order of a relaxation time observable in the laboratory and if, furthermore, ϵ is a very small number, $0 < \epsilon \leq 1$, then we can replace ϕ_{nd} by a characteristic function ϕ_{na} of an absolutely continuous distribution μ_{na}. A convenient definition for ϕ_{na} is, for example,

$$\phi_{na}(t) \stackrel{\text{def}}{=} \exp(-t^2/2T^2)\, \phi_{nd}, \tag{28}$$

where T is some number satisfying the condition

$$T_1 \ll T \ll T_2 \tag{29a}$$

such that we have

$$|\phi_{nd}(t) - \phi_{na}(t)| < \epsilon \quad \text{for } 0 \leq t \leq T_2. \tag{29b}$$

The above inequality implies[8] that

$$\int_{-\infty}^{\infty} |\mu_{nd}(\lambda) - \mu_{na}(\lambda)|\, d\lambda \lesssim \pi/T_2 \tag{30}$$

and therefore the discrete measure μ_{nd} is well approximated by the absolutely continuous measure μ_{na},

$$\mu_{na}(\lambda) = p_{nd}^{-1} \sum_{\nu=p+1}^{\infty} \mu_\nu \Phi(T(\lambda - \lambda_\nu)), \tag{31}$$

where $\Phi(x) = (2\pi)^{-1/2} \int_{-\infty}^{x} \exp(-\frac{1}{2}y^2)\, dy$ is the Gaussian distribution. It is reasonable in this case to replace the Liouvillian L by a skew-adjoint operator $\tilde{L}$ having the spectral decomposition

$$\tilde{L} = i \int_{-\infty}^{\infty} \lambda\, d\tilde{\mathcal{E}}(\lambda), \tag{32a}$$

with

$$\langle f | \tilde{\mathcal{E}}(\lambda) | f \rangle = \tilde{\mu}(\lambda), \tag{32b}$$

where f is the same cyclic vector as in (24) and $\tilde{\mu}$ is the measure obtained from μ by replacing μ_{nd} by μ_{na},

$$\tilde{\mu}(\lambda) = \sum_{\nu=1}^{p} \mu_\nu \theta(\lambda - \lambda_\nu) + p_{nd} \mu_{na}(\lambda) + p_a \mu_a(\lambda). \tag{32c}$$

This then suggests the replacement of the covariance matrix $\mathbf{G}(\cdot)$ by a new covariance matrix $\tilde{\mathbf{G}}(\cdot)$ having the representation

$$\tilde{G}^{\alpha\beta}(t) = \int_{-\infty}^{\infty} \exp(it\lambda)\, d\tilde{E}^{\alpha\beta}(\lambda),$$

$$\tilde{E}^{\alpha\beta}(\lambda) \stackrel{\text{def}}{=} \langle k^\beta | \tilde{\mathcal{E}}(\lambda) | k^\alpha \rangle. \tag{33a}$$

By such a procedure it is always possible to construct a new model in which the deterministic erratic stochastic process $\mathbf{s}(t)$ is replaced by a completely nondeterministic stochastic process $\tilde{\mathbf{s}}(t)$. If all the conditions stated are fulfilled, then for all practical purposes, that is, for all reasonable observables, one can obtain a much simpler model that approximate the true motion for $0 \leq t < T_2$ in an excellent manner, and rigorous bounds for such a consistent approximation can be found for many particular applications.

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[1] D. K. Saraswati and H. Primas, "A system theoretic representation of mechanical systems: I. Decomposition of a mechanical system into a hierarchy of orthogonal stationary linear dynamical systems," J. Math. Phys. **19**, 2646 (1978).

[2] In many problems of quantum mechanics the Liouville space $\mathfrak{L}$ is not only a Hilbert space but is also a (noncommutative) *-algebra, often a Hilbert algebra. Though we do not make any use of this additional structure here, we will have to care that we keep the original ordering.

[3] J. L. Doob, *Stochastic Processes* (Wiley, New York, 1953); Yu. A. Rozanov, *Stationary Random Processes* (Holden Day, San Francisco, 1967).

[4] H. Cramer, "On some classes of nonstationary stochastic processes," Proceedings of the Fourth Berkeley Symposium on Statistics and Applied Probability **2**, 57—78 (1960); "On the structure of purely nondeterminstic stochastic processes." Arkiv fur Matematik, **4**, 249—66 (1961).

[5] H. Cramer, "On the theory of stationary random processes," Ann. Math. **41**, 215—30 (1940).

[6] Computational complexity is to be understood as the minimal-program complexity in the sense of A. Kolmogorov and G. Chaitin. Compare the review given by C. P. Schnorr, *Zufalligkeit und Wahrscheinlichkeit. Eine algorithmische Begrundung der Wahrscheinlichkeitstheorie* (Springer, Berlin, 1971).

[7] This is a well known and much discussed problem in linear filtering and estimation theory. Extensive references can be found in the excellent review article by T. Kailath, "A view of three decades of linear filtering theory," IEEE Transactions on Information Theory, IT-20, 146—81 (1974).

[8] C. G. Essen, "Fourier analysis of distribution functions. A mathematical study of the Laplace—Gaussian law," Acta Math. **77**, 1—125 (1965).

