New Integral Formulation of the Schrödinger Equation*

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The 1-dimensional Schrödinger equation is replaced by a pair of coupled integral equations. The equations are solved by iteration. The zeroth-order solution is the WKB approximation. The solutions are valid even in the presence of classical turning points and discontinuous potentials. Thus, connection formulas are not required. Low-order calculations are carried out in several cases of interest. In each case, a first-order calculation gives results comparable to or better than those obtained with connection formulas.

I. MOTIVATION

Let Γ be a smooth rectifiable Jordan arc with end points $\{p, q\}$ in the complex X plane. Consider the Schrödinger equation for $x \in \Gamma$ and an arbitrary potential $V(x)$:

$$0 = \psi''(x) + k^2(x)\psi(x), \tag{1}$$

$$k^2(x) = 2m\hbar^{-2}[E - V(x)]. \tag{2}$$

Since the discussion is restricted to $x \in \Gamma$, it is understood that all derivatives are Γ derivatives; for example,

$$\psi'(x) = \lim_{\substack{y \to x \\ x, y \in \Gamma}} \frac{\psi(y) - \psi(x)}{y - x}. \tag{3}$$

There are four fourth roots of $k^2(x)$. Let one of them be indicated by $k^{\frac{1}{2}}(x)$. For the present, it is assumed that $k^{\frac{1}{2}}(x)$ is nonzero and Γ differentiable.

The successes of the WKB approximation suggest that the solution to Eq. (1) might profitably be written in the form

$$\psi(x) = \chi_+(x)W_+(x) + \chi_-(x)W_-(x), \tag{4}$$

$$S(x) = \int_p^x k(z)\, dz, \tag{5}$$

$$W_\pm(x) = k^{-\frac{1}{2}}(x)e^{\pm iS(x)}. \tag{6}$$

Further conditions are needed to make Eq. (4) a well-defined decomposition of $\psi(x)$. The formal manipulations of the next paragraph suggest that these conditions might consist of requiring that χ_+ and χ_- satisfy a pair of coupled integral equations (12). The "derivation" of these equations is to some extent based on intuitive arguments. It should simply be regarded as motivation for the more rigorous approach in the next section.

Let $\leq$ denote the natural ordering from p to q along Γ. We choose a partition P_N of Γ:

$$p = x_0 < x_1 < \cdots < x_N = q. \tag{7}$$

We define

$$\begin{aligned} &k(P_N, x) = k(x_n), \quad \text{if} \quad p < x_{n-1} < x \leq x_n, \\ &k(P_N, x) = k(p), \quad \text{if} \quad p = x. \end{aligned} \tag{8}$$

If one wishes to solve Eq. (1) with $k(x) \to k(P_N, x)$, it is necessary to match $\psi(P_N, x)$ and $\psi'(P_N, x)$ across the discontinuity at x_n. If χ_+ and χ_- are held constant between the discontinuities, this condition leads to

$$\begin{aligned} (x_{n+1} - x_n)^{-1}&[\chi_\pm(P_N, x_{n+1}) - \chi_\pm(P_N, x_n)\tfrac{1}{2}\gamma_n^{(+)}] \\ &= \chi_\pm(P_N, x_n)(x_{n+1} - x_n)^{-1} \\ &\quad \times \{\gamma_n^{(-)} \exp[\mp 2iS(P_N, x_n)]\}, \end{aligned} \tag{9}$$

$$\gamma_n^{(\pm)} = k^{\frac{1}{2}}(x_{n+1})k^{-\frac{1}{2}}(x_n) \pm k^{-\frac{1}{2}}(x_{n+1})k^{\frac{1}{2}}(x_n). \tag{10}$$

If $k(P_N, x)$ is a good approximation to $k(x)$ and if $(x_{n+1} - x_n)$ is small, then Eq. (9) reduces to

$$\chi'_\pm(x) = \chi_\mp(x)k'(x)\tfrac{1}{2}k^{-1}(x) \exp[\mp 2iS(x)]. \tag{11}$$

Integration of Eq. (11) yields

$$\chi_\pm(x) = A_\pm + \int_p^x \chi_\mp(z)\tfrac{1}{2}k'(z)k^{-1}(z) \exp[\mp 2iS(z)]\, dz, \tag{12}$$

where A_+ and A_- are constants.

II. EQUIVALENCE

The following theorems put the preceding result on a firmer footing.

Theorem 1: If ψ satisfies Eq. (1), then there exist functions χ_+ and χ_-, together with constants A_+ and A_-, such that Eqs. (4) and (12) hold.

Proof: We define

$$\psi_\pm = \tfrac{1}{2}(\psi \pm \psi'/ik), \tag{13}$$

and rewrite Eq. (13) in the form

$$\psi = \psi_+ + \psi_-, \tag{14}$$

$$\psi' = ik\psi_+ - ik\psi_-. \tag{15}$$

Notice that Eqs. (1) and (14) give

$$\psi'' = -k^2(\psi_+ + \psi_-). \tag{16}$$

We differentiate Eq. (13) and then apply Eqs. (15) and (16) to obtain

$$\begin{aligned}\psi'_\pm &= [ik\tfrac{1}{2}(1 \pm 1) \mp k'/2k]\psi_+ \\ &\quad + [ik\tfrac{1}{2}(-1 \pm 1) \pm k'/2k]\psi_- \\ &= (\pm ik - k'/2k)\psi_\pm + \tfrac{1}{2}k'k^{-1}\psi_\mp \\ &= W'_\pm W_\pm^{-1}\psi_\pm + \tfrac{1}{2}k'k^{-1}\psi_\mp. \end{aligned} \tag{17}$$

Now we solve Eq. (17) for $\psi_\pm$ in terms of $\psi_\mp$:

$$\psi_\pm(x) = W_\pm(x) \times \left(\psi_\pm(p)W_\pm^{-1}(p) + \int_p^x \tfrac{1}{2}k'(z)W_\mp(z)\psi_\mp(z)\,dz\right). \tag{18}$$

It remains only to make the identifications

$$\chi_\pm(x) = \psi_\pm(x)/W_\pm(x), \tag{19}$$

$$A_\pm = \chi_\pm(p). \tag{20}$$

Theorem 2: If χ_+ and χ_- satisfy Eq. (11), then there exists a function ψ satisfying Eqs. (1) and (4).

Proof: We define

$$U = \chi_+W_+ + \chi_-W_-. \tag{21}$$

We differentiate Eq. (21) and apply Eq. (11) to obtain

$$U' = (W'_+ + e^{2iS}W_-k'/2k)\chi_+ + (W'_- + W_+e^{-2iS}k'/2k)\chi_-. \tag{22}$$

We differentiate Eq. (22) and apply Eq. (11) to obtain

$$\begin{aligned} U'' &= [(W'_+ + W_-e^{2iS}k'/2k)' \\ &\quad + (W'_- + W_+e^{-2iS}k'/2k)e^{2iS}k'/2k]\chi_+ \\ &\quad + [(W'_- + W_+e^{-2iS}k'/2k)' \\ &\quad + (W'_+ + W_-e^{2iS}k'/2k)e^{-2iS}k'/2k]\chi_- \\ &= -k^2W_+\chi_+ - k^2W_-\chi_- \\ &= -k^2U. \end{aligned} \tag{23}$$

It remains only to make the identification

$$\psi = U. \tag{24}$$

Thus, the second-order differential equation (1) is equivalent to the two coupled integral equations (12). The solution of these integral equations is the main concern of the remainder of this paper.

III. SOLVING THE INTEGRAL EQUATIONS

It is convenient to write Eq. (12) in operator notation:

$$\chi_\pm = A_\pm + K_\mp\chi_\mp. \tag{25}$$

This equation represents a pair of coupled integral equations which can be uncoupled to yield

$$\chi_\pm = (A_\pm + K_\mp A_\mp) + (K_\mp K_\pm)\chi_\pm. \tag{26}$$

Notice that $(K_\mp K_\pm)$ is a Voltera operator. Furthermore, the restrictions on $k^{\frac{1}{2}}$ guarantee that the integral kernel is continuous. Thus, the (unique, bounded, uniformly convergent[1]) solution of Eq. (26) is the Neumann series

$$\chi_\pm = \sum_{n=0}^{\infty}(K_\mp K_\pm)^n(A_\pm + K_\mp A_\mp). \tag{27}$$

This solution can also be obtained from the recursion scheme:

$$\chi_\pm^{(0)} = A_\pm, \tag{28}$$

$$\chi_\pm^{(n+1)} = A_\pm + K_\mp\chi_\mp^{(n)}, \tag{29}$$

$$\chi_\pm = \lim_{n\to\infty}\chi_\pm^{(n)}. \tag{30}$$

In a problem of practical interest, $k^{\frac{1}{2}}$ is likely to have at least one zero or point of nondifferentiability. The presence of such a trouble point (henceforth called a "pond") calls for a modified procedure. Some commonly encountered ponds are considered in the following sections.

IV. SIMPLE TURNING POINT

Suppose that Γ is pondless except at a classical turning point t. That is, $k(t) = 0$. We assume that $V(x)$ can be extended to an analytic function on some open set in the complex X plane. The corresponding extension of $k^{\frac{1}{2}}(x)$ will be analytic except at t and along a possible branch cut. Let Γ_t be a smooth contour which coincides with Γ except for a small excursion to avoid t and the branch cut.

Now Eq. (1) can be integrated twice to obtain

$$\psi(x) = [\psi(p) + (x - p)\psi'(p)] + \int_p^x \psi(z)k^2(z)(z - x)\,dz. \tag{31}$$

Let ψ_t and ψ be the Neumann-series solutions to equation (31) along Γ_t and Γ, respectively. But the integrals in these series are path independent; thus, $\psi_t = \psi$ wherever Γ_t and Γ coincide.

Let ψ_{27} be the general solution to Eq. (1) which results from using Eq. (27) to solve Eq. (12) on Γ_t. The equivalence theorems guarantee that A_+ and A_- can be chosen so that $\psi_{27} = \psi_t$. Thus, $\psi = \psi_{27}$ whereever Γ_t and Γ coincide. In short, Eq. (27) is valid on Γ (except at t) if K_+ and K_- are defined in terms of the slightly distorted contour Γ_t.

V. POORLY MATCHED POTENTIALS

One sometimes considers a potential which has a different analytic form on each of several segments of Γ. It is sufficient to consider the case where only two segments are involved.

Let $k_p^{\frac{1}{2}}(x)$ and $k_q^{\frac{1}{2}}(x)$ be Γ differentiable. Suppose that t is an interior point of Γ. We define

$$\begin{aligned} k^{\frac{1}{2}}(x) &= k_p^{\frac{1}{2}}(x), \quad \text{if} \quad p \leq x \leq t, \\ k^{\frac{1}{2}}(x) &= k_q^{\frac{1}{2}}(x), \quad \text{if} \quad t < x \leq q. \end{aligned} \tag{32}$$

If $k_p^{\frac{1}{2}}$ and $k_q^{\frac{1}{2}}$ are poorly matched, then $k^{\frac{1}{2}}$ will not be a smooth function; t will be a pond. More precisely, t will be a pond if $k_p^{\frac{1}{2}}(t) \neq k_q^{\frac{1}{2}}(t)$ and/or if

$$\frac{d}{dx} k_p^{\frac{1}{2}}(x)\Big|_{x=t} \neq \frac{d}{dx} k_q^{\frac{1}{2}}(x)\Big|_{x=t}.$$

A few preliminary remarks must precede the discussion of the general case.

Suppose that $k^{\frac{1}{2}}$ is continuous at t but its derivative is not. We assign an arbitrary value to $(d/dx)k^{\frac{1}{2}}(x)|_{x=t}$. The integrals of Eq. (27) are now well defined, and the resulting sums for χ_+ and χ_- are continuous functions. The functions still correspond to solutions of Eq. (1) on each side of t. In view of Eqs. (14) and (15), these solutions join smoothly at $x = t$. But this is the condition which must be satisfied by the correct solution of Eq. (1). Thus, Eq. (27) remains applicable if the pond is essentially ignored.

Now we allow the possibility that $k^{\frac{1}{2}}(x)$ is not continuous at t. We let $t < u \in \Gamma$ and approximate $k^{\frac{1}{2}}(x)$ as follows:

$$\begin{aligned} k_u^{\frac{1}{2}}(x) &= k_p^{\frac{1}{2}}(x), && \text{if} \quad p \leq x \leq t, \\ k_u^{\frac{1}{2}}(x) &= k_p^{\frac{1}{2}}(x) + [k_q(u) - k_p(t)] \\ &\quad \times (x - t)(u - t)^{-1}, && \text{if} \quad t \leq x \leq u, \\ k_u^{\frac{1}{2}}(x) &= k_q^{\frac{1}{2}}(x), && \text{if} \quad u \leq x \leq q. \end{aligned} \tag{33}$$

A Neumann-series solution to Eq. (31) is valid both for $k(x)$ and for $k_u(x)$. If the boundary conditions are applied at p, then the difference between the two solutions will satisfy

$$\Delta(x) = \Delta^{(0)}(x) + \int_p^x \Delta(z) k_u^2(z)(z - x)\, dz, \tag{34}$$

$$\Delta(x) = \psi_u(x) - \psi(x), \tag{35}$$

$$\Delta^{(0)}(x) = \int_p^x \psi(z)[k_u^2(z) - k^2(z)](z - x)\, dz. \tag{36}$$

Notice that Eq. (34) has a Neumann-series solution which is continuous with respect to $\Delta^{(0)}$. It follows that

$$\begin{aligned} \psi &= \lim_{\Delta^{(0)} \to 0} (\psi_u - \Delta) \\ &= \lim_{\Delta^{(0)} \to 0} \psi_u \\ &= \lim_{u \to t^+} \psi_u, \end{aligned} \tag{37}$$

where the last step is justified by an inspection of Eq. (36). But it was shown in the previous paragraph that ψ_u can also be obtained from Eq. (27). Thus, to determine ψ, one may approximate $k^{\frac{1}{2}}$ as in Eq. (33), apply Eq. (27), and then take the limit as in Eq. (37).

This limit is just the term-by-term limit of Eq. (27). It corresponds to modifying the integral kernel of $K_\pm$ as follows:

$$\begin{aligned} &e^{\pm 2iS(x)} k'(x)/2k(x) \\ &\qquad \to \delta(x - t) e^{\pm 2iS(t)} \log [k_q(t)/k_p(t)]^{\frac{1}{2}} \\ &\qquad\quad + \lim_{v \to x^-} e^{\pm 2iS(v)} k'(v)/2k(v), \end{aligned} \tag{38}$$

where multiple integrals of the δ function are to be evaluated according to the formula

$$\begin{aligned} \frac{1}{n!} = \int_p^q \int_p^{z_1} \int_p^{z_2} \cdots \int_p^{z_{n-1}} &\delta(z_1 - t) \cdots \delta(z_n - t) \\ &\times dz_1 \cdots dz_n. \end{aligned} \tag{39}$$

The procedure just developed is simple to apply and completely in keeping with the general intent of this paper; but there is an alternative procedure which may occasionally prove useful. Equation (27) allows the general solution of Eq. (1) to be obtained to any desired accuracy on $[p, t)$ and on $(t, q]$. The arbitrary constants on the second segment can be chosen so that the two solutions and their derivatives are equal at t. An approximate over-all solution is obtained by combining these two partial solutions.

VI. THE RADIAL EQUATION

The domain of the radial equation (40) is usually taken to be the entire positive axis: $\Gamma = (0, \infty)$. For simplicity, we assume that Γ has been slightly distorted to avoid classical turning points and that no other ponds are present. Also, we assume that the real part of l exceeds $-\frac{1}{2}$:

$$0 = \psi''(r) + k^2(r)\psi(r), \tag{40}$$

$$k^2(r) = [E - V(r)]2m\hbar^{-2} - l(l + 1)r^{-2}. \tag{41}$$

Boundary Conditions at Infinity

If the boundary conditions are to be applied at ∞, one is tempted to set $p = \infty$ and apply Eq. (27). This procedure can often be justified. For example, suppose

that $k(\infty)$ is positive and that

$$\int_1^\infty [k(z) - k(\infty)]\, dz$$

is finite. Then the indicated procedure is readily validated if the phase integral is redefined[2] as follows:

$$S(r) = rk(\infty) + \int_\infty^r [k(z) - k(\infty)]\, dz. \quad (42)$$

Boundary Conditions at the Origin

More commonly, one wishes to let the boundary condition be "regularity" at the origin:

$$0 = \lim_{r\to 0} \psi(r). \quad (43)$$

Two fundamentally different solution schemes are developed to satisfy this condition.

Scheme 1

The first scheme involves removing the centrifugal singularity with the transformation[3]

$$r = e^x, \quad (44)$$

$$\psi(r) = \varphi(x)e^{\frac{1}{2}x}. \quad (45)$$

The result is a Schrödinger-type equation

$$0 = \varphi''(x) + k^2(x)\varphi(x), \quad (46)$$

$$k^2(x) = 2m\hbar^{-2}[E - V(e^x)]e^{2x} - (l + \tfrac{1}{2})^2. \quad (47)$$

Now suppose that $ik(-\infty)$ is negative and that

$$\int_0^{-\infty} [k(z) - k(-\infty)]\, dz$$

is finite. We redefine the phase integral as

$$S(x) = \int_0^x k(z)\, dz. \quad (48)$$

It is easy to show that Eq. (27) leads to the desired solution of Eq. (46) if one sets $A_+ = 0$ and $p = -\infty$.

Scheme 2

Equation (12) was originally solved by iteration. The zeroth-order approximations for χ_+ and χ_- were taken to be A_+ and A_-, respectively. Actually, any pair of bounded functions could have been used for the zeroth-order approximations. It turns out that iteration of Eq. (12) is also possible when one is seeking the regular solution of Eq. (40). But the zeroth-order approximations have to satisfy more stringent requirements. The exact form of these requirements is obtained in the following paragraphs.

We assume that

$$\int_0^1 \left\{k(z) - \frac{i[l(l+1)]^{\frac{1}{2}}}{z}\right\} dz$$

converges and redefine[2] the phase integral as

$$S(r) = i[l(l+1)]^{\frac{1}{2}} \log(r) + \int_0^r \left(k(z) - \frac{i[l(l+1)]^{\frac{1}{2}}}{z}\right) dz. \quad (49)$$

Also, we let $p = 0$. The equivalence theorems now assume the following form:

Theorem 3: Equation (4) provides a one-to-one correspondence between regular solutions of Eq. (40) and regular solutions of

$$\chi_\pm = K_\mp \chi_\mp. \quad (50)$$

Proof: Proceed as in Theorems 1 and 2 to show the equivalence of Eq. (40) and the differential form of Eq. (50). Direct examination of these differential equations reveals that their regular solutions ψ and $\chi_\pm$ behave near the origin as r^{l+1} and $r^{l+\frac{1}{2}\pm\sqrt{l(l+1)}}$, respectively. Application of this result to Eqs. (14), (19), (21), and (24) shows that regular solutions of (40) correspond to regular solutions of (50).

Theorem 4: Let arc length along Γ be denoted by

$$\alpha(r) = \int_0^r |dz|. \quad (51)$$

Suppose:

(i) Γ is sufficiently close to $(0, \infty)$ to satisfy

$$1.1 \geq \sup_{r\in\Gamma} \frac{\alpha(r)}{|r|} + \sup_{\substack{r_1, r_2 \in \Gamma \\ r_1 < r_2}} \left| \left(\frac{r_1}{r_2}\right)^{l+\frac{1}{2}\pm\sqrt{l(l+1)}} \right|; \quad (52)$$

(ii) there is a point r_0 such that for $0 \leq r \leq r_0$ the following function has a bounded derivative:

$$\rho(r) = \{k(r) - i[l(l+1)]^{\frac{1}{2}}/r\}/r; \quad (53)$$

(iii) $\zeta_\pm(r)$ is any bounded function such that the following function has a bounded second derivative for $0 \leq r \leq r_0$:

$$\eta_\pm(r) = [\zeta_\pm(r) r^{-1-l\mp\sqrt{l(l+1)}} - 1]/r. \quad (54)$$

Then a regular nontrivial solution of Eq. (50) is given by

$$\chi_\pm = \lim_{n\to\infty} (K_\mp K_\pm)^n \zeta_\pm. \quad (55)$$

Furthermore, all other regular solutions of Eq. (50) are multiples of this solution.

Proof: We define

$$Q_\pm = k'k^{-1}e^{\pm 2iS}r^{1\pm 2\sqrt{l(l+1)}}, \tag{56}$$

$$w_\pm = W_\pm r^{-\frac{1}{2}\pm\sqrt{l(l+1)}}\{i[l(l+1)]^{\frac{1}{2}}\}^{\frac{1}{2}}, \tag{57}$$

and choose $y \in \Gamma$ such that

$$1.1 \geq \|w_\pm\|_y + \|Q_\pm\|_y + \|w_\pm^{-1}\|_y, \tag{58}$$

where for any function h

$$\|h\|_t = \sup_{0\leq r\leq t} |h(r)|. \tag{59}$$

Let $R \in \Gamma$. We choose $N > 0$ such that

$$1 + N^N\alpha^N(y) \geq \|w_\pm\|_R \|Q_\pm\|_R \|Q_\mp\|_R \|w_\pm^{-1}\|_R \times [1 + (1 + N)^{-2}N^N\alpha^N(y)]. \tag{60}$$

We define

$$\delta_\pm = \frac{W_\pm}{r^{l+2}(1 + N^N\alpha^N)} \times \left[\zeta_\pm - \left(\frac{2k}{k'e^{\pm 2iS}}\right)\frac{d}{dr}\left(\frac{2k}{k'e^{\mp 2iS}}\zeta'_\pm\right)\right], \quad \text{if } r < r_0,$$

$$\delta_\pm = 0, \quad \text{if } r \geq r_0. \tag{61}$$

It follows from (ii) and (iii) that $\delta_\pm(r)$ is bounded. Let $T_\pm$ be the operator defined by

$$T_\pm h = W_\pm r^{-l-2}(1 + N^N\alpha^N)^{-1} \times K_\mp K_\pm W_\pm^{-1} r^{l+2}(1 + N^N\alpha^N)h, \tag{62}$$

where $h(r)$ is again arbitrary.

It is now shown that $T_\pm$ is a contraction on $(0, R)$. Let $\|h\|_R = 1$. Then

$$\begin{aligned}
|T_\pm f(r)| &= \left| \int_0^r \int_0^{r_1} w_\pm(r) Q_\mp(r_1) Q_\pm(r_2) \right. \\
&\quad \times w_\pm^{-1}(r_2)\left(\frac{\alpha(r)}{r}\right)\left(\frac{\alpha(r_1)}{r_1}\right) \\
&\quad \times \left(\frac{r_1}{r}\right)^{l+\frac{1}{2}\pm\sqrt{l(l+1)}}\left(\frac{r_2}{r_1}\right)^{l+\frac{1}{2}+\sqrt{l(l+1)}} \\
&\quad \times \tfrac{1}{2}\alpha^{-1}(r)[1 + N^N\alpha^N(r)]^{-1} \\
&\quad \left. \times \alpha^{-1}(r_1)[1 + N^N\alpha^N(r_2)]h(r_2)\, dr_2\, dr_1 \right| \\
&\leq \|w_\pm\|_r \|Q_\mp\|_r \|Q_\pm\|_r \|w_\pm^{-1}\|_r \\
&\quad \times (1.1)^4 \tfrac{1}{4}\alpha^{-1}(r)/[1 + N^N\alpha^N(r)] \\
&\quad \times \int_0^r \int_0^{r_1} \alpha^{-1}(r_1)[1 + N^N\alpha^N(r_2)]\, |dr_2|\, |dr_1| \\
&= \|w_\pm\|_r \|Q_\mp\|_r \|Q_\pm\|_r \|w_\pm^{-1}\|_r \\
&\quad \times (1.1)^4 \tfrac{1}{4} \frac{[1 + (1 + N)^{-2}N^N\alpha^N(r)]}{[1 + N^N\alpha^N(r)]}.
\end{aligned} \tag{63}$$

If $r \leq y$, then Eq. (58) reduces Eq. (63) to

$$\begin{aligned}
|T_\pm f(r)| &\leq \tfrac{1}{4}(1.1)^8[1 + N^N\alpha^N(r)]^{-1} \\
&\quad \times [1 + (1 + N)^{-2}N^N\alpha^N(r)] \\
&< \tfrac{1}{4}(1.1)^8 \\
&< 1.
\end{aligned} \tag{64}$$

If $r > y$, then Eq. (60) reduces Eq. (63) to

$$\begin{aligned}
|T_\pm f(r)| &\leq \tfrac{1}{4}(1.1)^4 \\
&< 1.
\end{aligned} \tag{65}$$

Thus, $T_\pm$ is a contraction. Now we write Eq. (50) in the form

$$\chi_\pm = K_\mp K_\pm \chi_\pm. \tag{66}$$

We now define

$$\begin{aligned}
\zeta_\pm^{(0)}(r) &= \zeta_\pm(r), \quad \text{if } r < r_0, \\
\zeta_\pm^{(0)}(r) &= 0, \quad \text{if } r \geq r_0,
\end{aligned} \tag{67}$$

$$\Omega_\pm = W_\pm r^{-l-2}(\chi_\pm - \zeta_\pm^{(0)})/(1 + N^N\alpha^N). \tag{68}$$

Equation (68) transforms Eq. (66) to

$$\begin{aligned}
\Omega_\pm &= (T_\pm - 1)W_\pm r^{-l-2}\zeta_\pm^{(0)}/(1 + N^N\alpha^N) + T_\pm\Omega_\pm \\
&= T_\pm\delta_\pm + T_\pm\Omega_\pm.
\end{aligned} \tag{69}$$

Since $T_\pm$ is a contraction and $\delta_\pm$ is bounded, Eq. (68) has the following solution on $(0, R)$:

$$\begin{aligned}
\Omega_\pm &= \sum_{n=0}^{\infty} T_\pm^n(T_\pm\delta_\pm) \\
&= \sum_{n=0}^{\infty} T_\pm^n(T_\pm - 1)W_\pm r^{-l-2}(1 + N^N\alpha^N)^{-1}\zeta_\pm^{(0)} \\
&= W_\pm r^{-l-2} \\
&\quad \times \left(-\zeta_\pm^{(0)} + \lim_{n\to\infty}(K_\mp K_\pm)^n\zeta_\pm^{(0)}\right)\Big/(1 + N^N\alpha^N).
\end{aligned} \tag{70}$$

Thus,

$$\begin{aligned}
\chi_\pm &= \zeta_\pm^{(0)} + r^{l+2}(1 + N^N\alpha^N)W_\pm^{-1}\Omega_\pm \\
&= \lim_{n\to\infty}(K_\mp K_\pm)^n\zeta_\pm^{(0)} \\
&= \lim_{n\to\infty}(K_\mp K_\pm)^n\zeta_\pm + \lim_{n\to\infty}(K_\mp K_\pm)^n(\zeta_\pm^{(0)} - \zeta_\pm) \\
&= \lim_{n\to\infty}(K_\mp K_\pm)^n\zeta_\pm,
\end{aligned} \tag{71}$$

where the last step is justified by the fact that, on $[r_0, R]$, the operator $K_\mp K_\pm$ is Voltera with a bounded kernel.

Assume that Eq. (55) fails to be a regular nontrivial solution of Eq. (50). Then Eq. (68) implies that $\Omega_\pm$ is unbounded. But Eq. (70) gives $\Omega_\pm$ as a bounded function. The contradiction implies that Eq. (55) is indeed a regular nontrivial solution. The essential

uniqueness of Eq. (55) follows from the fact that Eq. (70) is the unique regular solution of Eq. (69).

VII. RATE OF CONVERGENCE

In each case, χ_+ and χ_- have been given in terms of a limiting procedure. Sequences of approximate solutions for $\chi_\pm$ were shown to converge to the exact solutions. It is not difficult to generate estimates for the rates of convergence, but the estimates typically admit the possibility of slow convergence. Thus, one must have a certain amount of blind (or at least near-sighted) faith in the accuracy of low-order calculations. The following comments are offered to support this faith.

Consider the problem of solving Eq. (1) when $V(x)$ is a small potential step at $x = t$. Let the boundary conditions be $\chi_+(p) = 1$ and $\chi_-(q) = 0$. That is, there is an incident wave from the left. If connection formulas are not used, the WKB approximation gives $\chi_+(x) = 1$ and $\chi_-(x) = 0$ for $x \in [p, q]$. An exact calculation shows that, in the region $x \in [p, t)$, the WKB approximation errs by the omission of a reflected wave which is first order in the magnitude of the potential step. But, for $x \in (t, q]$, the error is second order.

Thus, when there is an interface between two very slightly dissimilar media, the WKB approximation essentially consists of ignoring reflections from the interface. A continuous medium has infinitely many such interfaces. The WKB approximation ignores all of the resulting reflections. The integral in Eq. (12) is simply the summation of the omitted reflections.

If $k(x)$ is large and slowly varying, one expects these reflections to be weak and incoherent. For such $k(x)$, the integral kernel in Eq. (12) is indeed found to be small and highly oscillatory. Consequently, the integral itself tends to be small.

The multiple integrals of Eq. (27) correspond to multiple reflections. If $k(x)$ is large and slowly varying, the above line of thought suggests that these multiple integrals should be quite insignificant. That is, low-order calculations should be very accurate.

The rapid convergence argument is less convincing when the "large and slowly varying" condition fails. The examples illustrate what may be expected in such cases.

VIII. EXAMPLE: LINEAR POTENTIAL

Suppose a and b are positive constants such that

$$V(x) = -ax + b. \tag{72}$$

It is convenient to translate the origin to the classical turning point

$$y = x + (E - b)/a. \tag{73}$$

Then,

$$k^2(y) = \sigma y, \tag{74}$$

$$\sigma = 2ma/\hbar^2, \tag{75}$$

$$0 = \psi''(y) + k^2(y)\psi(y). \tag{76}$$

Suppose E is real, y is real, and $\sigma > 0$. We choose the phase of $k^{\frac{1}{2}}(y)$ to be $\frac{1}{4}\pi$ for $y < 0$ and 0 for $y > 0$.

The classically forbidden region is now to the left of the origin. The boundary condition $\psi(-\infty) = 0$ is of particular interest. It is easy to show that Eq. (27) holds if one takes $\Gamma = (-\infty, \infty)$, $A_+ = 0$, and $A_- = 1$ and that

$$S(y) = \int_0^y k(z)\, dz. \tag{77}$$

The first-order reflection amplitude is

$$\chi_+^{(1)}(\infty) = \int_{-\infty}^{\infty} \tfrac{1}{2}k'(z)k^{-1}(z)e^{-2iS(z)}\, dz. \tag{78}$$

But

$$S(y) = 2\sigma^{\frac{1}{2}}\tfrac{1}{3}y^{\frac{3}{2}}; \tag{79}$$

so

$$y = (3S\tfrac{1}{2}\sigma^{-\frac{1}{2}})^{\frac{2}{3}} \tag{80}$$

and

$$\chi_+^{(1)}(\infty) = \int e^{-2iS} d \log [\sigma(3S\tfrac{1}{2}\sigma^{-\frac{1}{2}})^{\frac{2}{3}}]^{\frac{1}{4}}$$

$$= \int e^{-2iS}(\tfrac{1}{6}) d \log (S), \tag{81}$$

where Fig. 1 indicates the path of integration in the complex S plane. The residue at the origin gives

$$\chi_+^{(1)}(\infty) = -i\tfrac{1}{3}\pi$$

$$= -i1.047. \tag{82}$$

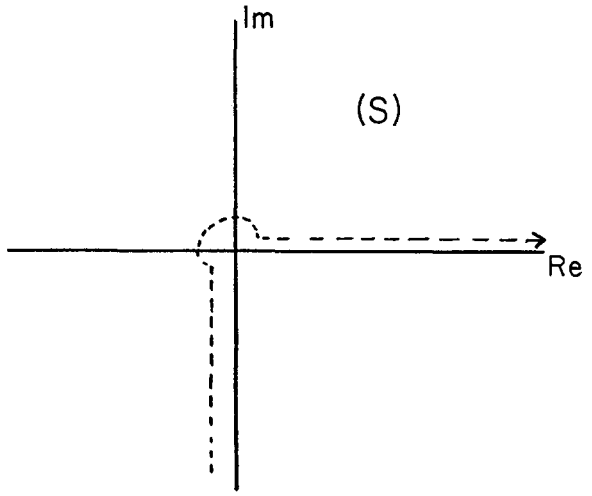

FIG. 1. Path of integration for Eq. (81). The contour may be closed in the fourth quadrant.

This is to be compared with the known value

$$\chi_+(\infty) = -i. \tag{83}$$

Residue calculations are prohibitively difficult with many potentials. Suppose that this had been the case with the linear potential. Then the integral of Eq. (78) could have been truncated and evaluated numerically. For example, if the integral is restricted to the region such that $|S(x)| \leq \frac{1}{2}\pi$, then the numerical result is

$$\chi_+^{(1)}(\infty) \sim 0.063 - i1.107. \tag{84}$$

The close agreement between Eqs. (82)–(84) serves to substantiate the earlier comments on the rate of convergence of Eq. (27). It is easy to believe that, for a large class of smooth potentials, the main error in zeroth-order WKB is the omission of the first-order contribution from the immediate vicinity of the classical turning point. This conclusion is, of course, basic to the "derivation" of the usual WKB connection formulas.

IX. EXAMPLE: PARABOLIC BARRIER

Suppose a is a positive constant such that

$$V(x) = -ax^2. \tag{85}$$

The zero-energy problem is then

$$0 = \psi''(x) + k^2(x)\psi(x), \tag{86}$$

$$k^2(x) = \sigma x^2, \tag{87}$$

$$\sigma = 2ma/\hbar^2. \tag{88}$$

Suppose Γ is the real axis and $\sigma > 0$. We choose the phase of $k^{\frac{1}{2}}(x)$ so that $k^{\frac{1}{2}} \geq 0$.

The boundary condition $\chi_+(-\infty) = 0$ is of particular interest. It is easy to show that Eq. (27) holds if one takes $\Gamma = (-\infty, \infty)$, $A_+ = 0$, $A_- = 1$, and $S(x)$ as in Eq. (77). The calculus of residues can be employed as before to obtain the first-order reflection amplitude

$$\chi_+^{(1)}(\infty) = -i\tfrac{1}{4}\pi = -i0.785. \tag{89}$$

This is to be compared with the known value

$$\chi_+(\infty) = -i2^{-\frac{1}{2}} = -i0.710. \tag{90}$$

A naive[4] application of connection formulas would have led to the ambiguous value

$$\chi_+(\infty) = 0 \quad \text{or} \quad -i, \tag{91}$$

depending upon whether the energy is taken to be slightly positive or slightly negative. Thus, the first-order calculation can be a considerable improvement over connection formula techniques.

X. EXAMPLE: PLATEAUED POTENTIAL

Suppose $V(x)$ rises rapidly from one level region to another as illustrated in Fig. 2. Let x, E, and m be real. We choose the phase of $k^{\frac{1}{2}}(x)$ to be 0 for $x < 0$ and either 0 or $\frac{1}{4}\pi$ [depending upon the sign of $E - V(\delta)$] for $x > \delta$. Take $\Gamma = (-\infty, \infty)$ and let $S(x)$ be as in Eq. (77).

The condition "rises rapidly" means that $\int_0^\delta k(z)\,dz$ is negligible. Thus, Eq. (12) reduces to

$$\chi_\pm(x(\mu)) = A_\pm + \int_0^\mu \chi_\mp(x(z))\,dz, \tag{92}$$

$$\mu(x) = \log\,[k(x)/k(0)]^{\frac{1}{2}}. \tag{93}$$

Iteration of Eq. (92) involves simple integrations which eventually yield

$$\chi_\pm(x) = A_\pm \sum_{n=0}^{\infty} \frac{\mu^{2n}}{(2n)!} + A_\mp \sum_{n=0}^{\infty} \frac{\mu^{2n+1}}{(2n+1)!} \tag{94}$$

$$= A_\pm \cosh\mu + A_\mp \sinh\mu \tag{95}$$

$$= A_\pm \tfrac{1}{2}\{[k(x)/k(0)]^{\frac{1}{2}} + [k(0)/k(x)]^{\frac{1}{2}}\} + A_\mp \tfrac{1}{2}\{[k(x)/k(0)]^{\frac{1}{2}} - [k(0)/k(x)]^{\frac{1}{2}}\}. \tag{96}$$

This is recognized as the exact solution for a potential step (i.e., $\delta = 0$).

Now suppose, for example, that

$$k(\delta)/k(0) = e^2 = 7.4. \tag{97}$$

Truncating the sums of Eq. (94) at $n = 1$ gives

$$\chi_\pm^{(1)}(x) = A_\pm, \quad \text{if} \quad x \leq 0, \tag{98}$$

$$\chi_\pm^{(1)}(x) = 1.500A_\pm + 1.167A_\mp, \quad \text{if} \quad x \geq \delta. \tag{99}$$

Inclusion of all orders gives

$$\chi_\pm(x) = A_\pm, \quad \text{if} \quad x \leq 0, \tag{100}$$

$$\chi_\pm(x) = 1.545A_\pm + 1.175A_\mp, \quad \text{if} \quad x \geq \delta. \tag{101}$$

The first-order wavefunction is

$$\psi^{(1)}(x) = A_+ e^{ixk(0)} + A_- e^{-ixk(0)}, \quad \text{if} \quad x \leq 0, \tag{102}$$

$$\psi^{(1)}(x) = (1.500A_+ + 1.167A_-)e^{ixk(\delta)} + (1.500A_- + 1.167A_+)e^{-ixk(\delta)}, \quad \text{if} \quad x \geq \delta. \tag{103}$$

FIG. 2. Shape of "plateaued potential."

Inclusion of all orders gives

$$\psi(x) = A_+e^{ixk(0)} + A_-e^{-ixk(0)}, \quad \text{if } x \leq 0, \tag{104}$$

$$\psi(x) = (1.545A_+ + 1.175A_-)e^{ixk(\delta)} + (1.545A_- + 1.175A_+)e^{-ixk(\delta)}, \quad \text{if } x \geq \delta. \tag{105}$$

These results are slightly modified if the exact phase integral is used, but it is easy to believe that the low-order calculations retain their accuracy. On the other hand, this potential presents severe problems if one attempts to apply WKB in the usual way.

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$$S(r) = S(1) + \int_1^r k(z)\,dz.$$

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Canonically Conjugate Pairs, Uncertainty Relations, and Phase Operators*

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Apparent difficulties that prevent the definition of canonical conjugates for certain observables, e.g., the number operator, are eliminated by distinguishing between the Heisenberg and Weyl forms of the canonical commutation relations (CCR's). Examples are given for which the uncertainty principle does not follow from the CCR's. An operator F is constructed which is canonically conjugate, in the Heisenberg sense, to the number operator; and F is used to define a quantum time operator.

1. INTRODUCTION

A great deal of effort has been expended in the study of canonical commutation relations and the associated uncertainty principle. In particular, the question of the existence of a phase operator canonically conjugate to the number operator has excited considerable interest and also generated a certain amount of confusion. This situation was greatly clarified by the work of Susskind and Glogower[1] and others.[2] In this paper, we first present some general considerations which are based on the important distinction between the Weyl and Heisenberg representations of the canonical commutation relations. We show, by means of examples, how various apparent difficulties can be eliminated by paying attention to this distinction. We then discuss the general relation between the uncertainty principle and the canonical commutation relations and, again by way of examples, we show that the former need not follow from the latter.

In addition to these general remarks, we explicitly construct an operator which is canonically conjugate, in the Heisenberg sense, to the number operator. As an interesting application, we use this "phase" operator to define a quantum time operator in the context of an idealized oscillator clock.

2. CANONICAL COMMUTATION RELATIONS

The observables Q and P are said to be canonically conjugate if they satisfy the (abstract) canonical commutation relation (CCR)

$$[Q, P] = i. \tag{2.1}$$

In this section, we very briefly review the types of representations of the CCR's which may be defined on a separable Hilbert space $\mathcal{H}$. This is an important question because the apparent difficulties which occur for certain pairs (Q, P) can be eliminated by a more precise specification of the representation involved.

The most commonly used representation employs the idea of a Weyl pair[3]: A *Weyl pair* (or Weyl system) consists of two strongly continuous, 1-parameter groups of unitary operators $(U(\alpha), V(\beta))$ satisfying the relation

$$U(\alpha)V(\beta) = e^{(i\alpha\beta)}V(\beta)U(\alpha). \tag{2.2}$$

Such unitary groups can always be represented in the exponential form

$$U(\alpha) = e^{(i\alpha P)}, \qquad V(\beta) = e^{(i\beta Q)}, \tag{2.3}$$

where the generators Q and P are densely defined,

Inclusion of all orders gives

$$\psi(x) = A_+e^{ixk(0)} + A_-e^{-ixk(0)}, \quad \text{if } x \leq 0, \tag{104}$$

$$\psi(x) = (1.545A_+ + 1.175A_-)e^{ixk(\delta)} + (1.545A_- + 1.175A_+)e^{-ixk(\delta)}, \quad \text{if } x \geq \delta. \tag{105}$$

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$$U(\alpha) = e^{(i\alpha P)}, \qquad V(\beta) = e^{(i\beta Q)}, \tag{2.3}$$

where the generators Q and P are densely defined,

unbounded self-adjoint operators. A formal power-series expansion of (2.2) using (2.3) yields (2.1); therefore, Q and P are (formally) canonically conjugate. In fact, this procedure is rigorously correct if both sides of (2.2) are allowed to act on any vector chosen from a suitable dense subspace.[4] The standard example of a Weyl pair is given by choosing as generators the position and momentum operators for a free particle in one dimension. Furthermore, von Neumann's theorem[3] states that every Weyl pair is unitarily equivalent to the standard example. An immediate consequence of this theorem is that any generator for a Weyl pair has a continuous spectrum comprising the entire real line. This fact is the source of many remarks to the effect that certain operators, e.g., those with discrete or bounded spectra, could not have canonical conjugates.

The strong conditions imposed by von Neumann's theorem on the spectra of canonically conjugate pairs can be avoided by using a weaker definition of canonical conjugacy: A *Heisenberg pair* (Q, P) consists of two densely defined, self-adjoint operators together with a dense subspace $\mathcal{C}$ on which their commutator is defined and satisfies

$$[Q, P]\psi = i\psi, \quad \psi \in \mathcal{C}. \tag{2.4}$$

It is clear that the generators of any Weyl pair form a Heisenberg pair, but the converse statement is false. That is, there are Heisenberg pairs which cannot be exponentiated to form a Weyl pair, and von Neumann's theorem is false for such pairs. The problem of determining sufficient conditions for the truth of the converse has been studied by several authors.[5] Roughly speaking, the commutator domain $\mathcal{C}$ must be invariant under Q and P, and the operator $P^2 + Q^2$ must be essentially self-adjoint on $\mathcal{C}$.

A simple example of a Heisenberg pair is provided by the problem of a particle in a 1-dimensional box of unit length.[6] The relevant Hilbert space is $\mathcal{H} = L_2(0, 1)$, and the canonical operators (Q, P) are defined by

$$Q\psi(x) = x\psi(x),$$
$$P\psi(x) = -i\frac{d\psi}{dx}(x),$$

where the domain of Q is the whole space and the domain of P is

$$\mathcal{D}(P) = \{\psi \in \mathcal{H}: \psi \text{ is absolutely continuous}, \psi' \in \mathcal{H}, \psi(0) = \psi(1)\}. \tag{2.5}$$

The domains have been chosen so that both operators are densely defined and self-adjoint. To complete the definition of (Q, P) as a Heisenberg pair, we must specify the commutator domain $\mathcal{C}$. Since Q is defined everywhere on $\mathcal{H}$, we need only ensure that $Q\psi \in \mathcal{D}(P)$ whenever $\psi \in \mathcal{C}$; this condition guarantees that $[Q, P]\psi$ is well defined. The function $Q\psi$ cannot satisfy the periodicity condition in (2.5) unless $\psi(0) = \psi(1) = 0$; therefore, the commutator domain must be

$$\mathcal{C} = \{\psi \in \mathcal{D}(P): \psi(0) = \psi(1) = 0\}.$$

We omit the proof that $\mathcal{C}$ is dense. The CCR of (2.1) is obtained by a simple formal calculation which is rigorously justified for any element of $\mathcal{C}$. Although (Q, P) is a Heisenberg pair, it certainly cannot be a Weyl pair[7] since the spectrum of Q is bounded and the spectrum of P is discrete. The difficulties which prevent the formation of a Weyl pair from (Q, P) can be understood in terms of the sufficient conditions mentioned above. The domain $\mathcal{C}$ is not invariant under P and, if one attempts to remedy this by a further restriction of $\mathcal{C}$, it is found that $P^2 + Q^2$ will not be self-adjoint on the reduced domain.

3. CCR's AND UNCERTAINTY RELATIONS

It is usually assumed that a canonically conjugate pair of observables represented by self-adjoint operators will satisfy an uncertainty relation. We now show that the truth of this assumption depends critically on the properties of the commutator domain $\mathcal{C}$ associated with the relevant representation of the CCR. For any normalized $\psi \in \mathcal{C}$, we have

$$\begin{aligned} i &= (\psi, [Q, P]\psi) \\ &= (Q\psi, P\psi) - (P\psi, Q\psi), \end{aligned}$$

and an application of the Schwartz inequality gives

$$1 \leq 2\,\|Q\psi\|\,\|P\psi\|.$$

The number $\|Q\psi\|$ is just the root-mean-square average of Q, since

$$\|Q\psi\|^2 = (Q\psi, Q\psi) = (\psi, Q^2\psi),$$

and the same holds for P. The familiar form of the uncertainty relation is obtained by the replacements $Q \to Q - \langle Q\rangle$, $P \to P - \langle P\rangle$ and the definitions $\delta Q = \|Q - \langle Q\rangle\|$, $\delta P = \|P - \langle P\rangle\|$:

$$\delta Q\,\delta P \geq \tfrac{1}{2}. \tag{3.1}$$

We wish to emphasize the elementary but important point that this derivation is only valid for $\psi \in \mathcal{C}$. If all relevant physical states are in $\mathcal{C}$, this remark imposes no real restriction, but if there are physical states not in $\mathcal{C}$, the derivation fails and we may expect (3.1) to be violated. The former situation exists for any Weyl pair, but the examples given below show that either situation is possible for Heisenberg pairs.

An example for which (3.1) is satisfied is provided by the particle in a 1-dimensional box. The physically admissible wavefunctions for this problem must vanish at the boundaries; therefore, according to the discussion in Sec. 2, they all lie in the commutator domain and consequently satisfy the uncertainty relation. A contrary example is given by the pair (Θ, L_z), where L_z is the z component of angular momentum and

$$L_z\psi(\theta) = -i\frac{d\psi(\theta)}{d\theta},$$
$$\Theta\psi(\theta) = \theta\psi(\theta).$$

Except for obvious changes in notation, the domains of L_z and Θ and the commutator domain $\mathcal{C}$ are defined just as in the previous example. The difference is that there is no requirement that the physical wavefunctions vanish at the end points of the interval $(0, 2\pi)$. In particular, the eigenfunctions of L_z do not belong to $\mathcal{C}$ and they clearly violate (3.1), since $\delta L_z = 0$ while $\delta\Theta \leq 2\pi$. This difficulty is, of course, well known,[2] and satisfactory replacements for (3.1) have been formulated by considering trigonometric functions of Θ.