On the relativistic Boltzmann equation

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Using harmonic analysis techniques, we construct orthogonal polynomials on Minkowski's hyperboloid in order to interpret in the framework of the theory of group representation the tensorial polynomials introduced by Marle for the resolution of the relativistic Boltzmann equation by the Grad method. Calculations are performed in an adapted coordinate system by using zonal spherical functions on the hyperboloid of Minkowski, which as a matter of fact are Jacobi polynomials. Moreover, the homogeneous components of the Maxwell distribution function give an interpretation of Juttner's formulas and, consequently, of the thermodynamic quantities of the fluid.

INTRODUCTION

This paper on the relativistic Boltzmann equation deals with the Grad method of resolution[1] adapted by Marle[2] to the relativistic case.

Grad's method consists in trying to find a solution of the nonrelativistic equation as an expansion in a series of orthogonal polynomials in an N-dimensional space that, in the case when $N=1$, reduces to Hermite polynomials.

In the framework of general relativity, Marle[2] has introduced a family of orthogonal tensorial polynomials, $H^{\alpha_1,\alpha\cdots\alpha_n}$ such that the system of functions

$$L^{\alpha_1,\alpha_2\cdots\alpha_n}=\nu(\mu)\,H^{\alpha_1,\alpha_2\cdots\alpha_n}$$

is complete in the space of square integrable functions on the Minkowski hyperboloid. $\nu(\mu)$ stands for the Maxwell distribution function.

Marle's calculations are rather complicated and are of practical use only for the very first polynomials. Stewart[3] and Anderson[4] have given a construction for these polynomials.

In our work, we have tried to look for the origin of Marle's polynomials. Apparently, they can be obtained in the framework of the theory of group representation by the consideration of spherical functions on the Minkowski hyperboloid.

Our work runs as follows:

(1) The first part is essentially a brief summary of the relativistic Boltzmann equation and of the Grad method of resolution adapted by Marle to the relativistic case.

(2) In the second part, we construct orthogonal polynomials on Minkowski's hyperboloid.

In this paper, calculations are performed in a special coordinate system. Their covariant form will be given later and will be useful to give an interpretation of Marle's polynomials.

(a) First of all, we notice that the distribution function of a Maxwell–Boltzmann fluid (as well as that of a quantum fluid of bosons or fermions) is invariant under the action of the group SO(3) which leaves stationary the velocity vector U^α of the fluid. This leads us to the consideration of the homogeneous space $G/\mathrm{SO}(3)$, G being the orthochronous Lorentz group that acts transitively on the Minkowski hyperboloid.

(b) It is known that most of the special functions may be interpreted in the framework of group representations using the zonal spherical functions $\mathscr{K}_\sigma$ as a starting point. Thus, with harmonic analysis techniques, we first study the zonal functions on the Minkowski hyperboloid. When $\sigma=n$ is a nonnegative integer, then these zonal functions $\mathscr{K}_n$ are polynomials of degree n, and we prove that when n is even, they coincide with the Jacobi polynomials. In particular, we obtain a Rodrigues formula and indicate the connection with Gegenbauer polynomials, precisely the special functions associated with the group SO(3).

(c) Using the zonal functions $\mathscr{K}_n$, we determine the components of degree n, $\mathfrak{M}_n$, of the Maxwell distribution function. It is remarked that $\mathfrak{M}_0$ and $\mathfrak{M}_1$ are Juttner's first two integrals.[5] Thus $\mathfrak{M}_1$ corresponds to the density r of the fluid. As for $\mathfrak{M}_2$, it is the quantity rf where f is the index of the fluid introduced by Lichnerowicz.[6]

(d) With the homogeneous components $\mathfrak{M}_n$, we can construct orthogonal polynomials on the Minkowski hyperboloid, which enables us to rediscover Marle's polynomials in a special coordinate system.

The main references concerning the relativistic Boltzmann equation used here are Refs. 7–16.

I. THE RELATIVISTIC BOLTZMANN EQUATION

Space–time is a four-dimensional manifold V_4, supposed to be orientable (we also assume time orientability), and endowed with a hyperbolic metric ds^2 of class C^h where h is sufficiently large, such that

$$ds^2=(\omega_0)^2-(\omega_1)^2-(\omega_2)^2-(\omega_3)^2.$$

The ω_α constitute a Pfaffian system of local, linearly independent forms. In a system of local coordinates, we have

$$ds^2=g_{\alpha\beta}dx^\alpha dx^\beta.$$

∇ stands for the covariant derivation defined by the metric connection and $\Gamma^\alpha_{\beta\gamma}$ for the corresponding Christoffel symbols. We denote by $T_x(V_4)$ the tangent space at a point $x\in V_4$ and by $T(V_4)$ the tangent bundle, Lichnerowicz.[17] Let us con-

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sider a chart in V_4 in which the local coordinates are x^α (the Greek tensorial indices run for 0, 1, 2, 3 and the Latin ones for 1, 2, 3). In this chart, the local coordinates will always be such that the vector ∂_0 will be timelike and future directed, and that the tetrad $(\partial_0, \partial_1, \partial_2, \partial_3)$ will be positively oriented. (We write ∂_α for $\partial/\partial x^\alpha$.)