4. PHASE OPERATOR

It has often been assumed that the annihilation operator a for a harmonic oscillator has the representation

$$a = e^{-i\Theta}N^{\frac{1}{2}}, \tag{4.1}$$

in which the number operator N and the phase operator Θ are self-adjoint. A formal calculation based on this representation shows that (Θ, N) is a canonically conjugate pair. This simple picture was destroyed by Susskind and Glogower,[1] who proved that no unitary operator $\exp(-i\Theta)$ could satisfy (4.1). They replaced this incorrect representation by the rigorous polar decomposition

$$a = (N+1)^{\frac{1}{2}}E,$$

where E is defined by

$$E\phi_0 = 0,$$
$$E\phi_n = \phi_{n-1}, \quad n \geq 1, \tag{4.2}$$

and $\{\phi_n\}$ is the complete orthonormal set of eigenfunctions of N. Although the relations (4.2) show that E is not unitary, one can introduce useful self-adjoint operators C and S by

$$E = C + iS. \tag{4.3}$$

These are the cosine and sine operators introduced by Susskind and Glogower.[1]

The results outlined above apparently make it impossible to define an operator canonically conjugate to N; nevertheless, we will construct an operator F which does have this property. The contradiction is resolved by the distinction between the Weyl and Heisenberg forms of the CCR's. Indeed, if F and N were the generators for a Weyl pair, we could use (2.2) to derive the incorrect representation (4.1); but we will find that (F, N) is a Heisenberg pair for which (2.2) is false.

The construction of F is most conveniently carried out in the representation defined by choosing $\mathcal{K} = H^2$, where H^2 is the Hilbert space of functions analytic in the unit disk. The inner product in H^2 is defined by

$$(f, g) = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}f^*(e^{i\theta})g(e^{i\theta}),$$

and the eigenfunctions of N are given by $\phi_n = z^n$. Thus, we have

$$N = z\frac{d}{dz} = -i\frac{d}{d\theta},$$

where $\theta = \arg(z)$ and

$$\mathfrak{D}(N) = \left\{f \in H^2 : z\frac{df}{dz} \in H^2\right\}.$$

By analogy with the discussion of L_z in Sec. 3, we might expect the canonical conjugate to N to be given by

$$\Theta f(z) = \theta f(z), \tag{4.4}$$

but Θ does not define an operator in H^2, since $\theta = \arg(z)$ is not an analytic function of z. A more useful way to view this difficulty is to note that the boundary value of f is given by a convergent Fourier series containing no Fourier coefficients f_n with negative n,

$$f(e^{i\theta}) = \sum_{n=0}^{\infty} f_n e^{in\theta}.$$

This simply reflects the fact that N has no negative eigenvalues. From this point of view, the problem is that the Fourier expansion of Θf will contain coefficients $(\Theta f)_n$ for negative values of n. This suggests that one modify (4.4) by following Θ with a projection operator which deletes the negative-n components. It is not necessary to introduce the projection operator explicitly, since an equivalent definition is given by

$$(g, Fh) = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\, g^*(e^{i\theta})\theta h(e^{i\theta}) \tag{4.5}$$

for any g, $h \in H^2$. The operator defined by (4.5) is obviously bounded and symmetric; consequently, it is self-adjoint.

To show that (F, N) is a Heisenberg pair, we must specify a dense commutator domain $\mathcal{C}$. Just as in the angular-momentum case, the only problem is to

ensure that $Fh \in \mathfrak{D}(N)$ whenever $h \in \mathfrak{C}$. The definition of $\mathfrak{D}(N)$ can be rephrased as

$$\mathfrak{D}(N) = \left\{ f \in H^2 : \sum_{n=0}^{\infty} n^2 |f_n|^2 < \infty \right\}, \tag{4.6}$$

from which it follows that each $f \in \mathfrak{D}(N)$ is strictly periodic on the unit circle. Let us consider those elements $f \in \mathfrak{D}(N)$ which satisfy

$$f(-1) = 0;$$

then the function $\theta f(e^{i\theta})$ will also be periodic, since f vanishes at the point of discontinuity for θ. Furthermore, the result of projecting this function onto H^2 will satisfy (4.6); i.e., it will lie in $\mathfrak{D}(N)$. We are thus led to define $\mathfrak{C}$ by

$$\mathfrak{C} = \left\{ f \in \mathfrak{D}(N) : 0 = f(-1) = \sum_{n=0}^{\infty} (-1)^n f_n \right\}.$$

To show that $\mathfrak{C}$ is dense in H^2, we introduce the functions

$$h_m(z) = 1 + (-1)^{m+1} z^m,$$

which are elements of $\mathfrak{C}$ for $m \geq 1$. Next, suppose that f is orthogonal to each h_m; then

$$(h_m, f) = f_0 + (-1)^{m+1} f_m = 0, \quad m \geq 1,$$

which yields

$$f_m = (-1)^m f_0, \quad m \geq 1.$$

This is impossible for a normalizable function unless $f_0 = 0$, which implies $f \equiv 0$. Therefore, any function orthogonal to every element of $\mathfrak{C}$ vanishes identically and $\mathfrak{C}$ is dense in H^2. It remains to be shown that the CCR is satisfied on $\mathfrak{C}$. Let $h \in \mathfrak{C}$ and $g \in \mathfrak{D}(N)$; then

$$\begin{aligned} (g, [F, N]h) &= (g, FNh) - (g, NFh), \\ &= (g, FNh) - (Ng, Fh). \end{aligned}$$

Now we can use the definition (4.5) to obtain

$$(g, [F, N]h) = \int \frac{d\theta}{2\pi} g^* \theta \frac{1}{i} \frac{dh}{d\theta} - \int \frac{d\theta}{2\pi} \left(\frac{1}{i} \frac{dg}{d\theta} \right)^* \theta h.$$

After integrating by parts in the second term (the integrated term vanishes since $h \in \mathfrak{C}$), we find

$$(g, [F, N]h) = i(g, h). \tag{4.7}$$

Since $\mathfrak{D}(N)$ is dense in H^2, we can conclude that

$$[F, N]h = ih \tag{4.8}$$

for any $h \in \mathfrak{C}$. Thus, (F, N) is a Heisenberg pair.

The operator F, so far defined implicitly by (4.5), can be exhibited more explicitly by means of its spectral resolution; equivalently, we can search for a new representation in which F acts multiplicatively. A technique for finding this representation has been developed by Rosenblum[8] in connection with the spectral analysis of self-adjoint Toeplitz operators. An operator T on H^2 is said to be a Toeplitz operator if there is a function $W(\theta)$ such that

$$(g, Th) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} g^*(e^{i\theta}) W(\theta) h(e^{i\theta}).$$

In our case, F is defined by the choice $W(\theta) = \theta$; we remark in passing that the operators C and S discussed earlier correspond respectively to $W(\theta) = \cos\theta$ and $W(\theta) = \sin\theta$. The application of Rosenblum's method to our problem yields as the new representation space $L_2(d\rho)$, where $d\rho$ is a measure on the real line given by

$$\begin{aligned} d\rho(\lambda) &= \tfrac{1}{2} \cos \tfrac{1}{2}\lambda \, d\lambda, \quad \text{for} \quad |\lambda| \leq \pi, \\ &= 0, \quad \text{for} \, |\lambda| > \pi. \end{aligned}$$

The concentration of the measure in $[-\pi, \pi]$ is simply due to the boundedness of F. The isomorphism between H^2 and $L_2(d\rho)$ is given by the unitary mapping

$$f \in H^2 \to \psi \in L_2(d\rho)$$

with

$$\begin{aligned} \psi(\lambda) &= \lim_{b \to 1} \frac{1}{2\pi i} \int_{|z|=b} \frac{dz}{z} f(z^*) \Phi(z; \lambda) \\ &= \lim_{b \to 1} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} f(be^{-i\theta}) \Phi(be^{i\theta}; \lambda), \end{aligned} \tag{4.9}$$

where

$$\begin{aligned} \Phi(z; \lambda) &= [(1 + z)(1 - ze^{i\lambda})]^{-\frac{1}{2}} e^{-\Omega(z;\lambda)}, \\ \Omega(z; \lambda) &= \int_{-\pi}^{\pi} \frac{d\theta}{4\pi} \log|\theta - \lambda| \left(\frac{1 + ze^{i\theta}}{1 - ze^{i\theta}} \right). \end{aligned} \tag{4.10}$$

In particular, we denote the image of z^n by $\phi_n(\lambda)$; these are the eigenfunctions of N and they necessarily form a complete orthonormal set for the measure $d\rho$. It is easy to see that

$$\Phi(z; \lambda) = \sum_{n=0}^{\infty} z^n \phi_n(\lambda);$$

i.e., Φ serves as the generating function for $\{\phi_n\}$. In the new representation, we have

$$(F\psi)(\lambda) = \lambda \psi(\lambda),$$

$$(N\psi)(\lambda) = \int d\rho(\lambda') N(\lambda, \lambda') \psi(\lambda')$$

with

$$N(\lambda, \lambda') = \lim_{b \to 1} \int \frac{d\theta}{2\pi} \frac{1}{i} \frac{\partial \Phi(be^{i\theta}; \lambda)}{\partial \theta} \Phi^*(be^{i\theta}; \lambda').$$

Unfortunately, we have not been able to carry out the last integral above; consequently, we have no explicit representation for $N(\lambda, \lambda')$.

We have exploited the properties of the generating function Φ to derive a recursion relation for the functions ϕ_n which was used in a numerical calculation of

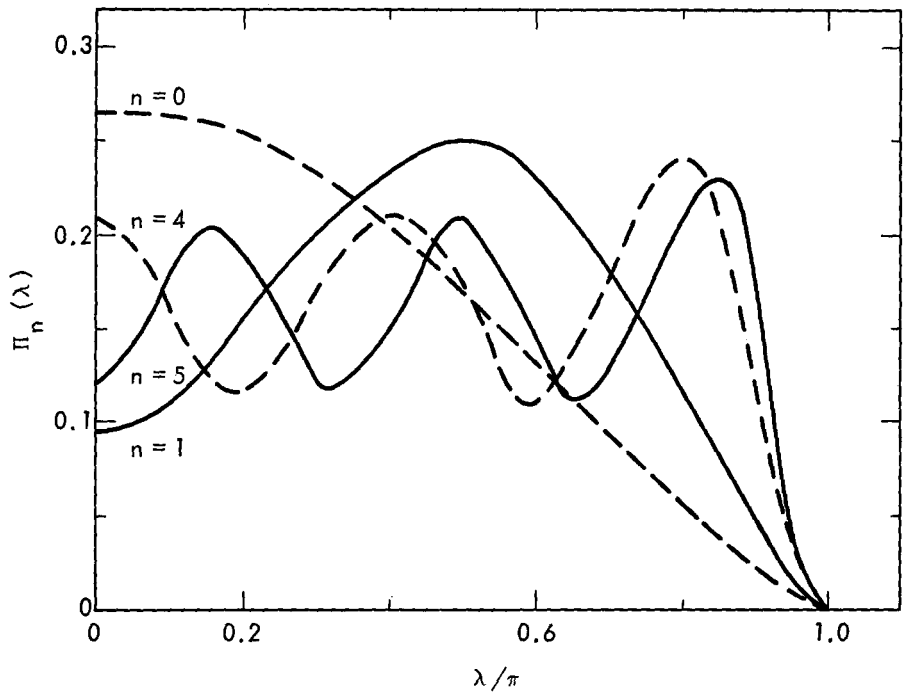

FIG. 1. Probability distribution in λ for occupation numbers $n = 0, 1, 4, 5$. All graphs extend symmetrically to negative λ.

the first 20 functions. An outline of the calculation is given in Appendix A. Qualitatively, ϕ_n resembles a distorted version of $e^{in\lambda}$; for example, it has the same symmetry under complex conjugation

$$\phi_n^*(\lambda) = \phi_n(-\lambda).$$

To each ϕ_n, there corresponds a probability distribution $\Pi_n(\lambda)$ in λ, given by

$$\Pi_n(\lambda)\, d\lambda = |\phi_n(\lambda)|^2\, d\rho(\lambda) = \tfrac{1}{2}\, |\phi_n(\lambda)|^2 \cos \tfrac{1}{2}\lambda\, d\lambda.$$

These functions exhibit strong oscillations with $n + 1$ maxima for Π_n; several examples are shown in Fig. 1. It is interesting to compare this behavior of Π_n to that of the analogous function in the angular-momentum case. The probability distribution corresponding to a given eigenfunction of L_z is a constant; it does not even depend on the eigenvalue. The source of the difference is the fact that the spectrum of N is bounded below while that of L_z is not.

To gain some insight into the physical significance of F, we will briefly consider the questions of the uncertainty relation for (F, N) and the classical limit for F. As far as the uncertainty relation is concerned, the situation is similar to that found for (Θ, L_z). The operator F is bounded and there are physical states, namely the $\{\phi_n\}$, which have $\delta N = 0$; consequently, the conventional uncertainty relation is violated. We have not yet considered the problem of formulating modified uncertainty relations similar to those obtained for (Θ, L_z).

The behavior of F in the classical limit can be obtained by using the well-known coherent Glauber states

$$\Psi_\alpha \equiv \exp(-\tfrac{1}{2}|\alpha|^2) \sum_{n=0}^{\infty} \frac{\alpha^n}{(n!)^{\frac{1}{2}}}\, \phi_n, \qquad (4.11)$$

where $\alpha = |\alpha|\, e^{-i\theta}$. Since Ψ_α is an eigenstate of a, it is easy to show that

$$\langle a^n \rangle = \alpha^n, \quad \langle N \rangle = |\alpha|^2, \quad \delta N = |\alpha|,$$

where $\langle B \rangle \equiv (\Psi_\alpha, B\Psi_\alpha)$ and $\delta N \equiv [\langle N^2 \rangle - \langle N \rangle^2]^{\frac{1}{2}}$. In the limit of large $|\alpha|$ we have $\delta N/\langle N \rangle \to 0$; therefore, the state described by Ψ_α is characterized by a well-defined intensity and phase given by $|\alpha|^2$ and θ, respectively. The C and S operators defined in (4.3) satisfy[2]

$$\lim_{|\alpha| \to \infty} \left(\Psi_\alpha, \begin{Bmatrix} C^n \\ S^n \end{Bmatrix} \Psi_\alpha\right) = \begin{Bmatrix} (\cos\theta)^n \\ (\sin\theta)^n \end{Bmatrix}.$$

Thus, in the classical limit, C and S approach the corresponding functions of the classical phase with a dispersion which can be made arbitrarily small by choosing $|\alpha|$ sufficiently large. This behavior is shared by F; i.e., one can show that

$$\lim_{|\alpha| \to \infty} (\Psi_\alpha, F^n \Psi_\alpha) = \theta^n. \qquad (4.12)$$

The proof of (4.12) is given in Appendix B. Since neither C nor S commutes with F, they certainly cannot be expressed as functions of F; nevertheless, in

the classical limit, we have

$$\langle C\rangle = \cos\langle F\rangle,$$
$$\langle S\rangle = \sin\langle F\rangle.$$

Another interesting fact is that F and N satisfy the conventional uncertainty relation in the classical limit. To obtain this result, we employ the so-called weak CCR; i.e., we form the expression

$$\Gamma = (F\psi, N\psi) - (N\psi, F\psi).$$

For $\psi \in \mathcal{C}$, this is just the expectation value of the commutator, but Γ is actually well defined for any $\psi \in \mathcal{D}(N)$. A calculation like that leading to (4.7) gives

$$\Gamma = i[1 - |\psi(-1)|^2].$$

The combination of this result with the definition of Γ and the Schwartz inequality yields

$$|1 - |\psi(-1)|^2| \leq 2\,\|F\psi\|\,\|N\psi\|. \tag{4.13}$$

The same result is obtained if we replace F by $F - \langle F\rangle$ and N by $N - \langle N\rangle$. Again, we see that the conventional uncertainty relation can be obtained only if $\psi(-1) = 0$, which is the condition for membership in $\mathcal{C}$. The advantage of (4.13) is that it holds for all $\psi \in \mathcal{D}(N)$; therefore, it is valid for all relevant physical states. Now let us choose ψ to be a Glauber state with $\alpha = |\alpha|\,e^{-i\theta}$. Inserting in (4.13) the asymptotic form (B2) obtained in Appendix B, we have

$$|1 - 2(2\pi)^{\frac{1}{2}}\,|\alpha|\,\exp\,[-2\,|\alpha|^2\,(\pi \pm \theta)^2]| \leq 2\delta F\,\delta N.$$

When $|\alpha| \to \infty$, this yields

$$\begin{aligned} \tfrac{1}{2} &\leq \delta F\,\delta N, \quad \text{for} \quad \pi \pm \theta \neq 0, \\ (2\pi)^{\frac{1}{2}} &\leq \delta F, \quad \text{for} \quad \pi \pm \theta = 0. \end{aligned} \tag{4.14}$$

The second inequality follows from the fact that $\delta N = |\alpha|$. Note the curious fact that a state centered on a phase value in the interior of $[-\pi, \pi]$ can have an arbitrarily small dispersion in F, whereas a state concentrated at $\theta = \pm\pi$ has a minimum phase dispersion given by (4.14). It should be emphasized that (4.14) is not a general statement; it depends on the special properties of the Glauber states in the classical limit.

5. THE OSCILLATOR CLOCK

The harmonic oscillator Hamiltonian is given by $H = \omega N$, where ω is the oscillator frequency. In view of the commutation relation (4.8) for (F, N), we are naturally led to define a canonical conjugate to H by $T \equiv \omega^{-1}F$. One might then think that T is some sort of quantum time operator. We now investigate this possibility, as was done in Ref. 1, by using T in the construction of an idealized clock.

The basic elements in the oscillator clock are a 1-parameter family of states $\{\Lambda_\tau\}$, with the property

$$e^{-itH}\Lambda_\tau = \Lambda_{\tau+t}, \tag{5.1}$$

and an observable T, whose measurement on Λ_τ yields τ with negligible dispersion. If we write Λ_τ as

$$\Lambda_\tau = \sum b_n(\tau)\phi_n,$$

then the condition (5.1) requires

$$b_n(\tau) = b_n e^{-in\omega\tau}.$$

The coefficients b_n must be chosen so as to minimize the dispersion in the measurement of T. The particular choice made in Ref. 1 corresponds to

$$b_n = (1 - b^2)^{\frac{1}{2}}b^n,$$

where b is a real number in $(0, 1)$. In the limit $b \to 1$, one does find $\langle C\rangle = \cos(\omega\tau)$ with vanishing dispersion, but one also finds $\delta N/\langle N\rangle \to 1$. In other words, the limiting state does not correspond to a well-defined classical intensity. In view of this fact, we will choose instead a special family of Glauber states

$$\Lambda_\tau = \Psi_\alpha,$$

with $\alpha = |\alpha|\,e^{-i\omega\tau}$. Note that the states labeled by τ and $\tau + 2\pi/\omega$ are identical.

To operate the clock, we prepare the oscillator in the $\tau = 0$ state and, subsequently, measure T. According to (4.12), we will find

$$\lim_{|\alpha|\to\infty} (\Lambda_\tau, T^n\Lambda_\tau) = \tau^n;$$

i.e., the measurement of T yields τ with a dispersion which vanishes as $|\alpha| \to \infty$. Furthermore, the condition (5.1) guarantees

$$\tau = t, \bmod 2\pi/\omega.$$

Thus, the oscillator clock only allows us to measure time intervals within one oscillator period. This limitation is not fundamental; one can avoid it by using two oscillators with incommensurable periods. Therefore, T seems to be a suitable time operator.

6. DISCUSSION

In this work, we have been concerned with three related problems: the types of possible representations for the CCR's, the connection between the CCR's and the uncertainty principle, and finally the construction of a "phase" operator for the harmonic oscillator. With regard to the first problem, we hope to have made it clear that it is essential to specify precisely the representation of the CCR that is relevant to a given problem. In particular, the apparent difficulties associated

with the definition of canonical conjugates for operators with discrete or bounded spectra can be eliminated by recognizing that the appropriate representation is of the Heisenberg type instead of the more familiar Weyl type. The question of uncertainty relations is also intimately related to the type of representation used. For representations of the Weyl type, the commutator domain automatically includes all relevant physical states, and the conventional uncertainty relation follows. However, for representations of the Heisenberg type, the commutator domain may or may not contain all of the relevant physical states. In the latter case, the derivation of the uncertainty relation breaks down and, in the examples studied in Sec. 3, the uncertainty relation is violated by some physical states.

It has often been asserted that an operator which has a spectrum that is bounded below could not have a canonical conjugate. The counterexample produced in Sec. 4 provides an illustration of the general ideas discussed above, since its existence is based on the fact that (F, N) is a Heisenberg rather than a Weyl pair.

Finally, in order to avoid misunderstanding, we wish to emphasize that the existence of the time operator T defined in Sec. 5 does not provide an explanation for the familiar relation $\delta E\,\delta T \geq \frac{1}{2}$. The only general inequality that can be derived for the Heisenberg pair (T, H) is the weak uncertainty relation (4.13), and there are many physically acceptable states for which the left-hand side vanishes. On the other hand, it is true that an oscillator state useful in the construction of a clock will necessarily have a large dispersion in energy. This follows from the properties of the complete set $\{\phi_n\}$ studied in Sec. 4; any function strongly peaked, say at $\lambda = \lambda_0$, will have a very large number of components $\phi_n(\lambda)$ with nearly equal coefficients. Thus, one cannot make an accurate energy measurement on an oscillator clock, since the corresponding wavefunction is strongly peaked. This would seem to imply some kind of uncertainty relation despite the lack of a formal derivation starting from the CCR's, but this conclusion is misleading. Consider a system described by the total Hamiltonian $H = H_c + H_s$, where H_c is the clock Hamiltonian and H_s describes some other physical system. We assume that there is no interaction between the two subsystems. If the clock is prepared in a state suitable for accurate measurements of T, then there will be a large dispersion δE_c and, consequently, a large dispersion in the total energy. However, there is no apparent relation between δE_s and δT since $[H_s, T] = 0$. In other words, the function of the quantum clock is simply to provide the value of the time parameter t occurring in the usual description of S. In our opinion, any relation between δE_s and δT must arise from a detailed analysis of the interaction between S and the apparatus used to measure its energy.

APPENDIX A

We can obtain a recursion relation for the functions ϕ_n by writing the generating function in the form

$$\Phi(z;\lambda) = e^{-\Gamma(z;\lambda)}, \tag{A1}$$

which yields the identity

$$\frac{\partial\Phi}{\partial z} = -\frac{\partial\Gamma}{\partial z}\Phi. \tag{A2}$$

If we substitute in (A2) the power series for Φ and Γ,

$$\Phi(z;\lambda) = \sum z^n\phi_n(\lambda),$$
$$\Gamma(z;\lambda) = \sum z^n\gamma_n(\lambda),$$

then we find the recursion relation

$$n\phi_n = -n\phi_0\gamma_n - \sum_{m=1}^{n-1}(n-m)\gamma_{n-m}\phi_m, \quad n \geq 1.$$

Comparing (A1) to (4.10) gives

$$\Gamma(z;\lambda) = \Omega(z;\lambda) + \tfrac{1}{2}\log(1+z) + \tfrac{1}{2}\log(1 - ze^{i\lambda}),$$

so that

$$\gamma_0(\lambda) = \Omega(0;\lambda) = -\tfrac{1}{2} + (4\pi)^{-1} \times [(\pi+\lambda)\log(\pi+\lambda) + (\pi-\lambda)\log(\pi-\lambda)],$$

$$\gamma_n(\lambda) = (2n)^{-1}[(-1)^{n+1} - e^{in\lambda}] + \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\log|\theta-\lambda|\,e^{in\theta}, \quad n \geq 1.$$

The function ϕ_0 is given explicitly by

$$\phi_0(\lambda) = e^{-\gamma_0(\lambda)} = (e/\pi)^{\frac{1}{4}}\exp\{-\tfrac{1}{4}[(1+\lambda/\pi)\log(1+\lambda/\pi) + (1-\lambda/\pi)\log(1-\lambda/\pi)]\}.$$

Thus, the function ϕ_n can be computed from the ϕ_m, $m < n$, and the given functions γ_n. The latter were computed by first finding an expression for them in terms of the known functions[9] $\mathrm{Si}(x)$ and $\mathrm{Ci}(x)$.