We consider a fluid composed of identical particles of proper mass m moving in the background gravitational field. We assume $m \neq 0$. The state of a particle is supposed to be entirely determined by its position $x \in V_4$ and its momentum $p \in T_x(V_4)$. The momentum being such that

$$g_{\alpha\beta} p^\alpha p^\beta = m^2, \tag{1}$$

the vector p^α lies on the upper sheet Ω_x of the two-sheeted hyperboloid defined by (1).

The phase space of one particle is the fiber bundle

$$\Omega = \bigcup_{x \in V_4} \Omega_x$$

over the base V_4 with the Lorentz orthochronous group as the structural group. The elements of volume in V_4 and $T_x(V_4)$ are given respectively by the forms

$$\nu = |g|^{1/2} \left(\bigwedge_\alpha dx^\alpha \right), \quad \bar{\omega} = |g|^{1/2} \left(\bigwedge_\alpha dp^\alpha \right),$$

and the volume element in Ω_x by a form ω satisfying the relation

$$dF \wedge \omega = \bar{\omega} \quad F = \tfrac{1}{2} g_{\alpha\beta} p^\alpha p^\beta.$$

The form ω may be written

$$\omega = \frac{1}{p_0} |g|^{1/2} \left(\bigwedge_i dp^i \right), \quad p_\alpha = g_{\alpha\beta} p^\beta. \tag{2}$$

Using a hyperbolic coordinate system, the p components are given by

$$\begin{aligned} p^0 &= m \cosh\theta, & 0 \leqslant \varphi < 2\pi, \\ p^1 &= m \sinh\theta \sin\psi \sin\varphi, & 0 \leqslant \psi < \pi, \\ p^2 &= m \sinh\theta \sin\psi \cos\varphi, & 0 \leqslant \theta < \infty, \\ p^3 &= m \sinh\theta \cos\psi, \end{aligned} \tag{3}$$

and the form ω by

$$\omega = m \sinh^2\theta \sin\psi \, d\theta \wedge d\psi \wedge d\varphi. \tag{4}$$

We suppose that the particles interact by collisions only. When the motion of a particle is free, its trajectory in phase space is a solution of the differential system

$$\frac{dx^\alpha}{ds} = p^\alpha, \quad \frac{dp^\alpha}{ds} = -\Gamma^\alpha_{\beta\gamma} p^\beta p^\gamma. \tag{5}$$

The trajectory is a force line of the vector field

$$X(x^\alpha, -\Gamma^\alpha_{\beta\gamma} p^\beta p^\gamma)$$

on Ω_x.

The state of the fluid is described by a positive scalar function $\nu(p)$ which is defined on Ω_x. $\nu(p)$ is the momentum distribution function. The evolution law of the fluid is the Boltzmann equation that $\nu(p)$ must satisfy. It is written

$$\mathcal{L}_X \nu = \mathcal{I}(\nu), \tag{6}$$

where $\mathcal{L}_X$ is the Lie derivative by the vector field X,[17] and $\mathcal{I}(\nu)$ is an integral operator representing the collisions.[18]

II. MACROSCOPIC DESCRIPTION OF A RELATIVISTIC FLUID

In this paper, we adopt Marle's[18] and Synge's[19] viewpoint; i.e., all thermodynamical quantities of the fluid are scalars which must be evaluated in the rest frame of the fluid. The relativistic Maxwell distribution function is

$$\nu = a \exp\{-(y/m) p^\alpha U_\alpha\}, \tag{7}$$

where a and y are two scalars, U^α a unitarity future directed vector representing the speed of the fluid. The temperature T of the fluid is related to the coefficient y by

$$y = \frac{mc^2}{kT}, \tag{8}$$

c is the speed of light in vacuum and k the Boltzmann constant. The distribution function ν corresponds to a description at the microscopic scale. At the macroscopic one, tensor-valued functions are used: They are the moments of the distribution function. The moment of order n is defined by

$$I^{\alpha_1\alpha_2\cdots\alpha_n} = \int_{\Omega_x} \nu p^{\alpha_1} p^{\alpha_2} \cdots p^{\alpha_n} \omega. \tag{9}$$

Synge[19] has indicated how to perform the calculation of these moments: We have

$$I^{\alpha_1\alpha_2\cdots\alpha_n} = (-1)^n m^n \frac{\partial^n I}{\partial(y U_{\alpha_1}) \partial(y U_{\alpha_2}) \cdots \partial(y U_{\alpha_n})}, \tag{10}$$

the quantity I being defined by

$$I = \int_{\Omega_x} \nu \omega. \tag{11}$$

Pichon and Marle have obtained the general formula[20]

$$I^{\alpha_1\alpha_2\cdots\alpha_n} = 4\pi a m^{n+2} \sum_{j=0}^{E(n/2)} (-1)^j \times \frac{K_{n+1-j}(y)}{y^{j+1}} \{(n-2j) U_j g\}^{\alpha_1\alpha_2\cdots\alpha_n}. \tag{12}$$

$E(n/2)$ stands for the entire part of $n/2$, $K_n(y)$ is the modified Bessel function of the second kind and order n (see Watson[21]),

$$K_n(y) = \int_0^\infty \exp(-y \cosh\theta) \cosh n\theta \, d\theta. \tag{13}$$

The symbol $\{(n-2j) U_j g\}^{\alpha_1\alpha_2\cdots\alpha_n}$ represents the symmetric tensor constructed by the symmetrized tensorial product of $(n-2j)$ times the vector U^α and j times the tensor $g^{\alpha\beta}$.

Let us introduce the functions φ_l defined by

$$\varphi_l=\int_0^\infty \exp(-y\cosh\theta)\sinh^2\theta\cosh^l\theta d\theta. \tag{14}$$

They satisfy the recurrence formula

$$y(\varphi_{l+2}-\varphi_l)=(l+3)\varphi_{l+1}-l\varphi_{l-1} \tag{15}$$

so that we may write the Juttner formulas for a Maxwell–Boltzmann fluid

$$r=A\varphi_1,\quad E=\frac{c^2}{\varphi_1}(\varphi_2-\varphi_1),\quad P=\frac{Ac^2}{3}(\varphi_2-\varphi_0), \tag{16}$$

where A is a positive constant, E the proper specific energy, r the proper material density, and P the pressure of the fluid.

Later on, it will be convenient to use the index f of the fluid which have been defined by Lichnerowicz,[22]

$$c^2rf=(c^2+E)r+P. \tag{17}$$

Using (16) we may write

$$f\varphi_1=\Phi,$$

where $3\Phi=4\varphi_2-\varphi_0$ (18)

III. APPLICATION OF THE GRAD METHOD OF RESOLUTION OF THE RELATIVISTIC BOLTZMANN EQUATION

Marle has adapted the GRAD method to the relativistic case: Let $n(u^\alpha)$ be the velocity distribution function. The method consists in trying to find a solution of the relativistic Boltzmann equation as an expansion in a series

$$n=n_0\left(\alpha+\alpha_\lambda H^\lambda+\cdots+\frac{1}{p!}\alpha_{\lambda_1\lambda_2\cdots\lambda_p}H^{\lambda_1\lambda_2\cdots\lambda_p}+\cdots\right), \tag{19}$$

where n_0 is the velocity distribution function at the thermodynamical equilibrium,

$$n_0=a\exp(-y u_\alpha U^\alpha). \tag{20}$$

The α are tensors which are functions only of the position $x\in V_4$, and the H are tensorial polynomial functions of P and of the parameters y and U^α.

By carrying the expression (19) into the Boltzmann equation, we obtain an infinite series of partial differential equations which lead to the determination of the tensors α.

As far as the tensorial polynomials H are concerned, they are defined by the following theorem:

Marle's theorem[23]: Let u^α, U^α be two unitary future directed vectors and y a positive constant. There is a unique set of tensors $H^{\lambda_1\lambda_2\cdots\lambda_p}$ $(p=0,1,2,\ldots,\infty)$ entirely symmetric, and such that

(a) the components $H^{\lambda_1\lambda_2\cdots\lambda_p}$ are polynomials of degree p with respect to the four variables u^α, where the term of the highest degree is $u^{\lambda_1}u^{\lambda_2}\cdots u^{\lambda p}$. Conventionally, $H=1$ for $p=0$.

(b) They possess the orthogonality property

$$(H^{\lambda_1\lambda_2\cdots\lambda_p},H^{\mu_1\mu_2\cdots\mu_q})=\int_{\Omega_x}\exp(-y u_\alpha U^\alpha)\times H^{\lambda_1\lambda_2\cdots\lambda_p}H^{\mu_1\mu_2\cdots\mu_q}\omega=0, \tag{21}$$

when $p\neq q$.

(c) The family of functions

$$L^{\lambda_1\lambda_2\cdots\lambda_p}=\exp\left\{-\frac{y}{2}u_\alpha U^\alpha\right\}H^{\lambda_1\lambda_2\cdots\lambda_p} \tag{22}$$

is complete in the space of square integrable functions defined on Ω_x.

IV. ORTHOGONAL POLYNOMIALS ON MINKOWSKI's HYPERBOLOID

Preliminaries

The orthochronous Lorentz group G acts transitively on the upper sheet Ω_x on the hyperboloid

$$u^\alpha u_\alpha=1,\quad u^0>0.$$

Moreover, the Maxwell distribution function is invariant under the action of the group SO(3) which leaves stationary the velocity vector U^α of the fluid. This leads us quite naturally to the consideration of the homogeneous space $G/\mathrm{SO}(3)$, Helgason.[24]

Using the techniques of harmonic analysis, we can obtain a decomposition of the Maxwell distribution function. This decomposition is expressed in terms of the zonal spherical functions on the homogeneous space $G/\mathrm{SO}(3)$ and leads us to complete expressions for the moments of the Maxwell distribution function of the fluid; that is, Marle's polynomials. Moreover, these zonal functions are closely connected to Jacobi polynomials.