APPENDIX B

In the representation that diagonalizes F, we have

$$(\Psi_\alpha, F^n\Psi_\alpha) = \int d\rho(\lambda)\,|\Psi_\alpha(\lambda)|^2\,\lambda^n,$$

where Ψ_α is a Glauber state with $\alpha = Re^{-i\theta}$. Since we want to prove (4.12), we replace λ^n by $(\lambda - \theta + \theta)^n$

and write

$$(\Psi_\alpha, F^n\Psi_\alpha) = \theta^n + \sum_{l=1}^{n}\binom{n}{l}\theta^{n-l}I_l,$$

$$I_l = \int d\rho(\lambda)(\lambda-\theta)^l|\Psi_\alpha(\lambda)|^2.$$

Our task now is to show that

$$\lim_{R\to\infty} I_l = 0, \quad l \geq 1. \tag{B1}$$

The asymptotic form for Ψ_α is most readily obtained in the H^2 representation; therefore, we use (4.9) to write I_l as

$$I_l = \lim_{b\to 1}\int\frac{d\phi}{2\pi}\int\frac{d\phi'}{2\pi}\Psi_\alpha^*(be^{-i\phi'})\Psi_\alpha(be^{-i\phi})H_l(\phi',\phi),$$

with

$$H_l(\phi',\phi) \equiv \int d\rho(\lambda)\Phi^*(be^{i\phi'};\lambda)(\lambda-\theta)^l\Phi(be^{i\phi};\lambda).$$

The function $\Psi_\alpha(z)$ is the representative of the Glauber state in H^2; according to (4.11), it is

$$\Psi_\alpha(z) = \exp(-\tfrac{1}{2}R^2)g(\alpha z),$$

$$g(w) \equiv \sum_{n=0}^{\infty}\frac{w^n}{(n!)^{\frac{1}{2}}}.$$

The function $g(w)$ is entire and has power series coefficients that are analytic functions of the index; consequently, we can find its asymptotic form by the following standard method[10]:

(1) For fixed w we find the maximum term;

(2) We approximate the sum in the vicinity of the maximum term by an integral and compute the integral by the saddle-point method.

In the present case, one finds, with $w = re^{iv}$ and $r \to \infty$,

$$g(w) \to (2\pi)^{\frac{1}{2}}(2r)^{\frac{1}{2}}\exp[\tfrac{1}{2}r^2 - r^2v^2 + i(r^2 - \tfrac{1}{2})v].$$

In the case of interest, we have $w = \alpha z$, with $z = be^{-i\phi}$ and $b \to 1$, so that

$$\Psi_\alpha(z) \to (2\pi)^{\frac{1}{2}}(2R)^{\frac{1}{2}} \times \exp[-R^2(\theta+\phi)^2 - i(R^2 - \tfrac{1}{2})(\theta+\phi)]. \tag{B2}$$

Thus,

$$I_l \approx (2\pi)^{\frac{1}{2}}(2R)\int\frac{d\phi}{2\pi}\int\frac{d\phi'}{2\pi} \times \exp[i(R^2 - \tfrac{1}{2})(\phi' - \phi)] \times \exp\{-R^2[(\phi+\theta)^2 + (\phi'+\theta)^2]\}H_l(\phi',\phi).$$

The Gaussian factors effectively limit the integrals to a small region around $\phi' = \phi = -\theta$; consequently, if $|H_l(\phi',\phi)| \leq M_l < \infty$ in this region, we obtain the following bound on I_l:

$$|I_l| \leq (2\pi)^{\frac{1}{2}}(2R)M_l\left|\int_{-\infty}^{\infty}\frac{d\phi}{2\pi}\exp(-R^2\phi^2)\right|^2, \leq (2\pi)^{-\frac{1}{2}}M_lR^{-1} \to 0.$$

Thus, (B1) is established as soon as we show that $H_l \equiv H_l(-\theta,-\theta)$ is finite. We have

$$H_l = \lim_{b\to 1}\int d\rho(\lambda)(\lambda-\theta)^l|\Phi(be^{-i\theta};\lambda)|^2,$$

where by (4.10)

$$|\Phi(z;\lambda)|^2 = (|1+z||1-ze^{i\lambda}|)^{-1}e^{-2\operatorname{Re}\Omega(z;\lambda)},$$

$$\operatorname{Re}\Omega(be^{-i\theta};\lambda) = (1-b^2)\int\frac{d\phi}{4\pi}\frac{\log|\phi-\lambda|}{1+b^2-2b\cos(\phi-\theta)}. \tag{B3}$$

As $b \to 1$, the integrand in (B3) develops a singularity at $\phi = \theta$, and this is the only part of the integration region that can cancel the $(1-b^2)$ factor. If we restrict the ϕ integral to a small interval centered on θ and make appropriate expansions in the integrand, we find that

$$\operatorname{Re}\Omega(be^{-i\theta};\lambda) \to \tfrac{1}{2}\log|\theta-\lambda|.$$

Thus, we have

$$H_l = \tfrac{1}{4}(1+\cos\theta)^{-\frac{1}{2}} \times \int_{-\pi}^{\pi}d\lambda(\cos\tfrac{1}{2}\lambda)\frac{(\lambda-\theta)^l}{|\lambda-\theta|}(1-\cos(\lambda-\theta))^{-\frac{1}{2}},$$

which is clearly finite for $l \geq 1$ and $\theta \neq \pm\pi$. This completes the proof of (4.12) for all $\theta \in (-\pi,\pi)$.

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[1] L. Susskind and J. Glogower, Phys. **1**, 49 (1964).

[2] P. Carruthers and M. Nieto, Rev. Mod. Phys. **40**, 411 (1968). This is an excellent review article which contains references to the original literature.

[3] C. R. Putnam, *Commutation Properties of Hilbert Space Operators and Related Topics* (Springer, New York, 1967). See pp. 64ff.

[4] L. Gårding, Proc. Natl. Acad. Sci. U.S. **33**, 331 (1947).

[5] See Ref. 3, pp. 72ff.

[6] S. G. Eckstein, B. B. Varga, and S. O. Aks, University of Illinois, Chicago, Illinois, manuscript in preparation, 1969. In this work the authors analyze this example by using the fact that the matrices corresponding to unbounded operators may fail to have the same algebraic properties as the operators themselves.

[7] For a further discussion of this example, see E. Nelson, Ann. Math. **70**, 572 (1959), especially pp. 603ff.

[8] M. Rosenblum, Proc. Am. Math. Soc. **13**, 590 (1962).

[9] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964), pp. 227ff.

[10] E. Hille, *Analytic Function Theory* (Ginn, Boston, 1962), pp. 182ff.

Solution of Mathieu's Type of Secular Equations*

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A discussion is given for the general solution of a secular equation with all other matrix elements equal to zero except H_{ii}, $H_{i\,i+h}$, and $H_{i+h\,i}$. Both the eigenvalue and the amplitudes of the corresponding eigenfunction are expressed in terms of continued fractions of the matrix elements. A solution of Mathieu equation is used as an example to compare the present method with other methods.

I. INTRODUCTION

The secular equation is an equation formed by equating to zero the determinant of the coefficients of a set of linear homogeneous equations which arise in the course of solving an eigenvalue equation using a linear combination of vectors or operators. A secular equation with all its nondiagonal matrix elements equal to zero is in its simplest form, the solution of which is obviously trivial. In the nontrivial case, the simplest form may be the one in which only the nondiagonal matrix elements of a particular column i and the corresponding row i are not necessarily all equal to zero. Since this special kind of equation is largely of academic interest, its solution is given as an example. In this paper, our main concern is the solution of another simple form of secular equation in which all matrix elements are always zero except H_{ii}, $H_{i\,i+h}$, and $H_{i+h\,i}$, where i represents any state and h is a fixed integer. Although this kind of equation is simple, it has been found in various fields of physics, e.g., the Mathieu equation solved by the perturbation method, the hyperfine interaction expressed in the (F, m) representation, the 1-dimensional coupled oscillation, etc. Therefore, a general solution of this kind of simple equation may be of interest and useful. It has been shown[1] that the eigenvalue for the lowest state of the Mathieu equation can be expressed in terms of a simple continued fraction by means of which the calculation is much simplified. Hence, a similar kind of solution could be obtained even for the general case. We must point out that the equation discussed here is one of the very special cases of the general secular equation studied in Ref. 1. Accordingly, all symbols and definitions used here should be referred to Ref. 1.

II. SOLUTION

We start with the eigenvalue expansion of a general secular equation. For any eigenvalue E_i, we have

$$E_i = H_{ii} - R_i(E_i), \tag{1}$$

where

$$R_i = \bar{N}_i/\bar{M}_{ii}^{ii}, \tag{2}$$

with

$$\bar{N}_i = \sum_{\neq i}^{n-1\,\mathrm{p}} \left(\frac{(ij)}{(j)} - \frac{(ijk)}{(j)(k)} + \frac{(ijkl) - (ij)(kl)}{(j)(k)(l)} - \cdots \right) \tag{3}$$

and

$$\bar{M}_{ii}^{ii} = \sum_{\neq i}^{n-1\,\mathrm{p}} \left(1 - \frac{(jk)}{(j)(k)} + \frac{(jkl)}{(j)(k)(l)} - \cdots \right). \tag{4}$$

Here,

$$(j) \equiv (j,j) \equiv H_{jj} - E_i \equiv H_{jj} - H_{ii} + R_i,$$
$$(i_1, i_2, \cdots, i_r) \equiv (i_1, i_2)(i_2, i_3) \cdots (i_r, i_1),$$

i.e., the cyclic product of any r elements with $(\alpha, \beta) \equiv H_{\alpha\beta}$ for $\alpha \neq \beta$; and $\sum_{\neq i}^{\mathrm{p}} \equiv$ a summation over all possible nonequivalent cyclic permutations among all indices except i. We note that R_i represents a correction for the first-order perturbation. The amplitude of the corresponding eigenfunction is given by

$$a_{ij}/a_{ii} = -\bar{M}_{ii}^{ii(j)}/\bar{M}_{ii}^{ii}, \tag{5}$$

where

$$\bar{M}_{ii}^{ii(j)} = \sum_{\neq i,j}^{n-2\,\mathrm{p}} \left(\frac{(j,i)}{(j)} - \frac{(j,k)(k,i)}{(j)(k)} + \frac{(j,k)(k,l)(l,i) - (j,i)(k,l)(l,k)}{(j)(k)(l)} - \cdots \right) \tag{6}$$

for $j \neq i$. For the secular equation specified in Sec. I, its matrix element is expressed, in general, as

$$(\alpha, \beta) = H_{\alpha\beta}(\delta_{\alpha\beta} + \delta_{\alpha\,\beta-h} + \delta_{\alpha\,\beta+h}) \tag{7}$$

for all α and β, it follows that any cyclic product with more than two indices vanishes. Thus, Eqs. (3) and (4) become

$$\bar{N}_i = \sum_{\neq i}^{n-1\,\mathrm{p}} \left(\frac{(ij)}{(j)} - \frac{(ij)(kl)}{(j)(k)(l)} + \frac{(ij)(kl)(ms)}{(j)(k)(l)(m)(s)} - \cdots \right) \tag{8}$$

and

$$\bar{M}_{ii}^{ii} = \sum_{\neq i}^{n-1\,\mathrm{p}} \left(1 - \frac{(jk)}{(j)(k)} + \frac{(jk)(lm)}{(j)(k)(l)(m)} - \cdots \right). \tag{9}$$

To simplify our discussion, we define

$$\bar{M}_{n-r}[i_1, i_2, \cdots, i_r] \equiv \sum_{\neq i,s}^{n-r}{}^{\mathrm{p}} \left(1 - \frac{(jk)}{(j)(k)} + \frac{(jk)(lm)}{(j)(k)(l)(m)} - \cdots\right), \quad (10)$$

a specific determinant of order $n - r$. A recursion relation can be obtained as follows:

$$\bar{M}_{n-r}[i_1, \cdots, i_r] = \bar{M}_{n-r-1}[i_1, \cdots, i_{r+1}] - [(i_{r+1}i_{r+2})/(i_{r+1})(i_{r+2})]\bar{M}_{n-r-2}[i_1, \cdots, i_{r+2}] \quad (11)$$

or

$$F(i_{r+1}) = 1 - [(i_{r+1}i_{r+2})/(i_{r+1})(i_{r+2})]/F(i_{r+2}), \quad (12)$$

where $F(i_{r+1}) \equiv \bar{M}_{n-r}/\bar{M}_{n-r-1}$. By successive application of Eq. (12), F can be transformed into a continued fraction of the matrix elements. There are a number of different ways in which $\bar{N}_i$ and $\bar{M}_{ii}$ can be expanded in terms of $\bar{M}_{n-r}$ or $F(i_r)$. The simplest and most direct way is as follows:

$$\bar{N}_i = \frac{(i\, i-h)}{(i-h)}\bar{M}_{n-2}[i, i-h] + \frac{(i\, i+h)}{(i+h)}\bar{M}_{n-2}[i, i+h] \quad (13)$$

and

$$\bar{M}_{ii}^{ii} = \bar{M}_{n-1}[i]. \quad (14)$$

Therefore, from Eqs. (2) and (12), we obtain

$$R_i = \frac{(i\, i-h)}{(i-h)}\Big/F_i(i-h) + \frac{(i\, i+h)}{(i+h)}\Big/F_i(i+h). \quad (15)$$

Now

$$F_i(i-h) = 1 - \cfrac{(i-h\, i-2h)/(i-h)(i-2h)}{1 - \cfrac{(i-2h\, i-3h)/(i-2h)(i-3h)}{1 - \cdot}} \quad (16a)$$

and

$$F_i(i+h) = 1 - \cfrac{(i+h\, i+2h)/(i+h)(i+2h)}{1 - \cfrac{(i+2h\, i+3h)/(i+2h)(i+3h)}{1 - \cdot}} \quad (16b)$$

It is interesting to note that the only matrix elements involved in the calculation are those having indices $i \pm th$, where $t = 0, 1, \cdots$.

As for the amplitudes of the eigenfunction corresponding to E_i, Eq. (6) is expanded in terms of $\bar{M}_{n-r}$. We have

$$\bar{M}_{ii}^{ii(j)} = \frac{(j,i)}{(j)}\bar{M}_{n-2}[j,i] - \frac{(j,k_1)(k_1,i)}{(j)(k_1)}\bar{M}_{n-3}[j,k_1,i] + \cdots + (-1)^r\frac{(j,k_1)\cdots(k_r,i)}{(j)(k_1)\cdots(k_r)} \times \bar{M}_{n-r-2}[j,k_1,\cdots,k_r,i] + \cdots. \quad (17)$$

For a given value of j, only one of the terms on the right-hand side of Eq. (17) can survive under the conditions given by Eq. (7). For $j = i + th + h$,

$$\bar{M}_{ii}^{ii(i+th+h)} = (-1)^t\frac{(i+th+h, i+th)\cdots(i+h,i)}{(i+th+h)\cdots(i+h)} \times \bar{M}_{n-t}[i+th+h, \cdots, i], \quad (18)$$

which is valid for both $\pm h$. Since the expansion of Eq. (5) is rather complicated, it is much simpler to expand, instead, the ratio of two amplitudes of neighboring states. From Eq. (5),

$$a_{i\,i+th+h}/a_{i\,i+th} = \bar{M}_{ii}^{ii(i+th+h)}/\bar{M}_{ii}^{ii(i+th)} = -[(i+th+h, i+th)/(i+th+h)]/F_i(i+th+h). \quad (19)$$

Note that $F_i(i + th + h)$ is part of $F_i(i \pm h)$. By using the normalization condition $\sum_j^n |a_{ij}|^2 = 1$, the normalized value of each a_{ij} is obtained.

Alternatively, Eqs. (15) and (19) may be written as

$$R_i = (i\, i-h)/G_i(i-h) + (i\, i+h)/G_i(i+h) \quad (20)$$

and

$$a_{i\,i+th+h}/a_{i\,i+th} = -(i+th+h, i+th)/G_i(i+th+h), \quad (21)$$

respectively, where

$$G_i(i+h) = (i+h) - \cfrac{(i+h\, i+2h)}{(i+2h) - \cfrac{(i+2h\, i+3h)}{(i+3h) - \cdot}} \quad (22)$$

The continued fraction solution is an interesting example of a perturbation process taking place through intermediate states. In this case, there is no matrix element connecting state i with any other states except

its neighboring states $i \pm h$. The perturbation on state i from any nonneighboring state has to be relayed through all the states in between. We may say that the perturbation received by a given state depends not only on its neighbor but also on the perturbation that its neighbor has received. Therefore, Eq. (15) or Eq. (20) represents a perturbation such that the state i is affected directly or indirectly by two different groups of its neighbors, one group on one side and the other on another side.

III. EXAMPLES

A. Application to the Mathieu Equation

To illustrate the application of Eqs. (15) and (19), we try to solve the Mathieu equation

$$\frac{d^2\psi_i}{d\theta^2} + (b_i - s\cos^2\theta)\psi_i = 0, \quad \psi_i(0) = \psi_i(2\pi) \quad (23)$$

by the perturbation method.[2] When $s\cos^2\theta$ is taken as perturbation, the unperturbed eigenfunctions for the even case are

$$U_0 = (2\pi)^{-\frac{1}{2}} \text{ and } U_j = (\pi)^{-\frac{1}{2}}\cos j\theta, \quad j = 1, 2, \cdots,$$

with the associated eigenvalues i^2. The perturbed eigenfunction is given by

$$\psi_i = \sum_{j=0}^{\infty} a_{ij}U_j. \quad (24)$$

All the matrix elements except the following are zero:

$$H_{ii} = i^2 + \tfrac{1}{2}s, \quad H_{02} = H_{20} = 8^{-\frac{1}{2}}s,$$

and

$$H_{i\,i+2} = H_{i+2\,i} = \tfrac{1}{4}s, \quad \text{for all} \quad i \neq 0. \quad (25)$$

Now $h = 2$. The calculation of R_0 with $s = 4$, using a continued fraction, has been given in Ref. 1. By using Eqs. (1) and (15), the eigenvalue b_6 is given by

$$b_6 = 36 + 2s - R_6 \quad (26)$$

and

$$R_6 = [(6\,4)/(4)]/F_6(4) = [(6\,8)/(8)]/F_6(8), \quad (27)$$

with

$$F_6(4) = 1 - \cfrac{(4\,2)/(4)(2)}{1 - \cdot \atop \quad \cdot \atop \quad \cdot}, \quad F_6(8) = 1 - \cfrac{(8\,10)/(8)(10)}{1 - \cdot \atop \quad \cdot \atop \quad \cdot}. \quad (28)$$

For $s = 30$, the explicit form of R_6 with an approximation up to $n = 12$ (fourth-order approximation) is

$$R_6^{(4)} = \cfrac{A/(-20 + R_6)}{1 - A/(-20 + R_6)(-32 + R_6)/[1 - 2A/(-32 + R_6)(-36 + R_6)]} + \cfrac{A/(28 + R_6)}{1 - A/(-28 + R_6)(64 + R_6)/[1 - A/(64 + R_6)(108 + R_6)]}, \quad (29)$$

where $A = 56.25$. Now R_6 can be solved by the iteration method.[1] For the lowest order of approximation of R_6, we may take $F_6(4) = F_6(8) = 1$. Consequently, we have

$$R_6^{(2)} = A/(-20 + R_6) + A/(28 + R_6). \quad (30)$$

Using ${}_{(0)}R_6 = 0$, we obtain ${}_{(1)}R_6^{(2)} = -0.8036$, which yields ${}_{(1)}b_6^{(2)} = 51.8036$. This value is the same as that obtained by the second-order approximation given by the Rayleigh–Schrödinger perturbation. For a better approximation, Eq. (29) is used. The values of ${}_{(p)}R_6^{(4)}$ corresponding to each successive iteration p are given in column (4) in Table I, which also includes the results obtained by three other methods.

Two more points in Table I need explanation:

(i) In principle, the final limit of the solution obtained by the iteration method does not depend on the initially chosen value. Therefore, to simplify and speed up the calculation, some other mathematical tricks may be employed. For example, after every two consecutive iterations, the next value may be estimated by extrapolation from these three numbers.[2] Assuming that

$$[{}_{(1)}R - R_e]/[{}_{(2)}R - R_e] = [{}_{(2)}R - R_e]/[{}_{(3)}R - R_e], \quad (31)$$

we get

$$R_e = {}_{(3)}R - [{}_{(3)}R - {}_{(2)}R]^2/\{[{}_{(3)}R - {}_{(2)}R] - [{}_{(2)}R - {}_{(1)}R]\}. \quad (32)$$

Results computed by this iteration–extrapolation method are shown in column (5). Values calculated with use of Eq. (32) are indicated by $(\ )_e$.

(ii) By continuing the process of iteration indefinitely, we may have as many significant figures as we want for the limit of b_6. However, the accuracy of b_6 calculated depends not only on the number of iterations performed but also on the order of approximation used. Since $F_6(4)$ is exact, the inaccuracy is due to $F_6(8)$ only. The possible error of $R_6^{(4)}$ can be estimated by calculating how large a correction would

TABLE I. Eigenvalues E_6 of the Mathieu equation for $s = 30$ obtained by different methods. Broken lines indicate convergence.

Method: Order of iteration or approximation	(1)[2,3] Brillouin–Wigner b_6	(2)[2,3] Feenberg b_6	(3)[3] Sasakawa b_6	Eq. (26) (4) Simple iteration	Eq. (26) (5) Iteration-extrapolation
0	51.00000	51.00000	51.00000	51.00000000	51.00000000
1	48.27998	51.80358	51.75061	52.04142419	52.04142419
2	53.28531	51.63557	51.75116	51.77609995	51.77609995
3		51.67029	- - - - -	51.84222168	51.84222168
4		51.66310		51.82565734	$(51.82903074)_e$
5		51.66459		51.82980141	51.82895716
6		51.66428		51.82876169	51.82897557
7		51.66434		51.82902449	$(51.82897189)_e$
8		51.66433		51.82895871	51.82897188
9		- - - - -		51.82897518	- - - - - - -
10				51.82897106	
11				51.82897209	
12				51.82897183	
13				51.82897189	
14				51.82897188	
				- - - - - - -	
				$b_6^{(4)} = 51.82897188$	
Possible error	...	...	...	±0.00000200	
Exact solution			51.82897[2]		

be if the next higher-order approximation were included. We have

$$\Delta R_6^{(4)} \simeq (56.25)^4/[(28 + R_6)^2(64 + R_6)^2 \times (108 + R_6)^2(160 + R_6)] \simeq +1.86 \times 10^{-6}.$$

Therefore, we may write $b_6 = 51.828972(2)$.

To obtain the eigenfunction associated with b_6 and ψ_6 (the Mathieu function), we use Eqs. (19) and (24). The results of a_{6j} are shown in Table II with values of j up to 18.

TABLE II. Amplitudes of the Mathieu function ψ_6 for $s = 30$.

j	$th + h$	$a_{6\,6+th+h}/a_{6\,6+th}$	a_{6j}/a_{66}	a_{6j} (normalized)
0	−6	0.2879961	0.0287272	0.0256918
2	−4	0.2518950	0.0997485	0.0892089
4	−2	0.3959924	0.3959924	0.3541512
6			1.0000000	0.8943385
8	2	−0.2854630	−0.2854630	−0.2553006
10	4	−0.1197233	0.0341766	0.0305654
12	6	−0.0702135	−0.0023997	−0.0021461
14	8	−0.0471953	0.0001133	0.0001013
16	10	−0.0342505	−0.0000038	−0.0000034
18	12	−0.0261168	0.0000001	0.0000001

B. Secular Equation with H_{ii}, H_{jj}, H_{ij}, and H_{ji} Nonzero Matrix Elements

A solution is given for a secular equation with all its matrix elements equal to zero except H_{ii}, H_{jj}, H_{ij}, and H_{ji}, where i represents a particular state and $j = 1, \cdots, n \neq i$, for all other states. It follows from Eqs. (1)–(6) that, for state i,

$$E_i = H_{ii} - R_i, \quad R_i = \sum_{j\neq i}^{n} [(ij)/(j)] \tag{33a}$$

and

$$a_{ij}/p_{ii} = -(j, i)/(j);$$

and, for all other states j,

$$E_j = H_{jj} - R_j, \tag{33b}$$

$$R_j = [(ji)/(i)] \Big/ \sum_{k\neq i,j}^{n} [1 - (ik)/(i)(k)]$$

and

$$\frac{a_{ji}}{a_{jj}} = -\left[\frac{(i,j)}{(i)}\right] \Big/ \sum_{k\neq i,j}^{n} \left[1 - \frac{(ik)}{(i)(k)}\right],$$

$$\frac{a_{jk}}{a_{jj}} = \left[\frac{(k,i)(i,j)}{(k)(i)}\right] \Big/ \sum_{k\neq i,j}^{n} \left[1 - \frac{(ik)}{(i)(k)}\right].$$

We note that the result of (33a) is simpler than that of (33b) because there is no direct perturbation between any two states of j. They are related to each other only indirectly through state i.