In this paper, calculations are performed in a special coordinate system, the time axis being taken along the velocity vector U^α of the fluid.

A. Harmonic analysis on the homogeneous space $G/\mathrm{SO}(3)$

The main references concerning the notions of harmonic analysis used here are Refs. 25–28.

1. Summary of the method

(a) Let $v(u)$ be a square integrable function defined on Ω_x. Using the Gel'Fand–Graev method,[28] we can obtain a scalar function $h(\xi)$ defined on the upper sheet of the cone Γ,

$$\xi^\alpha\xi_\alpha=0,\quad \xi^0>0.$$

(b) The function $h(\zeta)$ is decomposed into homogeneous components $\tilde{\mathfrak{I}}_\sigma(\xi)$ of degree σ.

(c) Since they are homogeneous, the $\tilde{\mathfrak{I}}_\sigma(\xi)$ are entirely defined by their values $\tilde{\mathfrak{I}}_\sigma(\xi)$ taken on the sphere S^2 which is invariant under the action of the isotropy group of the homogeneous space $G/\mathrm{SO}(3)$.

(d) Using the Gel'Fand–Graev inversion formula,[28] we may express the function $v(u)$ in terms of the zonal spherical functions $\mathscr{K}_\sigma$ on the homogeneous space. We shall see that the moments of the distribution function of a Maxwell–Boltzmann fluid (and also for a quantum fluid of bosons or fermions) corresponds to the case when $\sigma=n$ is a nonnegative integer. These results can be interpreted in the framework of group representations. We know[29] that the Lorentz group has no unitary representation of finite dimension, except the trivial representation. Moreover, when $\sigma=n$ is a nonnegative integer, the corresponding representation of the Lorentz group is not irreducible.

2. Determination of the homogeneous components $\mathfrak{F}_\sigma(\xi)$

The invariant integral on Ω_x may be expressed by using the distribution δ. The integral transformation

$$h(\xi)=\int_{\Omega_x} v(u)\delta(\xi^\alpha u_\alpha-1)\omega \tag{23}$$

gives us a function $h(\xi)$ defined on Γ.

The homogeneous components $\mathfrak{F}_\sigma(\xi)$ of $h(\xi)$ are obtained by a Mellin transformation

$$\mathfrak{F}_\sigma(\xi)=\int_0^\infty h(t\xi)t^{-(\sigma+1)}dt \tag{24}$$

We can easily see that $\mathfrak{F}_\sigma(\xi)$ is really homogeneous and of degree σ.

Using the relation (23) we have

$$\mathfrak{F}_\sigma(\xi)=\int_{\Omega_x} v(u)\,(\xi^\alpha u_\alpha)^\sigma\omega. \tag{25}$$

3. Decomposition of the functions defined on the hyperboloid

We owe to Gel'Fand and Graev the following result[30]: If $v(u)$ is a function with a compact support in Lobatchewski space, the inversion formula of the Gel'Fand–Graev integral transformation is given by

$$v(u)=-\frac{1}{8\pi^2}\int_\Gamma h(\xi)\delta^{(2)}(\xi^\alpha u_\alpha-1)\tilde{\omega}, \tag{26}$$

where $\tilde{\omega}$ represents the invariant mesure on Γ.

By the inversion formula of the Mellin transformation (24) we first have

$$h(\xi)=\frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty}\mathfrak{F}_\sigma(\xi)\,d\sigma, \tag{27}$$

where $-1<a<+1$ and since $\mathfrak{F}_\sigma(\xi)$ is entirely defined by its values $\tilde{\mathfrak{F}}_\sigma(\xi)$ taken on the sphere S^2 which is invariant under the action of the isotropy group, we have by application of the inversion formula of the Gel'Fand–Graev transformation, Vilenkin[31]

$$v(u)=-\frac{1}{4\pi^2 i}\int_{a-i\infty}^{a+i\infty}\sigma(\sigma+1)d\sigma \times\int_{S^2}\tilde{\mathfrak{F}}_\sigma(\xi)(u^\alpha\xi_\alpha)^{-(\sigma+2)}\hat{\omega}, \tag{28}$$

where $\hat{\omega}$ is the invariant mesure on the sphere S^2. $\tilde{\mathfrak{F}}_\sigma(\xi)$, defined on the sphere S^2, may be expanded in a Fourier series and, if $v(u)$ is invariant under the action of the isotropy group, then this expansion may be expressed in terms of the zonal spherical functions on the homogeneous space and the relation (28) becomes

$$v(u)=-\frac{1}{4\pi^2 i}\int_{a-i\infty}^{a+i\infty}\sigma(\sigma+1) \times\mathfrak{M}_\sigma\mathscr{K}_{-(\sigma+2)}d\sigma,\quad -1<a<+1. \tag{29}$$

The quantities $\mathfrak{M}_\sigma$ are defined as follows,

$$\mathfrak{M}_\sigma=\int_{\Omega_x} v(u)\,\mathscr{K}_\sigma\omega. \tag{30}$$

B. Orthogonal polynomials on Minkowski's hyperboloid

Now, we may use the preceding results for the determination of orthogonal polynomials on the Minkowski hyperboloid taken as a function $v(u)$, the velocity distribution function of a Maxwell–Boltzmann fluid which may be written

$$v(u)=\exp\{-y\,u_\alpha U^\alpha\}. \tag{31}$$

In a special coordinate system, we have by (3),

$$v(\theta)=\exp\{-y\cosh\theta\}. \tag{32}$$

1. Determination of the zonal spherical functions $\mathscr{K}_n(\theta)$

Representations of the Lorentz group G may be constructed in the space $\mathscr{L}^2(S^2)$ of square integrable functions defined on the sphere S^2. As a basis of this space, we may take the orthogonal system of functions,[31]

$$Z_k=a_k C^{1/2}_{k-k_0}(\cos\psi)\sin^{k_1}\varphi\exp\{\pm ik_1\varphi\}, \qquad 0\leqslant\varphi<2\pi,\quad 0\leqslant\psi<\pi, \tag{33}$$

where k stands for the following set of real numbers,

$$k=(k_0\pm k_1),\quad 0\leqslant k_1\leqslant k_0.$$

The C^γ_μ are Gegenbauer's polynomials which are reduced to the Legendre polynomials when $\gamma=\frac{1}{2}$. The constants a_k are defined by[31]

$$(a_k)^2=\frac{2^{k_1}(2k_0+1)}{\pi}\,\frac{\Gamma(k_0-k_1+1)\Gamma^2(k_1+1/2)}{\Gamma(k_0+k_1+1)}. \tag{34}$$

Let us denote by $R^\sigma{}_g$ a representation of the Lorentz group in the space $\mathscr{H}^\sigma$ of the scalar functions defined on the cone Γ and which are C^∞ and homogeneous of degree σ, so if $f\in\mathscr{H}^\sigma$

$$R^\sigma{}_g f(\xi)=f(g^{-1}\xi).$$

The representation $R^\sigma{}_g$ is equivalent to a representation $A^\sigma{}_g$ in the space $\mathscr{L}^2(S^2)$, and the zonal spherical functions $\mathscr{K}_\sigma(g)$ depend only on the Euler angle θ of the element $g\in G$.

By taking the system (33) of functions as a basis of the space $\mathscr{L}^2(S^2)$, the zonal spherical functions of the homogeneous space $G/SO(3)$ are given by[31]

$$\mathscr{K}_\sigma(\theta)=\tfrac{1}{2}\int_0^\pi(\cosh\theta-\sinh\theta\cos\varphi)^\sigma\sin\varphi\,d\varphi. \tag{35}$$

When $\sigma=n$ is a nonnegative integer, the corresponding representation of the Lorentz group is not irreducible,[32]

Later on, it will be convenient to use other expressions for the zonal spherical functions. We briefly indicate them.

(a) *Expression of the zonal spherical functions $\mathscr{K}_\sigma$ by the hypergeometric function*

Using the binomial expansion and by integrating term by term, formula (35) takes the form[33]

$$\mathscr{K}_\sigma(\theta)=\cosh^\sigma\theta\,F\left(-\frac{\sigma}{2},\frac{1-\sigma}{2};\frac{3}{2};\tanh^2\theta\right), \tag{36}$$

where $F(a,b;c;x)$ denotes the hypergeometric function

$$F(a,b;c;x)=\sum_{n=0}^{\infty}\frac{(a,n)(b,n)}{(c,n)}\frac{x^n}{n!}$$

and $(p,q)=\Gamma(p+q)/\Gamma(p)$.

By (36) we see that when $\sigma=n$ is a nonnegative integer, $\mathscr{K}_n(\theta)$ is an nth order polynomial in $\cosh(\theta)$.

(b) *Expression of the zonal functions $\mathscr{K}_\sigma(\theta)$ by Jacobi functions, Rodrigues' formula*[34]

By taking $-\sinh^2\theta$ as a new variable in the hypergeometric function and using the transformation formula

$$F(a,b;c;x)=(1-x)^{-a}F\left(a,c-a;c;\frac{x}{x-1}\right),$$

we obtain

$$\mathscr{K}_\sigma(\theta)=F\left(-\frac{\sigma}{2},1+\frac{\sigma}{2};\frac{3}{2};-\sin^2\theta\right). \tag{37}$$

By comparing (37) with the expression for Jacobi functions $J_\nu(a,b,x)$,

$$J_\nu(a,b,x),=F(-\nu,a+\nu;b;x)$$

we may write

$$\mathscr{K}_\sigma=J_{\nu/2}(1,\tfrac{1}{2},-\sinh^2\theta)=\frac{\sinh[(\sigma+1)\theta]}{(\sigma+1)\sinh\theta}. \tag{38}$$

The Jacobi polynomials satisfy the Rodrigues formula

$$J_n(a,b,x)=\frac{x^{1-b}(1-x)^{b-a}}{(b,n)}\frac{d^n}{dx^n}\times[x^{b-1+n}(1-x)^{b-a+n}].$$