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[1] Y. W. Chan, J. Math. Phys. 7, 27 (1966).
[2] P. M. Morse and H. Feshbach, *Method of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. II, Chap. 9.
[3] T. Sasakawa, J. Math. Phys. 4, 970 (1963).

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Diffraction Theory of Holography*

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A diffraction theory of side-band holography for transmission objects is formulated. Conditions are derived under which good quality images are formed. A simple geometrical construction is found by means of which the location of the images may be determined. It is also shown that, under conditions that are often satisfied in practice, one of the two images will be completely absent. This effect is entirely caused by diffraction (conversion of a homogeneous wave into evanescent waves on diffraction by the hologram) and has nothing to do with the finite resolving power or the finite thickness of the photographic plate. Numerical examples illustrating this phenomenon are given.

INTRODUCTION

Since the publication of Gabor's pioneering papers on holography,[1,2] numerous investigations dealing with many aspects of this subject have been carried out. These investigations lead to the elucidation of the basic principles of holography and to the development of many holographic schemes suitable for different applications. In spite of the great activity in this field, no completely satisfactory theory of some of the holographic schemes has been developed up to now. Much of the theoretical work is based on geometrical optics, sometimes utilizing useful but not quite complete analogies with the theory of communication systems. In those treatments where physical optics has been used, the numerous approximations, appropriate to the many different holographic schemes (e.g., Fresnel, Fraunhofer, Fourier transform) disguise the basic physical requirements and the limitations of this technique.

In the present paper we formulate a diffraction theory of the holographic scheme due to Leith and Upatnieks,[3] known often as side-band holography. Our treatment is based on the systematic use of the angular spectrum representation of wavefields.[4] Our analysis shows that basic for a clear understanding of side-band holography are two new theorems on diffraction. One is the diffraction reciprocity theorem that we discussed recently in another paper.[5] This theorem relates two fields whose boundary values in some planes are complex conjugates of each other. The second theorem (Theorem 3 of the Appendix of the present paper) connects two fields whose boundary values differ by a multiplicative space-periodic exponential factor. With the help of these two theorems, conditions are derived under which good quality holographic images are formed. These conditions involve no restriction on the distances of the images from the hologram. A simple geometrical construction is found by means of which the location of the images may be determined.

We also show that, under conditions that are often satisfied in practice, one of the two images will be completely absent. This disappearance of one of the images is a pure diffraction effect, caused by the conversion of a homogeneous wave into evanescent waves on diffraction by the hologram. It has nothing to do with the finite resolving power of the photographic plate or its finite thickness. We give some numerical examples that illustrate this interesting phenomenon. In particular, we find that, when the images are viewed visually, one of them will disappear if the reference and the reconstruction beams make angles greater than about 30° with the axis.

In order to bring out the essential features of the holographic process, we ignore in the present paper several complications. More specifically, we do not consider the imperfect resolution arising from the finite size of the photographic plate, nor do we consider effects arising from its finite thickness. Also, we assume that the incident beam, the reference beam, and the reconstruction beam are all of the same wavelength, and we restrict ourselves to holography with transmission objects.

1. BASIC EQUATIONS OF HOLOGRAPHY WITH TRANSMISSION OBJECTS

Consider a monochromatic light wave

$$\mathfrak{U}(x, y, z, t) = U^{(0)}(x, y, z) \exp(-i\omega t), \quad (1.1)$$

incident upon a semitransparent object which covers a portion $\mathcal{A}$ of the plane $z = z_0$ (see Fig. 1). The wave emerging from the object may be represented in the form (omitting the time periodic factor)

$$U(x, y, z_0) = U^{(0)}(x, y, z_0)T^{(0)}(x, y), \quad (1.2)$$

where $T^{(0)}(x, y)$ is a transmission function that characterizes the effect of the object on the incident light. $T^{(0)}$ depends, of course, on the nature of the incident field $U^{(0)}$. We will rewrite Eq. (1.2) in a more compact notation as

$$U_0(\mathbf{r}) = U_0^{(0)}(\mathbf{r})T^{(0)}(\mathbf{r}), \quad (1.3)$$

where $\mathbf{r}$ denotes the 2-dimensional vector (x, y) and the subscript zero indicates that the field point is situated in the plane $z = z_0$. We will employ a similar abbreviated notation when referring to field points in other planes perpendicular to the z axis.

Suppose that the light emerging from the object is incident on a photographic plate that is situated in the plane $z = z_1 > z_0$, whereas the light that does not pass through the object is obstructed by a stop situated in the plane $z = z_0$. Then the field at a typical point $\mathbf{r}_1(x_1, y_1)$ in the plane containing the photographic plate is given by

$$U_1(\mathbf{r}_1) = \int_{\mathcal{A}} U_0(\mathbf{r}_0)K_{10}(\mathbf{r}_1 - \mathbf{r}_0)d^2\mathbf{r}_0, \quad (1.4)$$

where $K_{10}(\mathbf{r}_1 - \mathbf{r}_0)$ is the wave propagator that characterizes propagation from the plane $z = z_0$ to the plane $z = z_1$ (cf. Ref. 5). On substituting from (1.3) into (1.4) and on setting

$$\begin{aligned} T(\mathbf{r}) &= T^{(0)}(\mathbf{r}), \quad \text{when} \quad \mathbf{r} \in \mathcal{A}, \\ &= 0, \qquad \text{when} \quad \mathbf{r} \notin \mathcal{A}, \end{aligned} \quad (1.5)$$

we obtain the following expression for the field distribution in the plane of the photographic plate:

$$U_1(\mathbf{r}_1) = \int_{(\infty)} U_0^{(0)}(\mathbf{r}_0)T(\mathbf{r}_0)K_{10}(\mathbf{r}_1 - \mathbf{r}_0)d^2\mathbf{r}_0, \quad (1.6)$$

where the integration extends formally over the whole plane[6] $z = z_0$.

Suppose now that in addition to the wavefield U a second field $U^{(r)}$, the reference field, assumed also to be monochromatic and of the same frequency, is incident on the plane containing the photographic plate. The total field $U^{(t)}(\mathbf{r}_1)$ at a point $\mathbf{r}_1$ in this plane is then given by

$$U_1^{(t)}(\mathbf{r}_1) = U_1(\mathbf{r}_1) + U_1^{(r)}(\mathbf{r}_1). \quad (1.7)$$

Hence, the intensity distribution in the plane of the photographic plate is given by

$$I_1^{(t)}(\mathbf{r}_1) = U_1^{(t)*}(\mathbf{r}_1)U_1^{(t)}(\mathbf{r}_1) \quad (1.8)$$

$$= I_1(\mathbf{r}_1) + I_1^{(r)}(\mathbf{r}_1) + U_1^{(r)*}(\mathbf{r}_1)U_1(\mathbf{r}_1) + U_1^{(r)}(\mathbf{r}_1)U_1^*(\mathbf{r}_1). \quad (1.9)$$

Here

$$I_1(\mathbf{r}_1) = U_1^*(\mathbf{r}_1)U_1(\mathbf{r}_1), \quad (1.10a)$$

$$I_1^{(r)}(\mathbf{r}_1) = U_1^{(r)*}(\mathbf{r}_1)U_1^{(r)}(\mathbf{r}_1) \quad (1.10b)$$

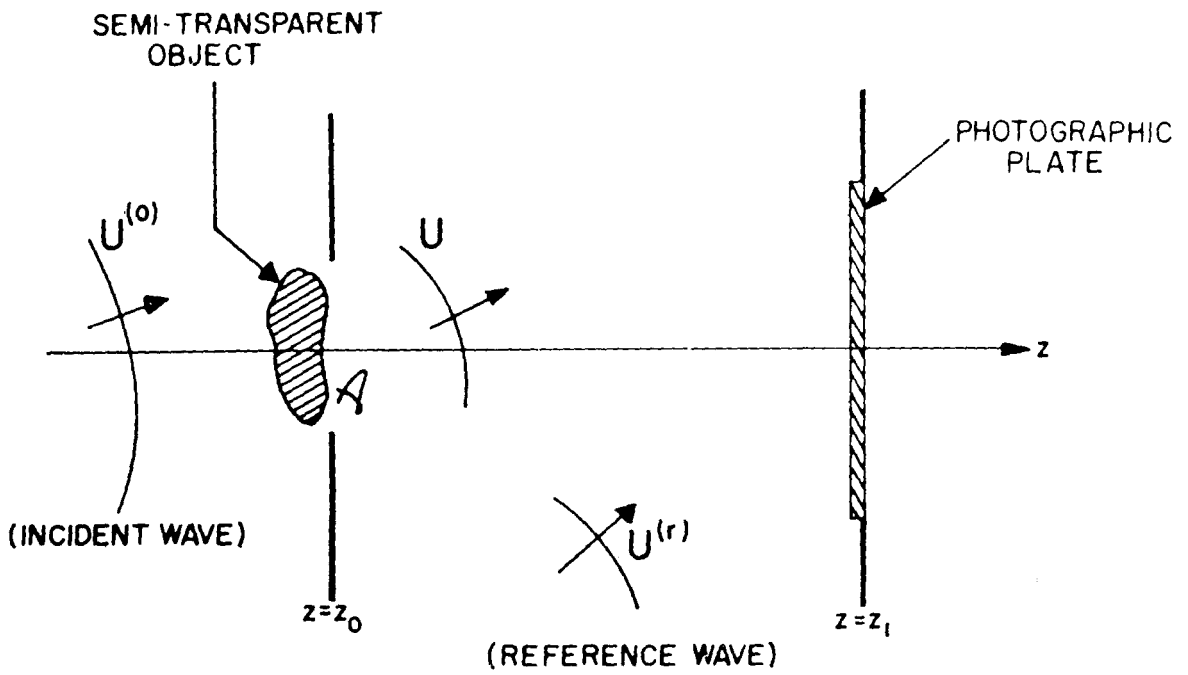

FIG. 1. Notation relating to the formation of a hologram.

are the intensity distributions in the plane $z = z_1$ of the wave that was transmitted by the object and of the reference wave, respectively.

The photographic plate responds to the intensity distribution $I_1^{(t)}(\mathbf{r}_1)$ of the total field. We will, for the present, somewhat idealize the photographic plate by assuming it to be a 2-dimensional storage medium. We also assume that, after the plate is processed, it will have an amplitude transmission function that is a linear function of the intensity $I_1^{(t)}$. We thus obtain a hologram whose amplitude transmission function is given by

$$T_H(\mathbf{r}) = c_0 + c_1 I_1^{(t)}(\mathbf{r}), \tag{1.11}$$

where c_0 and c_1 are real constants. Under usual circumstances, c_0 is positive and c_1 is negative. On substituting from (1.9) into (1.11), we obtain the following expression for the transmission function of the hologram:

$$T_H(\mathbf{r}) = T_H^{(I)}(\mathbf{r}) + T_H^{(II)}(\mathbf{r}) + T_H^{(III)}(\mathbf{r}), \tag{1.12}$$

where

$$T_H^{(I)}(\mathbf{r}) = c_1 U_1^{(r)*}(\mathbf{r}) U_1(\mathbf{r}), \tag{1.13a}$$

$$T_H^{(II)}(\mathbf{r}) = c_1 U_1^{(r)}(\mathbf{r}) U_1^*(\mathbf{r}), \tag{1.13b}$$

$$T_H^{(III)}(\mathbf{r}) = c_0 + c_1 I_1^{(r)}(\mathbf{r}) + c_1 I_1(\mathbf{r}). \tag{1.13c}$$

Suppose now that the processed hologram is placed in the plane $z = z_1$ and is illuminated by a monochromatic wave of the same frequency (see Fig. 2),

$$\mathcal{V}^{(h)}(x, y, z, t) = V^{(h)}(x, y, z) \exp(-i\omega t). \tag{1.14}$$

The space-dependent part of the distribution in the plane $z = z_1$ of the field emerging from the hologram is then given by

$$V_1(\mathbf{r}) = V_1^{(h)}(\mathbf{r}) T_H(\mathbf{r}) \tag{1.15}$$

or, by using (1.12) and (1.13),

$$V_1(\mathbf{r}) = V_1^{(I)}(\mathbf{r}) + V_1^{(II)}(\mathbf{r}) + V_1^{(III)}(\mathbf{r}), \tag{1.16}$$

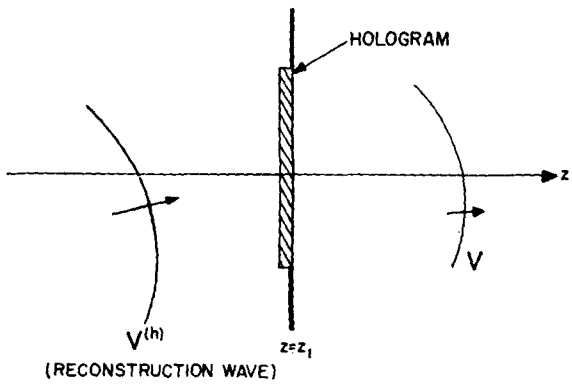

FIG. 2. Notation relating to reconstruction.

where

$$V_1^{(I)}(\mathbf{r}) = c_1 V_1^{(h)}(\mathbf{r}) U_1^{(r)*}(\mathbf{r}) U_1(\mathbf{r}), \tag{1.17a}$$

$$V_1^{(II)}(\mathbf{r}) = c_1 V_1^{(h)}(\mathbf{r}) U_1^{(r)}(\mathbf{r}) U_1^*(\mathbf{r}), \tag{1.17b}$$

$$V_1^{(III)}(\mathbf{r}) = V_1^{(h)}(\mathbf{r})[c_0 + c_1 I_1^{(r)}(\mathbf{r}) + c_1 I_1(\mathbf{r})]. \tag{1.17c}$$

Equation (1.16), together with (1.17a, b, c), (1.6), and (1.10a, b), are the basic equations of holography for transmission objects. They represent, under fairly general conditions, the boundary values in the plane $z = z_1$ of the wave emerging from the hologram.

2. THE BOUNDARY VALUES OF SIDE-BAND HOLOGRAPHY

We will now specialize the main equations that we just derived to the arrangement due to Leith and Upatnieks,[3] sometimes called side-band holography, and we will derive some conditions under which the partial fields $V^{(I)}$ and $V^{(II)}$ give reasonably faithful images of the original object.

The reference wave $U^{(r)}$ and the reconstructing wave $V^{(h)}$ are now plane waves, which we may represent in the form[7]

$$U^{(r)} = A^{(r)} \exp\{ik[p_r x + q_r y + m_r(z - z_1)]\}, \tag{2.1}$$

$$V^{(h)} = B^{(h)} \exp\{ik[p_h x + q_h y + m_h(z - z_1)]\}. \tag{2.2}$$

Here (p_r, q_r, m_r) and (p_h, q_h, m_h) are components of unit vectors $\mathbf{s}_r$ and $\mathbf{s}_h$, respectively, in the direction of propagation of the two waves.

On substituting from (2.1) and (2.2) into (1.17 a, b, c) and using (1.10b), we obtain the following expressions for the three contributions to $V_1(\mathbf{r})$:

$$V_1^{(I)}(\mathbf{r}) = C^{(I)} U_1(\mathbf{r}) \exp(ik\boldsymbol{\sigma}^{(I)} \cdot \mathbf{r}), \tag{2.3a}$$

$$V_1^{(II)}(\mathbf{r}) = C^{(II)} U_1^*(\mathbf{r}) \exp(ik\boldsymbol{\sigma}^{(II)} \cdot \mathbf{r}), \tag{2.3b}$$

$$V_1^{(III)}(\mathbf{r}) = B^{(h)}[c_0 + c_1 A^{(r)*} A^{(r)} + c_1 I_1(\mathbf{r})] \times \exp[ik(p_h x + q_h y)], \tag{2.3c}$$

where $\boldsymbol{\sigma}^{(I)}$ and $\boldsymbol{\sigma}^{(II)}$ are the 2-dimensional vectors

$$\boldsymbol{\sigma}^{(I)} \equiv p_h - p_r, \quad q_h - q_r, \tag{2.4a}$$

$$\boldsymbol{\sigma}^{(II)} \equiv p_h + p_r, \quad q_h + q_r, \tag{2.4b}$$

and $C^{(I)}$ and $C^{(II)}$ are the constants

$$C^{(I)} = c_1 A^{(r)*} B^{(h)}, \quad C^{(II)} = c_1 A^{(r)} B^{(h)}. \tag{2.5}$$

There are several cases of special interest, which for convenience we will refer to as arrangements A, B, and C. These are (see Fig. 3):

Arrangement A: Reconstruction wave propagates in the same direction as the reference wave: $p_h = p_r$, $q_h = q_r$, $m_h = m_r$. Hence, according to Eqs. (2.4),

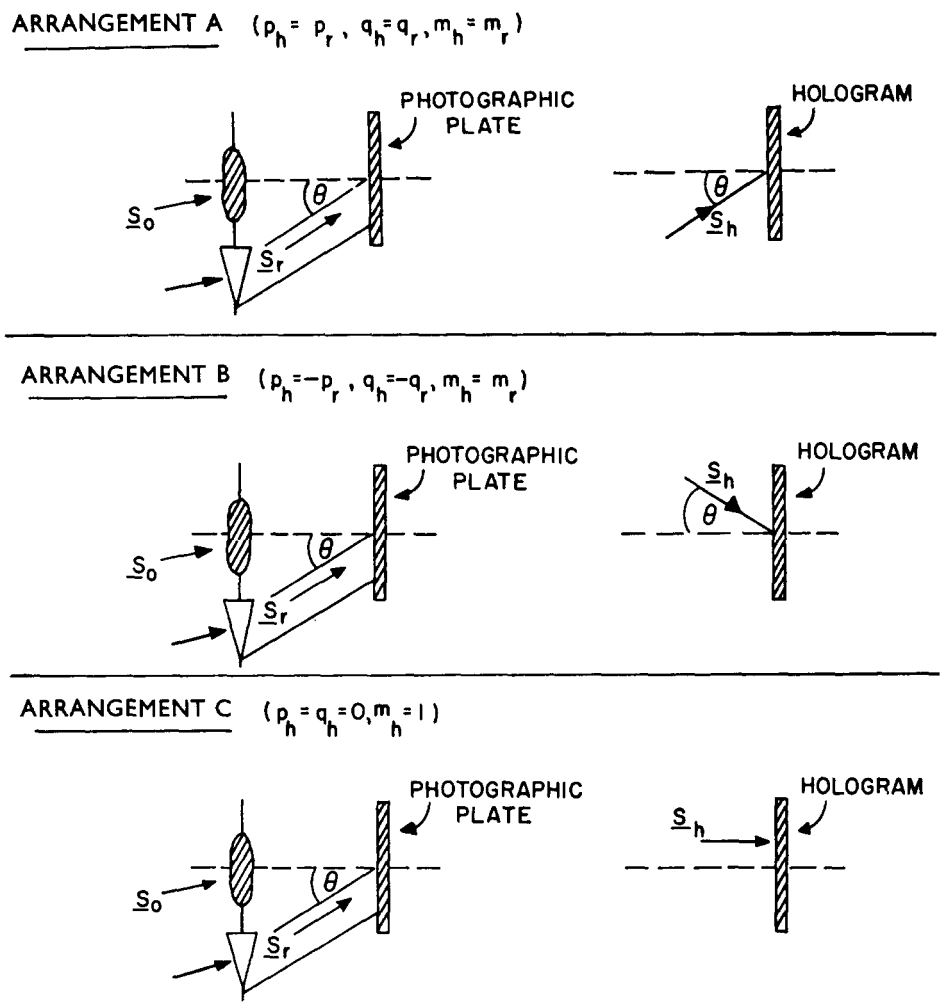

FIG. 3. Side-band holography. Three commonly employed arrangements.

we have in this case

$$\sigma^{(I)} \equiv 0, \tag{2.6a}$$

$$\sigma^{(II)} \equiv 2p_r, 2q_r. \tag{2.6b}$$

Arrangement B: Reconstruction wave is propagated in the direction "conjugate" to that of the reference wave, in the sense that $p_h = -p_r$, $q_r = -q_h$, $m_h = m_r$. In this case, we have

$$\sigma^{(I)} \equiv -2p_r, -2q_r, \tag{2.7a}$$

$$\sigma^{(II)} \equiv 0. \tag{2.7b}$$

Arrangement C: Reconstruction wave is incident normally in the plate: $p_h = q_h = 0$, $m_h = 1$. We now have

$$\sigma^{(I)} \equiv -p_r, -q_r, \tag{2.8a}$$

$$\sigma^{(II)} \equiv p_r, q_r. \tag{2.8b}$$

It will be useful from now on to indicate explicitly the dependence of $V_1^{(I)}$ and $V_1^{(II)}$ on $\sigma^{(I)}$ and $\sigma^{(II)}$, respectively, and we will therefore write $V_1^{(I)}(\mathbf{r}; \sigma^{(I)})$ in place of $V_1^{(I)}(\mathbf{r})$, etc. Equations (2.3) will now become

$$V_1^{(I)}(\mathbf{r}; \sigma^{(I)}) = C^{(I)}U_1(\mathbf{r}) \exp(ik\sigma^{(I)} \cdot \mathbf{r}), \tag{2.9a}$$

$$V_1^{(II)}(\mathbf{r}; \sigma^{(II)}) = C^{(II)}U_1^*(\mathbf{r}) \exp(ik\sigma^{(II)} \cdot \mathbf{r}). \tag{2.9b}$$

3. THE IMAGES WHEN $\sigma = 0$

We will first consider the simpler case, when the periodic exponential terms on the right-hand side of (2.9a) and (2.9b) are absent, i.e., when $\sigma^{(I)}$ and $\sigma^{(II)}$ vanish. As is seen from Eqs. (2.6a), (2.7b), and (2.9), this is so for $V_1^{(I)}$ in the arrangement A and for $V_1^{(II)}$ in arrangement B.

A. The Partial Field $V^{(I)}(\mathbf{r}; 0)$ (The Virtual Image Field in the Arrangement A)

We have, according to (2.9a), with $\sigma^{(I)} = 0$,

$$V_1^{(I)}(\mathbf{r}; 0) = C^{(I)}U_1(\mathbf{r}). \tag{3.1}$$

According to (3.1) and (1.4), $V_1^{(I)}(\mathbf{r}; 0)$ is proportional to the distribution in the plane $z = z_1$ of the field emerging from the hologram that would have been created in that plane by the light emerging from

the original object in the absence of any reference wave.[8] It follows that the partial field $V^{(I)}(x, y, z; 0)$, propagated into the half-space $z > z_1$ from the transilluminated hologram, appears to be propagated from a virtual image of the original object. This virtual image is situated in exactly the same position relative to the hologram, as was the original object relative to the photographic plate.

In particular, if the wave incident on the object when the hologram was taken was a plane wave propagated in the direction specified by the unit vector[9] $\mathbf{s}_0(p_0, q_0, m_0)$, we have

$$U_1^{(0)}(\mathbf{r}) = A^{(0)} \exp\{ik[p_0 x + q_0 y + m_0(z - z_0)]\}, \tag{3.2}$$

and Eqs. (1.6) and (3.2) give

$$U_1(\mathbf{r}) = A^{(0)} \int_{(\infty)} T(\mathbf{r}_0) \exp\{ik[p_0 x_0 + q_0 y_0]\} \times K_{10}(\mathbf{r}_1 - \mathbf{r}_0) d^2\mathbf{r}_0. \tag{3.3}$$

Thus, $U_1(r)$ now represents the field in the plane $z = z_1$ of the hologram due to the distribution

$$U_0(r) = A^{(0)} T(x_0, y_0) \exp\{ik[p_0 x_0 + q_0 y_0]\}$$

in the object plane $z = z_0$. Bearing in mind the significance of K_{10} as a propagator from the plane $z = z_0$ to the plane $z = z_1$, we conclude from Eqs. (3.1), (3.3), and (2.5) that the reconstructed field distribution in the plane $z = z_0$ is proportional to the distribution which would have been obtained in that plane by directly transilluminating the object with the plane wave (3.2); i.e.,

$$V^{(I)}(x, y, z_0; 0) = D^{(I)} T(x, y) \exp[ik(p_0 x + q_0 y)], \tag{3.4}$$

where

$$D^{(I)} = c_1 A^{(0)} A^{(r)*} B^{(h)}. \tag{3.5}$$

B. The Partial Field $V^{(II)}(\mathbf{r}; 0)$ (The Real Pseudoscopic Image in the Arrangement B)

We now have from (2.9b), with $\sigma^{(II)} = 0$,

$$V_1^{(II)}(\mathbf{r}; 0) = C^{(II)} U_1^*(\mathbf{r}). \tag{3.6}$$

It is seen, on comparing (3.6) with (3.1) and on using (2.5), that

$$B^{(h)*} V_1^{(II)}(\mathbf{r}; 0) = B^{(h)} V_1^{(I)*}(\mathbf{r}; 0), \tag{3.7}$$

where we have made use of the fact that c_1 is real.