By using fractional derivatives, see for example Ref. 35, we obtain for the zonal spherical functions $\mathscr{K}_\sigma(\theta)$ the Rodrigues formula

$$\mathscr{K}_\sigma(\theta)=\frac{1}{i(3/2,\sigma/2)}\frac{\cosh\theta}{\sinh\theta}\times\frac{d^{\frac{\sigma}{2}}}{d(-\sinh^2\theta)^{\frac{\sigma}{2}}}\{(-\sinh^2\theta)^{(\sigma+1)/2}\cosh^{\sigma-1}\theta\}. \tag{39}$$

(c) *Connection with Gegenbauer's polynomials*[36]

Gegenbauer's polynomials C_μ^γ may also be defined by the hypergeometric function

$$C_\mu^\gamma(x)=\frac{\Gamma(\mu+2\gamma)}{\Gamma(\mu+1)\Gamma(2\gamma)}\times F(-\mu,\mu+2\gamma;\gamma+\tfrac{1}{2};(1-x)/2) \tag{40}$$

so, we may write

$$C^{\frac{1}{\sigma/2}}(2\cosh^2\theta-1)=(1+\sigma/2)F(-\sigma/2,2+\sigma/2;\tfrac{3}{2};-\sinh^2\theta)$$

and consequently

$$\left\{(1+\sigma/2)+\sinh^2\theta\frac{d}{d\sinh^2\theta}\right\}\mathscr{K}_\sigma(\theta)=C^{\frac{1}{\sigma}}_{\frac{\sigma}{2}}(2\cosh^2\theta-1). \tag{41}$$

(d) *Expression of the first zonal functions $\mathscr{K}_n(\theta)$*: It is easy to obtain the first zonal functions, for example as polynomials in $\cosh\theta$. Thus

$$\mathscr{K}_0=1,\quad \mathscr{K}_1=\cosh\theta,\quad 3\mathscr{K}_2=4\cosh^2\theta-1, \tag{42}$$

$$\mathscr{K}_3=2\cosh^3\theta-\cosh\theta,\quad 5\mathscr{K}_4=16\cosh^4\theta-12\cosh^2\theta+1.$$

2. Determination of the homogeneous components $\mathfrak{F}_n(\xi)$

The homogeneous components $\mathfrak{F}_n(\xi)$ of the Maxwell distribution function are obtained by (25). When $\sigma=n$, a nonnegative integer, we have

$$\mathfrak{F}_n(\xi)=8\pi(\xi_0)^n\sum_{j=0}^{E(n/2)}\frac{n!(j+1)}{(n-2j)!(2j+2)!}\times\int_0^\infty\exp\{-y\cosh\theta\}\sinh^{2j+2}\theta\cosh^{n-2j}\theta\,d\theta. \tag{43}$$

The homogeneous components $\mathfrak{F}_n(\xi)$ are entirely determined by their values $\tilde{\mathfrak{F}}_n(\xi)$ on the sphere S^2 that is invariant under the action of the isotropy group of the homogeneous space. So, we have, using (30) and (43),

$$\tilde{\mathfrak{F}}_n(\xi)=\mathfrak{M}_n=4\pi\int_0^\infty\exp\{-y\cosh\theta\}\sinh^2\theta\,\mathscr{K}_n(\theta)\,d\theta. \tag{44}$$

3. Expression of the moments of the Maxwell distribution function

From (38) and (44) we have

$$y\,\mathfrak{M}_n = 4\pi K_{n+1}(y). \tag{45}$$

The formula (12) may therefore be written in the following form,

$$I^{\alpha_1\alpha_2\cdots\alpha_n} = a\,m^{n+2}\sum_{j=0}^{E(n/2)}(-1)^j\frac{\mathfrak{M}_{n+j}}{y^j}$$

$$\times[(n-2j)U_j g\ ]^{\alpha_1\alpha_2\cdots\alpha_n}. \tag{46}$$

In this formula, the homogeneous components $\mathfrak{M}_n$ are the coefficients of the term $U^{\alpha_1}U^{\alpha_2}\cdots U^{\alpha_n}$. Consequently, in a special coordinate system, these homogeneous components $\mathfrak{M}_n$ represent the temporal part of the nth order moment of the Maxwell distribution function.

4. Orthogonal polynomials on the Minkowski hyperboloid[36]

Now, we try to find mth order polynomials H_m such that

$$H_m = \sum_{j=0}^{m} a_j^{(m)}\cosh^j\theta, \quad a_m^{(m)} = 1 \tag{47}$$

and satisfying the orthogonality condition

$$(H_m, H_n) = \int_0^\infty \exp\{y\cosh\theta\}\sinh^2\theta\, H_m H_n\, d\theta = 0$$

when $m \neq n$. (48)

With the help of the functions φ_l which have been defined in (14), we see that the coefficients $a_j^{(m)}$ are solutions of the linear system

$$\sum_{j=0}^{m} a_j^{(m)}\varphi_{j+p} = 0, \tag{49}$$

where $p = 0,1,\ldots,m-1$ and $a_m^{(m)} = 1$. The first polynomials are given by

$$H_0 = 1,$$
$$\varphi_0 H_1 = \varphi_0\cosh\theta - \varphi_1, \tag{50}$$
$$(\varphi_0\varphi_2 - \varphi_1^2)H_2 = (\varphi_0\varphi_2 - \varphi_1^2)\cosh^2\theta$$
$$-(\varphi_0\varphi_3 - \varphi_1\varphi_2)\cosh\theta + \varphi_1\varphi_3 - \varphi_2^2.$$

It is not difficult to see that these polynomials are precisely the components of Marle's polynomials on the time axis in a special coordinate system. The functions φ_l appear when expressing in (36) the zonal spherical functions in terms of $\cosh\theta$.