Let us now assume that $U_1(\mathbf{r})$ is effectively band limited to a domain of spatial frequencies

$$u^2 + v^2 \leq k^2, \tag{3.8}$$

i.e., that the Fourier transform

$$\hat{U}_1(u, v) = \frac{1}{(2\pi)^2} \iint_{\infty}^{\infty} U_1(x, y) \times \exp[-i(ux + vy)] \, dx \, dy \tag{3.9}$$

effectively vanishes when $u^2 + v^2 > k^2$. We use the term "effectively" band limited, since $U_1(\mathbf{r})$ cannot be strictly band limited because of our assumption (1.5). However, if the structural details of the object in the x and y directions are large compared with the wavelength, as we will now assume, the amplitude of the Fourier components $\hat{U}_1(u, v)$ for $u^2 + v^2 > k^2$ will, in general, be negligible.

Under these circumstances, it immediately follows from Eq. (3.7) and the diffraction reciprocity theorem that was recently established in Ref. 5 that, for all values of d,

$$B^{(h)*} V^{(II)}(x, y, z_1 + d; 0) = B^{(h)} V^{(I)*}(x, y, z_1 - d; 0). \tag{3.10}$$

Thus, apart from a simple proportionality factor, the partial field $V^{(II)}$ is the complex conjugate of the mirror image of the partial field $V^{(I)}$ in the plane of the hologram.

In particular, if the wave incident on the object, when the hologram was taken, was the plane wave (3.2), we immediately obtain, from (3.10) and (3.4) with $d = z_1 - z_0$ and from (3.5),

$$V^{(II)}(x, y, 2z_1 - z_0; 0) = D^{(II)} T^*(x, y) \exp[-ik(p_0 x + q_0 y)], \tag{3.11}$$

where

$$D^{(II)} = c_1 A^{(0)*} A^{(r)} B^{(h)}. \tag{3.12}$$

Equation (3.11) shows that, apart from a simple phase factor, the reconstructed partial field distribution $V^{(II)}(x, y, z; 0)$ in the plane $z = z_1 + d = 2z_1 - z_0$ is proportional to the complex conjugate of the distribution that would have been obtained in the plane $z = z_0$ by directly transilluminating the object with the plane wave (3.2). This reconstructed field gives rise to a real pseudoscopic image of the original object and is located in the region that is obtained by reflecting the original object in the plane of the hologram.

In this section, we have considered the reconstructed images under conditions when either $\sigma^{(I)}$ or $\sigma^{(II)}$ were zero, i.e., when either $p_h = p_r$, $q_h = q_r$, or when $p_h = -p_r$, $q_h = -q_r$ (see Fig. 3). We will now consider the more complicated situation when $\sigma^{(I)}$ or $\sigma^{(II)}$ are different from zero.

4. THE IMAGES WHEN $\sigma \neq 0$

It follows from Eqs. (2.9) that $V_1^{(I)}(\mathbf{r};\boldsymbol{\sigma})$ and $V_1^{(II)}(\mathbf{r};\boldsymbol{\sigma})$ may be expressed in the form

$$V_1^{(\alpha)}(\mathbf{r};\boldsymbol{\sigma}) = V_1^{(\alpha)}(\mathbf{r};0)\exp(ik\boldsymbol{\sigma}\cdot\mathbf{r}), \quad \alpha = \mathrm{I}, \mathrm{II}. \tag{4.1}$$

For the sake of simplicity, we have now suppressed the superscripts (I) and (II) on $\boldsymbol{\sigma}$, it being understood that $\boldsymbol{\sigma}$ stands for $\boldsymbol{\sigma}^{(I)}$ in $V_1^{(I)}$ and for $\boldsymbol{\sigma}^{(II)}$ in $V_1^{(II)}$.

In Sec. 3 we have studied the images arising from the two field distributions $V_1^{\alpha}(\mathbf{r};0)$, $\alpha = \mathrm{I}, \mathrm{II}$ (the cases $\boldsymbol{\sigma} = 0$) in the plane $z = z_1$. The effects of the additional multiplicative factor $\exp(ik\boldsymbol{\sigma}\cdot\mathbf{r})$ is studied in Appendix A. It is shown there that, in general, it leads to a complicated modification of the field, which can most readily be appreciated from the following considerations based on results derived in the Appendix.

Let us represent the field $V^{(\alpha)}(x, y, z; 0)$, $\alpha = \mathrm{I}, \mathrm{II}$, which arises from the distribution $V_1^{(\alpha)}(x, y; 0)$ in the plane $z = z_1$, in the form of an angular spectrum of plane waves[10–12]:

$$V^{(\alpha)}(x, y, z; 0) = \iint_{-\infty}^{\infty} A^{(\alpha)}(p, q)\exp\{ik[px + qy + m(z - z_1)]\}\,dp\,dq, \tag{4.2}$$

where

$$m = (1 - p^2 - q^2)^{\frac{1}{2}}, \quad \text{if} \quad p^2 + q^2 \leq 1, \tag{4.3a}$$
$$= i(p^2 + q^2 - 1)^{\frac{1}{2}}, \quad \text{if} \quad p^2 + q^2 > 1. \tag{4.3b}$$

As is well known (see, for example, Sec. 3 of Ref. 5), each plane wave in the representation (4.2) carries information about one and only one spatial frequency component (Fourier component) of the distribution $V_1^{(\alpha)}(x, y; 0)$, namely, the component

$$u = kp, \quad v = kq. \tag{4.4}$$

We may restrict ourselves to spatial frequencies about which the information is carried by homogeneous waves ($p^2 + q^2 \leq 1$) only, i.e., about spatial frequencies such that

$$u^2 + v^2 \leq k^2; \tag{4.5}$$

for the evanescent waves ($p^2 + q^2 > 1$), which carry information about spatial frequencies for which $u^2 + v^2 > k^2$, are very rapidly attenuated and do not, in general, contribute to the image.

Next consider the field $V^{(\alpha)}(x, y, z; \boldsymbol{\sigma})$, which arises from the distribution $V_1^{(\alpha)}(x, y; \boldsymbol{\sigma})\exp(ik\boldsymbol{\sigma}\cdot\mathbf{r})$ in the plane $z = z_1$. According to Eq. (A9) of the Appendix, $V^{(\alpha)}(x, y, z; \boldsymbol{\sigma})$ may be represented in the form

$$V^{(\alpha)}(x, y, z; \boldsymbol{\sigma}) = \iint_{-\infty}^{\infty} A^{(\alpha)}(p, q)\exp\{ik[(p + \sigma_x)x + (q + \sigma_y)y + m'(z - z_1)]\}\,dp\,dq, \tag{4.6}$$

where

$$m' = [1 - (p + \sigma_x)^2 - (q + \sigma_y)^2]^{\frac{1}{2}}, \quad \text{if} \quad (p + \sigma_x)^2 + (q + \sigma_y)^2 \leq 1, \tag{4.7a}$$
$$= i[(p + \sigma_x)^2 + (q + \sigma_y)^2 - 1]^{\frac{1}{2}}, \quad \text{if} \quad (p + \sigma_x)^2 + (q + \sigma_y)^2 > 1, \tag{4.7b}$$

and $A^{(\alpha)}(p, q)$ in (4.6) and (4.2) are (for each α) the same functions of p and q.

We see from (4.6) that information about the spatial frequency component (u, v) of $V_1^{(\alpha)}(\mathbf{r}; 0)$ is now carried by a wave specified by the (possibly complex) unit propagation vector with components $p + \sigma_x$, $q + \sigma_y$, m'. It is obvious that the superposition of all these waves, as indicated by (4.6), will give rise to a field which, in general, will be very different from the field (4.2). In fact, information about spatial frequency components of $V_1^{(\alpha)}(\mathbf{r}; 0)$, for which

$$(u + k\sigma_x)^2 + (v + k\sigma_y)^2 > k^2, \tag{4.8}$$

will be now carried by evanescent waves and so will effectively be lost, except at field points in the immediate vicinity of the plane $z = z_1$.

However, under certain conditions of practical importance, derived in the Appendix and summarized by Theorem 3 of that Appendix, the effect of the additional term $\exp(ik\boldsymbol{\sigma}\cdot\mathbf{r})$ turns out to be relatively simple. Accordingly, we assume that:

(i) $$0 < \sigma_x^2 + \sigma_y^2 < 1; \tag{4.9}$$

(ii) The transmission function $T(x, y)$ of the object is effectively band limited to the spatial frequency domain (u, v) such that[13]

$$|u| \ll k\mu, \quad |v| \ll k\mu, \tag{4.10}$$

$$(u + k\sigma_x)^2 + (v + k\sigma_y)^2 \leq k^2, \tag{4.11}$$

where

$$\mu = +(1 - \sigma_x^2 - \sigma_y^2)^{\frac{1}{2}}. \tag{4.12}$$

More explicitly, the conditions (ii) imply that the Fourier transform

$$\hat{T}(u, v) = \frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty} T(x, y) \times \exp[-i(ux + vy)]\,dx\,dy \tag{4.13}$$

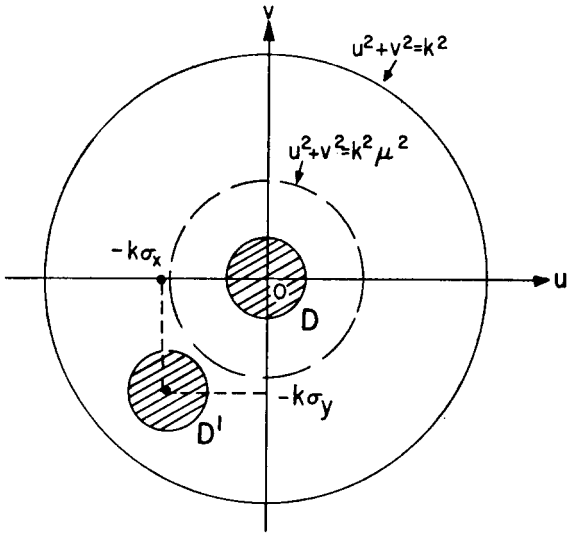

FIG. 4. Illustrating the inequalities (4.10) and (4.11). The transmission function $T(x, y)$ is band limited to the interior of the circle D centered at the origin. D' denotes the circle of the same radius but displaced by amounts $k\sigma_x$ and $k\sigma_y$ in the negative x and y directions, respectively.

of the transmission function $T(x, y)$ of the object effectively vanishes except when (u, v) satisfy the inequalities (4.10) and (4.11). The significance of the inequalities is illustrated in Fig. 4.

It is evident from (3.4), (3.11), and the properties of wave fields (cf. Ref. 5, Sec. 3), that $V_1^{(\alpha)}(x, y; 0)$ is band limited to the same spatial frequency domain as is $T(x, y)$. It then follows at once from Eq. (4.1) and from Theorem 3 of Appendix A, (bearing in mind that in the Appendix z is measured from the plane at which the boundary values are specified) that, for all values of ζ,

$$V^{(\alpha)}(x, y, z_1 + \zeta; \boldsymbol{\sigma}) = V^{(\alpha)}(x - \sigma_x\zeta/\mu, y - \sigma_y\zeta/\mu, z_1 - \zeta/\mu; 0) \times \exp[ik\Phi(x, y)], \quad (4.14)$$

with

$$\Phi(x, y) = \sigma_x(x - \sigma_x\zeta/\mu) + \sigma_y(y - \sigma_y\zeta/\mu). \quad (4.15)$$

We will now consider separately the two cases $\alpha = \mathrm{I}$ and $\alpha = \mathrm{II}$.

A. The Case $\alpha = \mathrm{I}$ (Virtual Images in Arrangements B and C)

In Eq. (4.14) let us choose

$$\zeta = -\mu d, \quad (4.16)$$

where

$$d = z_1 - z_0 \quad (4.17)$$

is the distance between the object and the photographic plate. Then, if we also use Eq. (3.4), we find at once from Eqs. (4.14) and (4.15) that

$$V^{(\mathrm{I})}(x, y, z_\mathrm{V}; \boldsymbol{\sigma}^{(\mathrm{I})}) = D^{(\mathrm{I})}T(x + \sigma_x^{(\mathrm{I})}d, y + \sigma_y^{(\mathrm{I})}d) \times \exp[ik\varphi^{(\mathrm{I})}(x, y)], \quad (4.18)$$

where

$$\varphi^{(\mathrm{I})}(x, y) = (p_0 + \sigma_x^{(\mathrm{I})})x + (q_0 + \sigma_y^{(\mathrm{I})})y + (\sigma_x^{(\mathrm{I})^2} + \sigma_y^{(\mathrm{I})^2})d, \quad (4.19)$$

and

$$z_\mathrm{V} = z_1 - \mu d. \quad (4.20)$$

Equations (4.18)–(4.20) show that the complex disturbance $V^{(\mathrm{I})}(x, y, z_\mathrm{V}; \boldsymbol{\sigma})$ in the plane $z = z_\mathrm{V}$, i.e., in the plane at distance $\mu d = (1 - \sigma_x^2 - \sigma_y^2)(z_1 - z_0)$ in front of the hologram is very closely related to the light distribution in the plane $z = z_0$ of the transilluminated object. More precisely, Eq. (4.18) shows that in the plane $z = z_\mathrm{V}$ there is a *virtual image* of the original object, displaced with respect to the object by amounts $\sigma_x^{(\mathrm{I})}d$ and $\sigma_y^{(\mathrm{I})}d$ in the x and the y directions, respectively. Apart from a simple geometrical phase factor, the complex amplitude distribution at corresponding points of the object and of the image planes are proportional to each other. Figures 5 illustrate the displacement of the virtual image

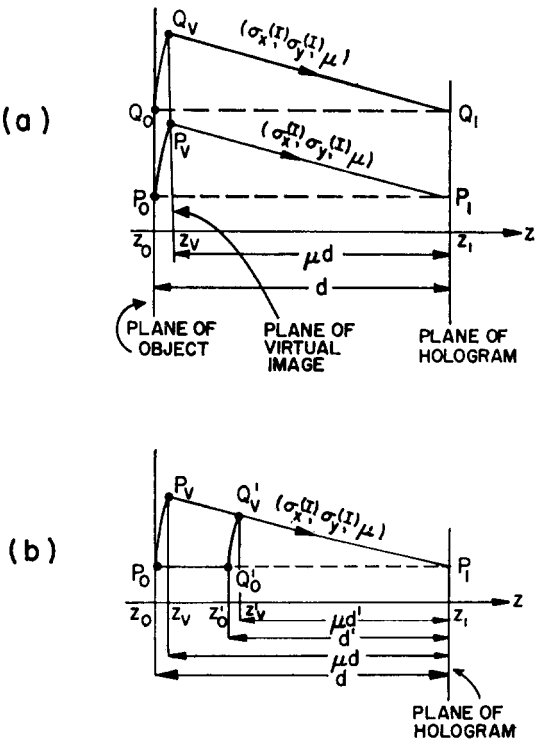

FIG. 5. Construction relating to the location of the virtual image [Eqs. (4.18) and (4.20)]. The object P_0Q_0 is parallel to the plane of the hologram [Fig. 5(a)], the object P_0Q_0' is perpendicular to it [Fig. 5(b)]. $P_\mathrm{V}Q_\mathrm{V}$ and $P_\mathrm{V}Q_\mathrm{V}'$ are the corresponding virtual images, reconstructed from the hologram.

relative to the original object as implied by Eqs. (4.18) and (4.20).

In Fig. 5(a), P_O and Q_O are two object points in the plane $z = z_0$, and P_V and Q_V are the corresponding virtual image points. The location of P_V and Q_V may be obtained from the following construction: Let P_1 and Q_1 be the feet of the perpendiculars dropped from P_O and Q_O onto the plane $z = z_1$ of the hologram. Then P_V and Q_V are the points in which the two lines through P_1 and Q_1, with direction cosines $\sigma_x^{(I)}$, $\sigma_y^{(I)}$, and μ, intersect spheres of radii $d = z_1 - z_0$ centered on P_1 and Q_1, respectively.

In Fig. 5(b), P_O and Q_O' are two object points in planes $z = z_0$ and $z = z_0'$, respectively, on a common perpendicular to the plane of the hologram, and P_V and Q_V' are the corresponding virtual image points. The location of the image points P_V and Q_V' may be obtained by the following construction: Let P_1 by the point in which the perpendicular P_OQ_O' intersects the plane $z = z_1$ of the hologram. Then P_VQ_V' are the two points in which the line through P_1, with direction cosines $\sigma_x^{(I)}$, $\sigma_y^{(I)}$, and μ, intersects the two spheres centered on P_1, of radii $d = z_1 - z_0$ and $d' = z_1 - z_0'$, respectively.

The line P_VQ_V in Fig. 5(a) is obviously parallel to the line P_OQ_O. On the other hand, the line P_VQ_V' in Fig. 5(b) is not parallel to P_OQ_O', so that in the image *depth information about the object is distorted.* This is also evident by considering the lateral and the longitudinal magnifications of this imaging process. If (x_O, y_O, z_O) are the coordinates of a typical object point and (x_V, y_V, z_V) are the coordinates of the corresponding (virtual) image points, Eqs. (4.18), (4.20), and (4.17) imply that

$$\begin{aligned} x_V &= x_O + \sigma_x^{(I)}(z_1 - z_0), \\ y_V &= y_O + \sigma_y^{(I)}(z_1 - z_0), \\ z_V &= z_1 - \mu(z_1 - z_0). \end{aligned} \tag{4.21}$$

Hence

$$\frac{dx_V}{dx_O} = \frac{dy_V}{dy_O} = 1, \quad \frac{dz_V}{dz_O} = \mu \equiv (1 - \sigma_x^{(I)^2} - \sigma_y^{(I)^2})^{\frac{1}{2}}. \tag{4.22}$$

Equation (4.22) shows that the lateral magnification is unity, whereas the longitudinal magnification is $\mu \equiv (1 - \sigma_x^{(I)^2} - \sigma_y^{(I)^2})^{\frac{1}{2}} \neq 1$.

We have seen earlier that $\boldsymbol{\sigma}^{(I)}$ is nonzero for arrangements B and C, being given by Eqs. (2.7a) and (2.8a), respectively. The location of the virtual images in these two arrangements is indicated in Fig. 7. Since $\mu = [1 - 4(p_r^2 + q_r^2)]^{\frac{1}{2}}$ in arrangement B and $\mu = [1 - (p_r^2 + q_r^2)]^{\frac{1}{2}}$ in arrangement C, it is evident that for the same direction of propagation (p_r, q_r, m_r) of the reference wave, the band-limitation requirement (4.10) is more severe for the virtual image in the arrangement B than it is in the arrangement C.

B. The Case $\alpha = \text{II}$ (Real Images in Arrangements A and C)

Let us choose in (4.14)

$$\zeta = \mu d, \tag{4.23}$$

where d, again given by (4.17), is the distance between the object and the photographic plate. If we also use Eq. (3.11), we find at once from (4.14) that

$$V^{(II)}(x, y, z_R; \boldsymbol{\sigma}) = D^{(II)}T^*(x - \sigma_x^{(II)}d, y - \sigma_y^{(II)}d) \times \exp[ik\varphi^{(II)}(x, y)], \tag{4.24}$$

where

$$\varphi^{(II)}(x, y) = (-p_0 + \sigma_x^{(II)})x + (-q_0 + \sigma_y^{(II)})y - (\sigma_x^{(II)^2} + \sigma_y^{(II)^2})d \tag{4.25}$$

and

$$z_R = z_1 + \mu d. \tag{4.26}$$

Equations (4.24)–(4.26) show that in the plane $z = z_R$, i.e., that in the plane at the distance $\mu d = (1 - \sigma_x^2 - \sigma_y^2)^{\frac{1}{2}}(z_1 - z_0)$ behind the hologram one obtains a real *pseudoscopic* image of the original object, displaced with respect to the object by amounts $\sigma_x^{(II)}d$ and $\sigma_y^{(II)}d$ in the x and y directions, respectively. Apart from a proportionality factor and a simple geometrical phase factor, the complex amplitudes at corresponding points of the object and the image are complex conjugates of each other.

Figures 6 illustrate the displacement of the real

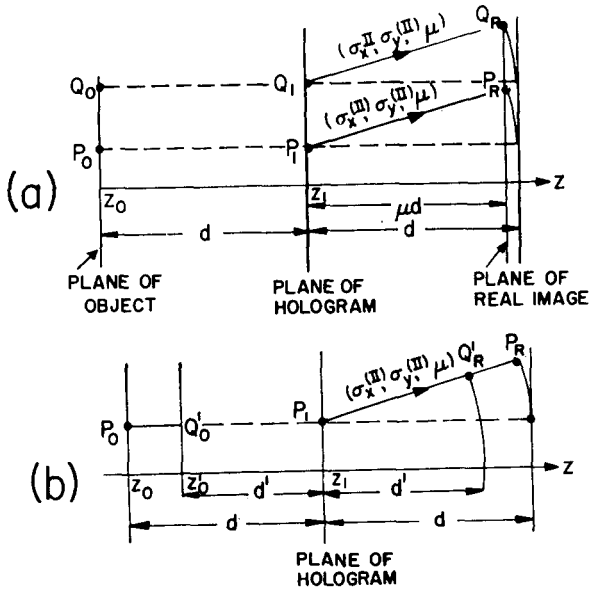

FIG. 6. Construction relating to the location of the real image [Eqs. (4.24)–(4.26)]. The object P_OQ_O is parallel to the plane of the hologram [Fig. 6(a)], the object P_OQ_O' is perpendicular to it [Fig. 6(b)]. P_RQ_R and P_RQ_R' are the corresponding real images, reconstructed from the hologram.

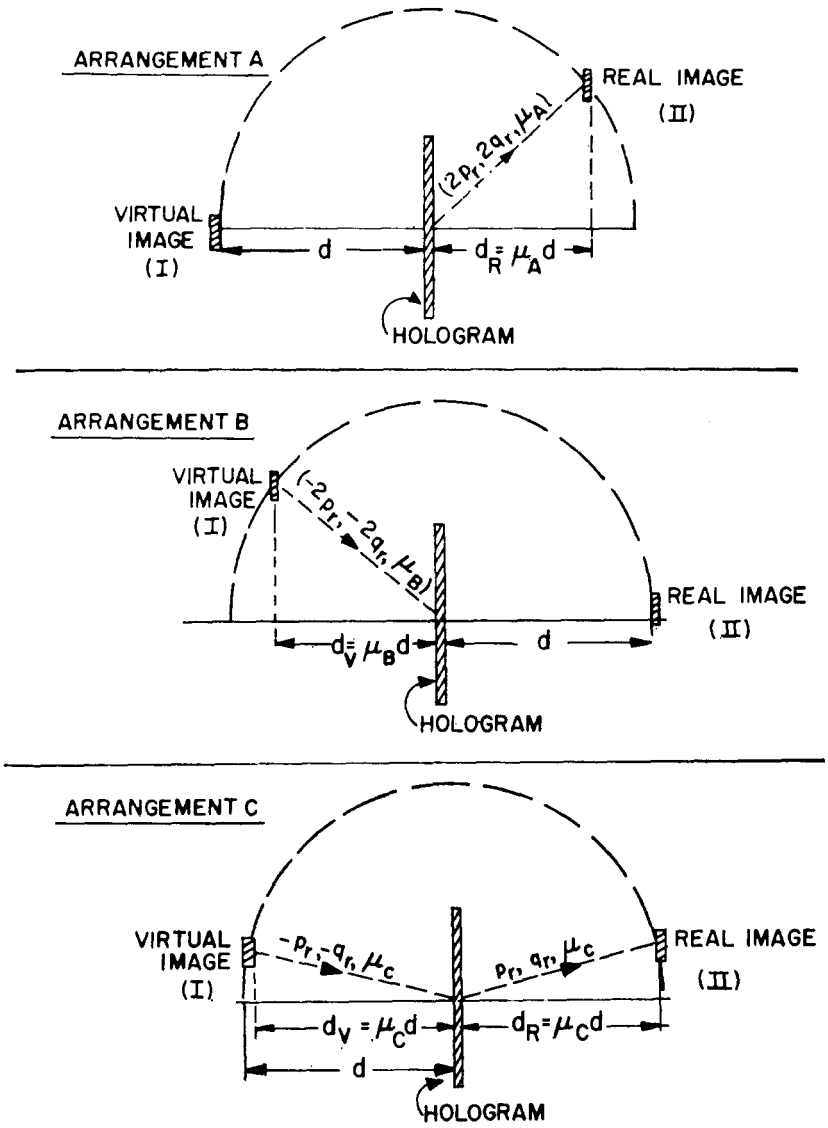

FIG. 7. Location of the virtual and real images in the arrangements A, B, and C, illustrated in Fig. 3.