The other components of Marle's polynomials may be expressed in terms of Gegenbauer polynomials by the relation (41). The calculations must now be performed on the homogeneous space SO(3)/SO(2) and they are rather similar to the preceding calculations on the homogeneous space G/SO(3).

Thus we obtain for the first two polynomials in a special coordinate system:

$$H^0 = u^0 - \frac{\varphi_1}{\varphi_0}U^0, \quad H^i = u^i, \tag{51}$$
$$H^{00} = u^0u^0 - Au^0U^0 + BU^0U^0,$$
$$H^{0i} = u^i(u^0 - fU^0),$$

$$H^{ij} = u^iu^j + \frac{A}{3}g^{ij}U_\lambda H^\lambda + \frac{\varphi_2-\varphi_0}{3\varphi_0}g^{ij}, \tag{52}$$
$$A = \frac{\varphi_0\varphi_3 - \varphi_1\varphi_2}{\varphi_0\varphi_2 - \varphi_1^2}, \quad B = \frac{\varphi_1\varphi_3 - \varphi_2^2}{\varphi_0\varphi_2 - \varphi_1^2}.$$

5. Thermodynamical interpretation

When $l = 0$, 1, or 2, the functions φ_l which have been defined in (14) are exactly the Juttner integrals[37] for a Maxwell–Boltzmann fluid. Consequently, the first homogeneous component, $\mathfrak{M}_1$, of the Maxwell distribution function represents the density r of the fluid; and the second homogeneous component, $\mathfrak{M}_2$, is such that

$$\mathfrak{M}_2 = f\mathfrak{M}_1, \tag{53}$$

f being the index of the fluid.[38]

These last results are valid for quantum fluids after substitution of the Maxwell distribution function by the quantum distribution function.

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Addendum: The Clebsch–Gordan coefficients of S_n [J. Math. Phys. 18, 1697 (1977)]

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The computer programs which generated the coefficients are now available[1] and may be obtained through Computer Physics Communications. The papers of Ref. 1 also contain some discussion of the precision of the coefficients. Further discussion of the material of this work is given in Ref. 2.

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Erratum: Discrete finite nilpotent Lie analogs: New models for unified gauge field theory [J. Math. Phys. 19, 1584 (1978)]

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I am grateful to Joseph C. Ferrar for pointing out several inaccuracies related to Propositions II, IV, and VI.

The definitions preceeding Proposition II are incomplete since the maps $\mathcal{D}$ and $\langle\ \rangle_\eta$ may not exist. In general, $\mathcal{D}$ exists only if every polynomial of minimal degree contained in the kernel of $\mathcal{H}$ is also contained in $R[x^p]$. The complete definition of the condition "$\mathcal{D}$ is faithful" must therefore specify that $\mathcal{H}$ has been chosen so that $\mathcal{D}$ exists. It then follows that $\langle\ \rangle_\eta$ exists for all admissible values of ξ if $\mathcal{D}$ is faithful. The proof of Proposition II should state that $\mathcal{D}$ is faithful only if ξ^p is a miminal polynomial in ξ over R.

Proposition IV is correct as stated, but the accompanying proof is based on a false statement. A straightforward proof follows from the polynomial expression for $\mathcal{C} \circ \mathcal{C}(\eta)$ as derived from the general polynomial expression for $\mathcal{C}(\eta)$.

The phrases "is reducible (irreducible) over" which are defined in the paragraph preceding Proposition VI should read "acts reducibly (irreducibly) on".

Proposition VI is inaccurate as stated: VI(2) should state that $\rho_m^{(r)}(\eta_p^2 L[\eta_p^2])$ acts irreducibly on $F(r,m)$ for all $r \geq 3$; and the term "inequivalent" should be deleted from VI(3). The proof accompanying VI(3) contains numerous errors and should be replaced by the following: for $r \geq 5$, $\rho_m^{(r)}(\eta_p^2 L[\eta_p^2])$ is non-Abelian, while for $r=3$ the (p,r)-analog of U(1) contains only the identity; for $r=4$ there exists a Lie isomorphism $\rho_m^{(4)}(\eta_p^2 L[\eta_p^2]) \cong \sum_k \sigma_k(\eta_p^2 L[\eta_p^2])$ (direct) where the skew-Hermitian singlet representations σ_k are defined by

$$\sigma_k : \eta_p^2 L[\eta_p^2] \to M_1[\eta_4] : \phi \otimes \lambda_{k'} \to \delta_{kk'}\,\phi\eta_p (\mathrm{mod}\,\eta_p^4).$$

In the final paragraph of Sec. II the domain of $\rho_{m'}^{(\eta)}$ should be specified as $\eta_p^2 L[\eta_p^2]$.

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