$\mu_A = \mu_B = [1 - 4(p_r^2 + q_r^2)]^{\frac{1}{2}}$,
$\mu_C = [1 - (p_r^2 + q_r^2)]^{\frac{1}{2}}$.

image relative to the mirror image of the object in the plane of the hologram, as implied by Eqs. (4.24) and (4.26). The symbols have strictly analogous meaning to those in Figs. 5. Corresponding points (x_R, y_R, z_R) in the real image and in the original object (x_O, y_O, z_O) are now related by the equations

$$\begin{aligned} x_R &= x_O + \sigma_x^{(II)}(z_1 - z_0), \\ y_R &= y_O + \sigma_y^{(II)}(z_1 - z_0), \\ z_R &= z_1 + \mu(z_1 - z_0). \end{aligned} \tag{4.27}$$

It follows from these equations that

$$\begin{aligned} \frac{dx_R}{dx_O} &= \frac{dy_R}{dy_O} = 1, \\ \frac{dz_R}{dz_O} &= -\mu \equiv -(1 - \sigma_x^{(II)2} - \sigma_y^{(II)2})^{\frac{1}{2}}. \end{aligned} \tag{4.28}$$

Thus the lateral magnification is again unity, while the longitudinal magnification is $-\mu = -(1 - \sigma_x^{(II)2} - \sigma_y^{(II)2})^{\frac{1}{2}}$, so that the depth information is again distorted.

$\boldsymbol{\sigma}^{(II)}$ is nonzero in arrangements A and C and is given by Eqs. (2.6b) and (2.8b). The location of the real pseudoscopic images in these two arrangements is also indicated in Fig. 7. Since the value of μ in the arrangement A is smaller than in the arrangement C, it follows that for the same direction of propagation of the reference wave, the band-limitation requirement (4.10) is more severe for the real image in the arrangement A than in the arrangement C.

5. ELIMINATION OF ONE OF THE ROTATED IMAGES BY DIFFRACTION

In the main part of the preceding section, we have restricted our analysis to situations where certain simplifying conditions [expressed by the inequalities

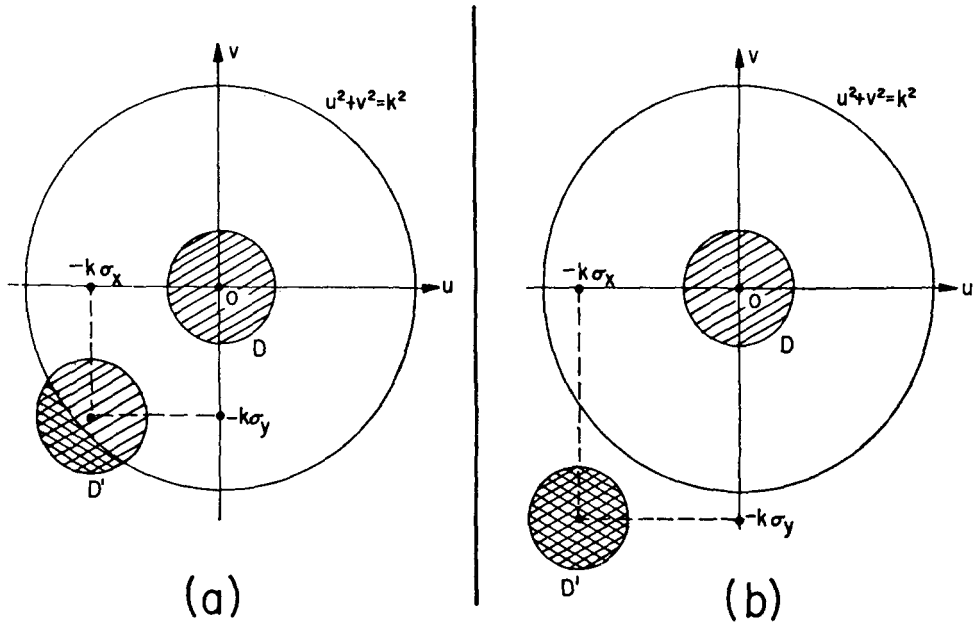

FIG. 8. Illustrating the conditions for partial [Fig. 8(a)] and total [Fig. 8(b)] disappearance of one of the images by diffraction. The transmission function $T(x, y)$ is band limited to the interior of the circle D. D' denotes a circle of the same radius displaced by amounts $k\sigma_x$ and $k\sigma_y$ in the negative x and y directions, respectively. Those spatial frequency components represented by points in D, for which the corresponding representative points in D' lie outside the circle $u^2 + v^2 = k^2$, will give rise to evanescent waves and will not appear in the rotated image.

(4.9)–(4.11)] were satisfied. The conditions ensure that the "rotated" images (images for which $\sigma \neq 0$) are of good quality. However, it is evident from the discussion given at the beginning of Sec. 4, that, in general, the reconstructed rotated images may be very different from the object. This is partly so because some of the spatial frequency components of the object may not appear in the rotated image. These are the components about which information is carried by evanescent waves, i.e., components of spatial frequencies (u, v) for which

$$(u + k\sigma_x)^2 + (v + k\sigma_y)^2 > k^2. \tag{5.1}$$

The situation is illustrated graphically in Fig. 8, where D represents the spatial frequency domain to which the transmission function $T(x, y)$ of the object is effectively band limited. D' is the same domain, but displaced by amounts $-k\sigma_x$, $-k\sigma_y$ in the x and y directions, respectively. Those spatial frequencies (u, v) of the domain D, which are such that their corresponding representative points in the displaced domain D' lie outside the circle $u^2 + v^2 = k^2$, will not appear in the rotated image.

Now according to (2.4a),

$$\sigma_x^{(\alpha)^2} + \sigma_y^{(\alpha)^2} = (p_h \mp p_r)^2 + (q_h \mp q_r)^2,$$

where the negative signs on the right apply when $\alpha = \text{I}$ (virtual image) and the positive signs apply when $\alpha = \text{II}$ (real image). We recall that the quantities (p_h, q_h) and (p_r, q_r) are the x and y components, respectively, of the unit vectors in the direction of propagation of the reconstruction wave incident on the hologram and of the reference wave, respectively. Since in the arrangements A and B the quantity $(p_h \mp p_r)^2 + (q_h \mp q_r)^2$ may easily exceed unity, $k^2\sigma_x^2 + k^2\sigma_y^2$ may easily exceed k^2 and, hence, the circle D' may lie entirely outside the circle $u^2 + v^2 = k^2$ [see Fig. 8(b)]. Under these circumstances the "rotated" image will completely disappear. We stress that this disappearance is entirely due to diffraction and not due to the finite limit of resolution or the finite thickness of the photographic plate.[14]

Suppose, in particular, that the transmission function $T(x, y)$ of the object is effectively band limited to a small domain throughout which

$$|u| \ll k\,|\sigma_x|, \quad |v| \ll k\,|\sigma_y|. \tag{5.2}$$

To first approximation, we may then neglect u and v in the inequality (5.1) and obtain the following order of magnitude relation for the condition under which the rotated image will disappear:

$$\sigma_x^2 + \sigma_y^2 \gtrsim 1. \tag{5.3}$$

In particular, we have for the real image in the arrangement A and the virtual image in the arrangement B $|\sigma_x| = 2p_r$, $|\sigma_y| = 2q_r$, so that if $T(x, y)$ is

band limited to a domain throughout which

$$|u| \ll 2kp_r, \quad |v| \ll 2kq_r, \tag{5.4}$$

these images will disappear if

$$4(p_r^2 + q_r^2) \geqslant 1. \tag{5.5}$$

It is more convenient to express (5.5) as a condition on the angle θ_r, which the reference wave makes with the normal to the photographic plate. Since $\cos\theta_r = m_r = (1 - p_r^2 - q_r^2)^{\frac{1}{2}}$, Eq. (5.5) is equivalent to the condition $\cos\theta \leqslant \sqrt{3}/2$, i.e.,

$$\theta_r \geqslant 30°. \tag{5.6}$$

Thus, we conclude that if the band limitation condition (5.4) is satisfied, the real image in the arrangement A and the virtual image in the arrangement B will disappear when the angle that the direction of propagation of the reference wave makes with the normal to the photographic plate exceeds about 30°.

The two conditions (5.4) imply that $u^2 + v^2 \ll 4k^2(p_r^2 + q_r^2)$, i.e., that

$$u^2 + v^2 \ll 4k^2 \sin^2\theta_r, \tag{5.7}$$

or, with θ_r obeying the inequality (5.6),

$$u^2 + v^2 \ll k^2. \tag{5.8}$$

Thus, roughly speaking, (5.4) imply that the transmission function of the object contains effectively only spatial periodicities $\Delta x = 2\pi/u$, $\Delta y = 2\pi/v$ which are large compared with the wavelength of the light.

When the holographic images are viewed visually, the eye will act as a low-pass spatial filter, with a cutoff at periodicities of the order of a dozen or so lines per millimeter, i.e., at spatial frequencies of the order of 10^2 cm^{-1}. Since k is of the order of 10^5 cm^{-1}, the inequality (5.8) is then satisfied and we conclude that for visual observations the real image in the arrangement A and the virtual image in the arrangement B disappear when $\theta_r \geqslant 30°$.

It is of interest to note that the critical condition (5.3) with the equality sign ($\sigma_y^2 + \sigma_x^2 = 1$) implies according to (4.12) that $\mu = 0$, i.e., that the directions P_1P_V and P_1P_R in Figs. 5 and 6 are perpendicular to the z axis. Thus, the critical condition implies that the image has been rotated into the plane of the hologram.

As another simple example, in which, however, the conditions (5.4) are not necessarily satisfied, consider a 1-dimensional amplitude grating, with (amplitude) transmission function

$$T(x) = \cos u_0 x, \tag{5.9}$$

where u_0 is a (real) constant. Let the directions of propagation of the reference wave and of the reconstruction wave lie in the (x, z) plane, so that

$$q_h = q_r = 0. \tag{5.10}$$

Since $\cos u_0 x = \frac{1}{2}[\exp iu_0 x + \exp(-iu_0 x)]$, the spectrum of $T(x)$ consists of two sharp lines of spatial frequencies

$$u = u_0, \quad v = 0 \quad \text{and} \quad u = -u_0, \quad v = 0. \tag{5.11}$$

Let us now find the condition that the virtual image of the grating in the arrangement B should disappear. Now according to Eqs. (2.7a) and (5.10), we have for the virtual image in arrangement B,

$$\sigma_x^{(I)} = -2p_r, \quad \sigma_y^{(II)} = 0, \tag{5.12}$$

so that the required condition, obtained from (5.1), (5.11), and (5.12) is

$$(\pm u_0 - 2kp_r)^2 > k^2. \tag{5.13}$$

Let us take $p_r > 0$ and assume that $k > |u_0| > 0$, so that (5.13) implies that

$$p_r > \tfrac{1}{2}(1 + |u_0|/k), \tag{5.14}$$

or, in terms of the spatial periodicity $\Delta x = 2\pi/u_0$ of the grating and the wavelength $\lambda = 2\pi/k$,

$$p_r > \tfrac{1}{2}[1 + \lambda/\Delta x]. \tag{5.15}$$

Again, using the relation

$$m_r \equiv \cos\theta_r = (1 - p_r^2 - q_r^2)^{\frac{1}{2}}$$

and the fact that according to (5.10) we now have $q_r = 0$, the condition (5.15) for the disappearance of the virtual image of the grating in the arrangement B is seen to be equivalent to the condition

$$\cos\theta_r < [1 - \tfrac{1}{4}(1 + \lambda/\Delta x)^2]^{\frac{1}{2}}. \tag{5.16}$$

The critical angle $\bar{\theta}_r$ such that $\cos\bar{\theta}_r$ is equal to the right-hand side of (5.16), for gratings of different periodicities is given in Table I. It may readily be

TABLE I. The critical angle $\bar{\theta}_r = \cos^{-1}\{[1 - \frac{1}{4}(1 + u_0/k)^2]^{\frac{1}{2}}\}$ for the disappearance of the virtual image in the arrangement B or of the real image in arrangement A, when the object is a 1-dimensional amplitude grating with transmission function $T(x) = \cos u_0 x$.

u_0/k	$\Delta x/\lambda$	$\bar{\theta}_r$
10^{-3}	10^3	30°01′56″
10^{-2}	10^2	30°19′52″
10^{-1}	10	33°21′56″
0.25	4	38°40′57″
0.50	2	48°35′25″
0.70	1.43	58°12′43″
0.80	1.25	64°10′30″
0.90	1.11	71°12′42″
0.99	1.01	84°16′06″
1	1	90°

verified that the condition (5.15) is also the condition for the disappearance of the real image in the arrangement A.

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APPENDIX: FIELDS WHOSE BOUNDARY VALUES DIFFER BY A MULTIPLICATIVE SPACE-PERIODIC FACTOR

Consider two fields $U^{(1)}(x, y, z)$ and $U^{(2)}(x, y, z)$, each of which satisfies the Helmholtz equation

$$(\nabla^2 + k^2)U^{(j)}(x, y, z) = 0, \quad j = 1, 2, \quad \text{(A1)}$$

in the half-space $z > 0$ and the Sommerfeld radiation condition at infinity in this half-space. Suppose that in the plane $z = 0$ the two fields satisfy the boundary conditions

$$U^{(1)}(x, y, 0) = F(x, y),$$
$$U^{(2)}(x, y, 0) = F(x, y) \exp [ik(\sigma_x x + \sigma_y y)], \quad \text{(A2)}$$

where σ_x and σ_y are real constants. Since according to (A2), the boundary values of the two fields on the plane $z = 0$ are related, the two fields in the half-space $z > 0$ are also related. In this Appendix, we will study the relationship between the two fields.

Let us represent each field in the form of an angular spectrum of plane wave[10–12]:

$$U^{(j)}(x, y, z) = \iint_{-\infty}^{\infty} A^{(j)}(p, q) \exp [ik(px + qy + mz)]\, dp\, dq, \quad j = 1, 2, \quad \text{(A3)}$$

where

$$m = (1 - p^2 - q^2)^{\frac{1}{2}}, \quad \text{when} \quad p^2 + q^2 \leq 1, \quad \text{(A4a)}$$
$$= i(p^2 + q^2 - 1)^{\frac{1}{2}}, \quad \text{when} \quad p^2 + q^2 > 1. \quad \text{(A4b)}$$

Then, setting $z = 0$ in (A3) and taking the Fourier inverse, we obtain the following expression for the complex spectral amplitudes $A^{(j)}(p, q)$ in terms of the boundary values of the two fields:

$$A^{(j)}(p, q) = \left(\frac{k}{2\pi}\right)^2 \iint_{-\infty}^{\infty} U^{(j)}(x, y, 0) \times \exp [-ik(px + qy)]\, dx\, dy. \quad \text{(A5)}$$

If we substitute from (A2) into (A5), we obtain the two formulas

$$A^{(1)}(p, q) = \left(\frac{k}{2\pi}\right)^2 \iint_{-\infty}^{\infty} F(x, y) \times \exp [-ik(px + qy)]\, dx\, dy, \quad \text{(A6)}$$

$$A^{(2)}(p, q) = \left(\frac{k}{2\pi}\right)^2 \iint_{-\infty}^{\infty} F(x, y) \times \exp \{-ik[(p - \sigma_x)x + (q - \sigma_y)y]\}\, dx\, dy. \quad \text{(A7)}$$

Comparison of (A6) with (A7) shows that

$$A^{(2)}(p, q) = A^{(1)}(p - \sigma_x, q - \sigma_y), \quad \text{(A8)}$$

a result which is nothing but the shift theorem on Fourier transforms. In the present context this result implies the following:

Theorem 1: Two fields $U^{(1)}$ and $U^{(2)}$, whose boundary values in the plane $z = 0$ differ only by the multiplicative periodic factor $\exp [ik(\sigma_x x + \sigma_y y)]$, as shown explicitly by (A1) and (A2), have angular spectrum representations such that the complex spectral amplitudes are related by Eq. (A8).

The theorem that we have just established has a number of interesting consequences. We have from (A3) and (A8)

$$U^{(2)}(x, y, z) = \iint_{-\infty}^{\infty} A^{(1)}(p - \sigma_x, q - \sigma_y) \times \exp [ik(px + qy + mz)]\, dp\, dq = \iint_{-\infty}^{\infty} A^{(1)}(p, q) \exp \{ik[(p + \sigma_x)x + (q + \sigma_y)y + m'z]\}\, dp\, dq, \quad \text{(A9)}$$

where

$$m' = [1 - (p + \sigma_x)^2 - (q + \sigma_y)^2]^{\frac{1}{2}}, \quad \text{if} \quad (p + \sigma_x)^2 + (q + \sigma_y)^2 \leq 1, \quad \text{(A10a)}$$
$$= i[(p + \sigma_x)^2 + (q + \sigma_y)^2 - 1]^{\frac{1}{2}}, \quad \text{if} \quad (p + \sigma_x)^2 + (q + \sigma_y)^2 > 1. \quad \text{(A10b)}$$

Comparison of (A9) with (A3) for $j = 1$ shows that the effect of multiplying the boundary value $F(x, y)$ in the plane $z = 0$ by the term $\exp [ik(\sigma_x x + \sigma_y y)]$ is equivalent to transforming each plane wave

$$A^{(1)}(p, q) \exp [ik(px + qy + mz)] \quad \text{(A11)}$$

in the angular spectrum of $U^{(1)}$ into the plane wave

$$A^{(1)}(p, q) \exp \{ik[(p + \sigma_x)x + (q + \sigma_y)y + m'z]\}, \quad \text{(A12)}$$

and the field $U^{(2)}$ is just the superposition of the waves (A12) for all values of p and q ($-\infty < p < \infty$, $-\infty < q < \infty$). If (A10a) applies, the wave (A12) is a homogeneous wave and if (A10b) applies, it is an evanescent wave.[5] It is evident that each wave (A11) in the angular spectrum representation of $U^{(1)}$, whether the wave is homogeneous or evanescent, may be transformed into either a homogeneous wave or an evanescent wave, depending on the exact values of p, q, σ_x, and σ_y. More precisely we have

Theorem 2: The effect of multiplying the boundary-value function $F(x, y)$ of a field distribution in the plane $z = 0$ by $\exp[ik(\sigma_x x + \sigma_y y)]$, where σ_x and σ_y are real constants, is equivalent to transforming each plane wave (A11) in the angular spectrum representation of the field into the plane wave (A12). A homogeneous wave ($p^2 + q^2 \leq 1$) will be transformed into a homogeneous or an evanescent wave according as $(p + \sigma_x)^2 + (q + \sigma_y)^2 \lesseqgtr 1$. An evanescent wave ($p^2 + q^2 > 1$) will be transformed into an evanescent or a homogeneous wave according as $(p + \sigma_x)^2 + (q + \sigma_y)^2 \gtreqless 1$.

The two theorems that we just established hold generally. We are now going to consider their implications when the boundary function $F(x, y)$ is band limited to a sufficiently small domain and when certain constraints are also imposed on σ_x and σ_y.

Suppose first that the boundary function $F(x, y) = U^{(1)}(x, y, 0)$ is band limited to a domain of the (u, v) plane, throughout which the following two conditions are satisfied:

$$u^2 + v^2 \leq k^2, \tag{A13}$$

$$(u + k\sigma_x)^2 + (v + k\sigma_y)^2 \leq k^2. \tag{A14}$$

This means that if we represent $F(x, y)$ as a Fourier integral,

$$F(x, y) = \iint_{-\infty}^{\infty} \hat{F}(u, v) \exp[i(ux + vy)]\, du\, dv, \tag{A15}$$

$\hat{F}(u, v)$ will vanish outside the circles specified by (A13) and (A14).

From the Fourier inverse relation

$$\hat{F}(u, v) = \frac{1}{(2\pi)^2} \iint_{-\infty}^{\infty} F(x, y) \exp[-i(ux + vy)]\, dx\, dy \tag{A16}$$

and from (A6), it follows that

$$\hat{F}(u, v) = (1/k^2) A^{(1)}(u/k, v/k). \tag{A17}$$

Hence, the band-limitation conditions (A13) and (A14) on $F(x, y)$ imply that $A^{(1)}(p, q)$ is band limited to a domain on the (p, q) plane, throughout which

$$p^2 + q^2 \leq 1, \tag{A18}$$

$$(p + \sigma_x)^2 + (q + \sigma_y)^2 \leq 1. \tag{A19}$$

According to (A18), (A19), (A4), and (A10), we now have for all waves in the angular spectrum representations of $U^{(1)}$ and $U^{(2)}$

$$m = (1 - p^2 - q^2)^{\frac{1}{2}}, \tag{A20}$$

$$m' = [1 - (p + \sigma_x)^2 - (q + \sigma_y)^2]^{\frac{1}{2}}, \tag{A21}$$

i.e., the two angular spectra now consist of *homogeneous waves only*.

We rewrite (A21) in the form

$$m' = [\mu^2 - (p^2 + q^2) - 2(p\sigma_x + q\sigma_y)]^{\frac{1}{2}}, \tag{A22}$$

where

$$\mu = +(1 - \sigma_x^2 - \sigma_y^2)^{\frac{1}{2}}. \tag{A23}$$

We will now also assume that

$$0 < \sigma_x^2 + \sigma_y^2 < 1, \tag{A24a}$$

so that

$$0 < \mu < 1 \tag{A24b}$$

and that throughout the domain to which $F(x, y)$ is band limited,

$$|u| \ll k\mu, \quad |v| \ll k\mu. \tag{A25}$$

The inequality (A13) is then automatically satisfied. In view of (A17), (A25) implies that throughout the domain to which $A^{(1)}(p, q)$ is band limited,

$$|p| \ll \mu, \quad |q| \ll \mu. \tag{A26}$$

The assumptions expressed by (A13), (A14), (A24), and (A25) are illustrated in Fig. 4.

We now expand the right-hand side of (A22) in a power series and retain only the leading terms in powers of p/μ and q/μ. This gives

$$m' \sim \mu - [(p\sigma_x + q\sigma_y)/\mu] - (p^2 + q^2)/2\mu. \tag{A27}$$

In view of (A26) and (A24), we also have $|p| \ll 1$, $|q| \ll 1$, so that we may expand the right-hand side of (A20) into a power series and retain only the leading terms in powers of p^2 and q^2. Hence,

$$m \sim 1 - \tfrac{1}{2}(p^2 + q^2). \tag{A28}$$

It follows from (A27) and (A28) that to a good approximation

$$\begin{aligned} m' &\sim \mu - [(p\sigma_x + q\sigma_y)/\mu] + (m - 1)/\mu \\ &= [(\mu^2 - 1)/\mu] + (m/\mu) - (p\sigma_x + q\sigma_y)/\mu \\ &= -[(\sigma_x^2 + \sigma_y^2)/\mu] + (m/\mu) - (p\sigma_x + q\sigma_y)/\mu \\ &= -[\sigma_x(\sigma_x + p) + \sigma_y(\sigma_y + q) + m]/\mu, \end{aligned} \tag{A29}$$

where we have made use of Eq. (A23).

We now substitute from (A29) into (A9) and obtain, on using also the expression (A3) for $U^{(1)}$, the following relation between the two fields $U^{(1)}$ and $U^{(2)}$, valid in the half-space $z > 0$:

$$U^{(2)}(x, y, z) \sim U^{(1)}(x - \sigma_x z/\mu, y - \sigma_y z/\mu, z/\mu) \times \exp[ik\Phi(x, y, z)] \quad \text{(A30)}$$

with

$$\Phi(x, y, z) = \sigma_x(x - \sigma_x z/\mu) + \sigma_y(y - \sigma_y z/\mu). \quad \text{(A31)}$$

Further, as we already saw, in view of our assumptions (A13) and (A14), the angular spectrum representations of $U^{(1)}$ and $U^{(2)}$ contain homogeneous waves only. Hence, according to a theorem established recently by Sherman,[15] both $U^{(1)}$ and $U^{(2)}$ may be continued into and throughout the half-space $z < 0$ and, moreover, the formula (A3) is a valid representation for the continuations. Hence, the formulas (A30) and (A3) are also valid when $z < 0$. We have thus the following:

Theorem 3: Let $U^{(1)}(x, y, z)$ and $U^{(2)}(x, y, z)$ be two fields that obey the Helmholtz equation

$$(\nabla^2 + k^2)U^{(j)}(x, y, z) = 0, \quad j = 1, 2, \quad \text{(A32)}$$

in the half-space $z > 0$ and the Sommerfeld radiation condition at infinity in this half-space. Further assume that in the plane $z = 0$, $U^{(1)}$ and $U^{(2)}$ satisfy the boundary conditions

$$U^{(1)}(x, y, 0) = F(x, y), \quad \text{(A33)}$$

$$U^{(2)}(x, y, 0) = F(x, y) \exp[ik(\sigma_x x + \sigma_y y)], \quad \text{(A34)}$$

where σ_x and σ_y are real constants such that

$$0 < \sigma_x^2 + \sigma_y^2 < 1. \quad \text{(A35)}$$

If $F(x, y)$ is band limited to a spatial frequency domain (u, v) throughout which

$$|u| \ll k\mu, \quad |v| \ll k\mu, \quad \text{(A36)}$$

$$(u + k\sigma_x)^2 + (v + k\sigma_y)^2 \leq k^2, \quad \text{(A37)}$$

where $\mu = (1 - \sigma_x^2 - \sigma_y^2)^{\frac{1}{2}}$, then in the half-space $z \geq 0$, the fields $U^{(1)}$ and $U^{(2)}$ are related by the formula

$$U^{(2)}(x, y, z) \sim U^{(1)}(x - \sigma_x z/\mu, y - \sigma_y z/\mu, z/\mu) \times \exp[ik\Phi(x, y, z)], \quad \text{(A38)}$$

with

$$\Phi(x, y, z) = \sigma_x(x - \sigma_x z/\mu) + \sigma_y(y - \sigma_y z/\mu). \quad \text{(A39)}$$

Moreover, the two fields $U^{(1)}$ and $U^{(2)}$ may be continued into the whole half-space $z < 0$ and this relation also remains valid throughout this half-space.

* Preliminary results of this investigation were reported at the Fall meeting of the Optical Society of America, held in Pittsburgh, Pa., in October 1968. [Abstract WC 11, J. Opt. Soc. Am. **58**, 1550 (1968).]

[1] D. Gabor, Proc. Roy. Soc. (London) **A197**, 454 (1949).

[2] D. Gabor, Proc. Phys. Soc. (London) **B64**, 449 (1951).

[3] E. N. Leith and J. Upatnieks, J. Opt. Soc. Am. **53**, 1377 (1963).

[4] The use of the angular spectrum representation in the analysis of the holographic process is, of course, not new. It was employed already in the first papers on this subject by Gabor (see Refs. 1, 2) and more recently, for example, by G. C. Sherman [J. Opt. Soc. Am. **57**, 1160 (1967)] and R. Mittra and R. L. Ransom in *Modern Optics*, J. Fox, Ed. (Polytechnic Press, Brooklyn, 1967; Wiley, New York, distr.), p. 619.

The paper by Mittra and Ransom came to our attention after the present work was completed. Some of the results derived in the Appendix of the present paper are very closely related to those given in Sec. 5.2 of that reference.

[5] J. R. Shewell and E. Wolf, J. Opt. Soc. Am. **58**, 1596 (1968).

[6] Throughout this paper the infinite symbol in brackets under an integral sign implies that the integration extends over a complete (infinite) plane.

[7] We assume here that the cross sections of the two beams $U^{(r)}$ and $V^{(h)}$ are large enough to allow us to neglect the spreading of the beams between the plane of the object and the plane of the hologram.

[8] We neglect here the effects arising from the finite size of the hologram.

[9] Usually the wave $U^{(0)}$ will be incident in the direction normal to the photographic plate, so that $p_0 = q_0 = 0$. However for some purposes [e.g., in order to study the 3-dimensional structure of the object; cf. E. Wolf, Optics Comm. **1**, 153 (1969)] it is necessary to understand the effects that arise when the object is also illuminated at other directions and for this reason we allow $\mathbf{s}_0$ to be an arbitrary unit vector.

[10] C. J. Bouwkamp, Rept. Progr. Phys. **17**, 41 (1954).

[11] E. Wolf, Proc. Phys. Soc. (London) **74**, 269 (1959), especially Appendix on p. 280.

[12] E. Lalor, J. Opt. Soc. Am. **58**, 1235 (1968).

[13] The rather restrictive assumption (4.10) is made in order to make it possible to apply Theorem 3 of our Appendix.

[14] That the disappearance of the image is purely due to diffraction was suggested previously, on qualitative grounds, by Mittra and Ransom in Sec. 7.1 of their paper quoted in Footnote 4.

[15] G. C. Sherman (a) Phys. Rev. Letters **21**, 761, 1220 (1968); (b) J. Opt. Soc. Am. **59**, 697 (1969).

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Commuting-Operator Approach to Group Representation Theory

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A study is given of the class-sum-operator approach to the representation theory of finite groups, the group D_{3h} being specifically studied. The class sum approach is shown to simplify the decomposition of Kronecker products. By using the class-sum-operator approach, it is shown that the "indirect" group-projection operators of Löwdin can be used in finite group theory, where they lead to useful factorizations of the finite group-projection operators. It is also shown that tensor operators of certain symmetry types can be constructed within the group itself, and may be used analogously to the usual operator equivalents of crystal field theory.

INTRODUCTION

In much of the traditional literature on quantum mechanics, there is a sharp dichotomy between those treatments which employ the Dirac viewpoint, emphasizing the commutation rules of operators, and those which emphasize the mathematical techniques of group representation theory. A partial link between the two approaches is provided by defining the group of an operator H (usually the Hamiltonian) as the set of operators which commute with H. It is possible, however, to combine the two approaches to a greater degree, by recasting traditional group representation theory itself from the Dirac viewpoint. This has the pedagogical advantage that it makes the group-theoretical apparatus assimilable by physicists who are acquainted with the standard operator approach in quantum mechanics, but who wish to learn the minimum number of new concepts. (This does not, of course, imply that a knowledge of group theory is not needed in setting up the formalism.) The operator approach also has some definite practical advantages, as this paper will illustrate.

Several of the basic ideas and mathematical results employed in this paper are to be found scattered throughout the literature.[1-3] The present paper sets out the main principles of the operator approach to group representation theory, and also applies this approach to a study of projection operators. Section 1A sets out some necessary results from the theory of group algebras, and suggests an alternative way of presenting the traditional group character tables. Section 1B deals with the analysis of the Kronecker products of irreducible representations. In order to render the paper more readable, much of the argument proceeds by using as an illustrative example the particular group D_{3h}, which is familiar to physicists working in crystal field theory.

1. CLASS-SUM OPERATORS AND KRONECKER PRODUCT DECOMPOSITION

A. The Class-Sum Operators

The class-sum operators of a finite group G are defined as

$$\mathcal{C}_K = \frac{1}{h_K} \sum_{k \in K} R_k, \tag{1.1}$$

where the sum runs over all group elements R_k belonging to the class K, which contains h_K group elements. In abstract group theory, $\mathcal{C}_K$ is an element of the group algebra, but in physical applications $\mathcal{C}_K$ is a sum of transformation operators. We adopt this operator interpretation throughout the discussion. From the group property and the definition of a class, there follow several mathematical consequences,[1,2] of which the most important for this discussion is the following: Each class-sum operator commutes with every operator in the group, so that the class sums constitute a commuting set of operators.

From this result and from Schur's lemma, it follows that each of the basis functions belonging to a given rep ν of G will be an eigenfunction of a class-sum operator $\mathcal{C}_K$ with some definite eigenvalue $\lambda^{(\nu)}(K)$. (The abbreviation rep for a unitary irreducible representation follows Melvin.[4,5]) Thus, each rep of G will be characterized by a set of simultaneous eigenvalues of the $\mathcal{C}_K$; the $\mathcal{C}_K$ are essentially the commuting operators of the Dirac viewpoint, and the eigenvalues are the associated quantum numbers. The numerical values of the $\lambda^{(\nu)}(K)$ may be found from the standard character table by writing the diagonal sums as

$$\chi^{(\nu)}(K) = n^{(\nu)} \lambda^{(\nu)}(K), \tag{1.2}$$

where $n^{(\nu)}$ is the dimension of the rep ν. As an example, we show in Table I the eigenvalues for D_{3h}. The numbers in brackets in the table serve to distinguish between different members of the degenerate

TABLE I. $\omega = e^{\frac{2}{3}i\pi}$.

Modified character table for D_{3h}						
	(1) E	(2) σ_h	(3) $2C_3$	(4) $2S_3$	(5) $3C_2'$	(6) $3\sigma_v$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	−1	−1
B_1	1	−1	1	−1	1	−1
B_2	1	−1	1	−1	−1	1
E_1	1	$1\begin{pmatrix}1\\1\end{pmatrix}$	$-\frac{1}{2}\begin{pmatrix}\omega\\\omega^2\end{pmatrix}$	$-\frac{1}{2}\begin{pmatrix}\omega\\\omega^2\end{pmatrix}$	$0\begin{pmatrix}1\\-1\end{pmatrix}$	$0\begin{pmatrix}1\\-1\end{pmatrix}$
E_2	1	$-1\begin{pmatrix}-1\\-1\end{pmatrix}$	$-\frac{1}{2}\begin{pmatrix}\omega\\\omega^2\end{pmatrix}$	$\frac{1}{2}\begin{pmatrix}-\omega\\-\omega^2\end{pmatrix}$	$0\begin{pmatrix}1\\-1\end{pmatrix}$	$0\begin{pmatrix}1\\-1\end{pmatrix}$

representations, and have been chosen by what is essentially a method of descent in symmetry.[6] They are the possible eigenvalues, within the irreducible space, of the single-named operator in the class name at the head of the column. The fact that C_3 and σ_v do not commute does not affect the value of listing together all the possible eigenvalues, as the next section shows. If the E_1 and E_2 functions are chosen so that C_3 becomes diagonal, the functions will be classified in terms of magnetic quantum number modulo 6. The eigenvalues of C_3 in the table for D_{3h} are clearly related to the crystal field quantum numbers μ of Hellwege[7,8] by the equation

$$\lambda^{(\nu)}(C_3) = e^{\frac{2}{3}i\mu\pi}. \tag{1.3}$$

If σ_v or C_2' are made diagonal, the basis functions can be made real, and this yields the same convention as that adopted by Griffith[3] for zero magnetic field. In this context, we refer to "C_3 quantization" and "σ_v quantization" of the E_1 and E_2 functions.

By the nature of the group character table used to construct Table I, it follows that no two rows of eigenvalues are identical. Thus, the Dirac criterion that each basis function should have a unique label is obeyed, as far as group symmetry labels are concerned. The orthogonality property of functions from different reps is now reduced to the orthogonality property of functions associated with different eigenvalues of a unitary operator.

B. The Decomposition of Kronecker Products

In the traditional procedure for the decomposition of the Kronecker product of two reps, the product of two characters is expressed as a linear combination of irreducible characters, either by inspection of the character table or by using the formula

$$c_\nu = \frac{1}{h}\sum_R \chi^{(\nu)*}(R)\chi(R) \tag{1.4}$$

to find the number of times which each rep occurs in the product. Use of this formula may involve finding several c_ν to be zero before hitting on the required nonzero ones. In the class-sum-operator approach, the relevant result here is that which arises from the logical way in which the group operators act on product functions. This gives

$$R(f_1 f_2) = \lambda_1\lambda_2(f_1 f_2), \tag{1.5}$$

when f_1 and f_2 are eigenfunctions of R with eigenvalues λ_1, λ_2, respectively. This result holds for single group operators, but not in general for class sum operators. To illustrate the operator approach, we decompose the triple product $E_2 \times E_2 \times E_2$ for D_{3h}. The resulting product functions, eight in number, all have eigenvalue $(-1)^3$ for σ_h and thus must belong to B_1, B_2, or E_2. The eigenvalue of C_3 in the triple product is $(\omega, \omega^2)^3 = 1, 1, \omega, \omega^2, \omega, \omega^2, \omega, \omega^2$. The last six of these numbers clearly belong to $3E_2$, while the first two may belong to B_1 or B_2. The eigenvalues of σ_v give the result $(1, -1)^3 = 1, -1, 1, -1, 1, -1, 1, -1$, and show that both B_1 and B_2 occur; the decomposition is, accordingly,

$$E_2 \times E_2 \times E_2 = 3E_2 + B_1 + B_2.$$

The procedure outlined above may often be shorter than the standard procedure. (Note that the method does not depend on whether C_3 and σ_v commute, since we may choose C_3 or σ_v quantization arbitrarily at any step of the argument.) When allied with Eq. (1.4), this procedure quickly sorts out the nonzero c_ν.

2. PROJECTION AND TENSOR OPERATORS FOR FINITE GROUPS

Löwdin has introduced projection operators for the 3-dimensional rotation group. These operators take the form[9]

$$O^{(N)} = \prod_L \frac{\mathfrak{L}^2 - L(L+1)}{N(N+1) - L(L+1)}, \tag{2.1}$$

where $\mathfrak{L}^2$ is the squared angular-momentum operator and L runs over all the eigenvalues of $\mathfrak{L}^2$, which are known to be represented in the subspace on which $O^{(N)}$ acts. Such an operator appears to contrast sharply with the projection operators of finite group theory; the latter proceed directly by projecting out the component of the desired symmetry, while the operator $O^{(N)}$ takes the more cumbersome indirect route of eliminating one by one the symmetry types which are not desired. This paper is intended to point out that, for a finite group, there is essentially no difference between the direct and indirect approaches; their equivalence may be established by using the class-sum-operator approach, which is summarized in the preceding section. Section 2A sets out the required

mathematical results and discusses the equivalence result, indicating some simplifications which can be introduced into the finite group projection operator theory by means of the class-sum approach. Section 2B discusses briefly the formation of tensor operators within the group algebra. In order to render the material accessible to physicists, the "proofs" are mainly heuristic and proceed by using the particular group D_{3h} as an example.

A. Projection Operators and the Group Algebra

As pointed out in the preceding section, the class-sum operators for a finite group form a commuting set. In this section, we need the further results:

(a) The product of two class-sum operators may be written as a linear combination of class-sum operators

$$\mathcal{C}_J\mathcal{C}_K = \sum_N h_N c_{JKN}\mathcal{C}_N; \tag{2.2}$$

(b) For a group in which the inverse of every element belongs to the same class as the element itself, the coefficients c_{JKN} are symmetric under interchange of any two indices and obey the sum rule

$$\sum_N c_{JKN} = 1.$$

The criterion of (b) is obeyed by the groups O_h and T_d and by the groups D_n, D_{nv}, and D_{nh} for any n. It clearly cannot be obeyed by groups which are Abelian and possess an element of order three or more, e.g., C_3 and C_{3h}. The slight modification of the symmetry properties of the c_{JKN} for these cases involves inverse classes.[2] The essential point is that such symmetry properties greatly simplify the construction of the class multiplication table. The result that $\mathcal{C}_K\mathcal{C}_N$ does not contain $\mathcal{C}_J$, if $\mathcal{C}_J\mathcal{C}_K$ does not contain $\mathcal{C}_N$, is analogous to the well-known property of the Kronecker product of group reps, and is another example of the close duality between the properties of classes and reps which has been studied in detail by Gamba.[10] The class multiplication table for D_{3h} is summarized by giving the symmetry properties (b) and the following nonzero coefficients (the class numbering is the same as in Table I of Sec. 1);

$$c_{1NN} = h_N^{-1}, \quad \text{for all } N,$$
$$c_{256} = c_{355} = c_{366} = c_{456} = \tfrac{1}{3},$$
$$c_{234} = \tfrac{1}{2}, \quad c_{333} = c_{344} = \tfrac{1}{4}.$$

The traditional projection operators of finite group theory are the primitive idempotents of the group algebra.[2] They are those linear combinations of the $\mathcal{C}_J$ which transform the class multiplication table into the unit matrix. To investigate the projection operators, we use the group D_{3h} as an illustrative example; the modified character table is given in the Sec. 1. The $\mathcal{C}_6$ class-sum operator has the eigenvalue -1 for the A_2 and B_1 reps. With the indirect approach, the operator $\mathcal{C}_6 + 1$ removes any A_2 or B_1 components from the operand. In a similar manner, $\mathcal{C}_2 + 1$ removes any B_1, B_2, or E_2 component, and $\mathcal{C}_6$ removes any E_1 or E_2 component. Application of the operator

$$\mathcal{C}_6(\mathcal{C}_2 + 1)(\mathcal{C}_6 + 1)$$
$$= \mathcal{C}_1 + \mathcal{C}_2 + 2\mathcal{C}_3 + 2\mathcal{C}_4 + 3\mathcal{C}_5 + 3\mathcal{C}_6 \tag{2.3}$$

thus ensures that only the A_1 components of the operand survive. The right-hand side of (2.3) is obtained from the class multiplication table and is seen to be the usual A_1 projection operator. The Löwdin indirect approach for the finite group case is accordingly seen to be equivalent to the usual approach, provided the class sum eigenvalues are used to label the reps. The essential mathematical reason for this is the fact that, within the group algebra of the finite group, it is possible to reduce any polynomial in the $\mathcal{C}_J$ to a linear sum of the $\mathcal{C}_J$. The corresponding process within the continuous rotation group is not possible, and so the indirect approach cannot be simply converted into an equivalent direct approach. The procedure outlined above actually provides a useful factorization of the projection operators, and is an alternative to the factorization procedure of Melvin,[4] which systematically employs the concept of kernel subgroups and quotient sets. By using the modified character table of a group, it is possible to vary tactics and choose the simplest projection operator for a given situation. For example, the set of eight functions arising from the product $E_1 \times E_1 \times E_1$ for D_{3h} contains only B_1, B_2, and E_1 type components. The following alternative operators can then be used to extract these components:

B_1: $\mathcal{C}_6(\mathcal{C}_6 - 1)$, $\mathcal{C}_5(\mathcal{C}_5 + 1)$, $\mathcal{C}_6(\mathcal{C}_5 + 1)$, etc.,
B_2: $\mathcal{C}_6(\mathcal{C}_6 + 1)$, $\mathcal{C}_5(\mathcal{C}_5 - 1)$, $\mathcal{C}_6(\mathcal{C}_5 - 1)$, etc.,
E_1: $(\mathcal{C}_6 - 1)(\mathcal{C}_6 + 1)$, $(\mathcal{C}_5 + 1)(\mathcal{C}_5 - 1)$, etc.

Having obtained the E_1 functions, we can further separate the two types of component by using, for example, σ_v quantization. The operators $\sigma_v - 1$ and $\sigma_v + 1$ would then give the two members of the E_1 family, σ_v being one chosen vertical reflection-plane operator. The operators C_3, S_3, or C_2' could equally well be used in this subclassification process, or even to simplify the complete process. Thus, if we know that only B_1, B_2, and E_1 functions occur in the operand, we may use the operator $\sigma_v - 1$ to leave only B_1 and $E_1(-1)$ type functions; the operator $\sigma_h + 1$ then removes the B_1 part to leave an $E_1(-1)$ type

function. The operator involved would then take the form

$$(\sigma_h + 1)(\sigma_v - 1) = C_2' + \sigma_v - \sigma_h - 1, \quad (2.4)$$

where the particular C_2' axis involved lies in the σ_v plane used to classify the E_1 states. This approach requires only individual group operators and not class sums, and, except for the choice of quantization, the representation matrices are not used at any stage of the proceedings. In many cases, it is not necessary to use all the operators of the group in the projection process. In general, the more information that is given about the components of a subspace, the simpler are the projection operators. For example, a d electron in a D_{3h} crystal field gives one singly degenerate level and two doubly degenerate levels. The modified character table shows that the singly degenerate function may be obtained simply by using $\mathcal{C}_6$ as the projection operator. The traditional projection operator for this case would involve a sum over all group operators, and would yield many terms which cancel out in the final result. When the Löwdin operators $O^{(N)}$ are used in atomic theory, the set of allowed L values in the operand is known, but could, in principle, take any of the values 0, $\frac{1}{2}$, 1, etc. For a finite group, only a finite number of reps can occur, and so the projection process must terminate even when no information is given about the operand.

B. Tensor Operators for a Finite Group

From the definition of a class follows the result

(c) For any group operators U and R_j,

$$UR_jU^{-1} = R_k, \quad (2.5)$$

where R_k is in the class of R_j, but in general depends on U.

If matrices are set up to describe the way in which the elements of a given class are permuted amongst themselves by the equivalence transformations of Eq. (2.5), the resulting representation may be reduced to yield linear combinations of the R_j which transform amongst themselves according to a rep of the group. They may accordingly be termed tensor operators of the group. Such operators were investigated by Gamba,[10] who determined the number of tensor operators furnished by each class of a group. Clearly, every class provides one A_1 tensor operator, namely the class sum itself. This set of A_1 operators are basic to the discussion of this and the preceding sections. The classes of D_{3h} provide the following operator types:

A_1 from classes 1, 2, 3, 4, 5, 6,

A_2 from classes 3, 4,

E_1 from classes 5, 6.

B_1, B_2, and E_2 type operators cannot be constructed from the group operators themselves, although such physical operators do exist, e.g., the coordinate operator z is of B_2 type. The set of reps A_1, A_2, E_1 is closed, in the sense that no Kronecker product of any two of them will yield anything other than A_1, A_2, or E_1 reps. The "excluded" set B_1, B_2, E_2 does not have this property. Thus the rep types of the possible tensor operators in the group algebra form a closed family with respect to addition and multiplication in an analogous "rep algebra."

The tensor operators commute with the class sum operators and thus cannot have matrix elements between functions belonging to different reps. In this respect, they are analogous to the operator equivalents of crystal field theory,[11] which formally belong to reps other than $D^{(0)}$, but which are diagonal in J, since they are actually polynomials in the operators J_x, J_y, and J_z. (For the rotation group, of course, J_x, J_y, and J_z belong to the Lie algebra of the group generators.) From an analysis of Kronecker products, it is readily seen that an A_2 type operator has nonzero matrix elements within an E_1 or E_2 manifold. The modified D_{3h} character table shows that if the E_1 and E_2 states are labeled in C_3 quantization, then an A_2 operator will be diagonal within E_1 or E_2. If σ_v quantization is used, the A_2 operator is off-diagonal within E_1 or E_2. The class of C_3 provides the A_1 operator $C_3 + C_3^2$ and the A_2 operator $C_3 - C_3^2$; using C_3 quantization, we have

$$\langle E_1\omega |\, C_3 - C_3^2 \,| E_1\omega\rangle = -\langle E_1\omega^2 |\, C_3 - C_3^2 \,| E_1\omega^2\rangle = i.$$

The relative value of these matrix elements is, of course, exactly that which results from the generalized Wigner–Eckart theorem on using the coupling coefficients of Griffith.[3] The procedure may also be applied to E_1 type operators if care is taken to choose a standard quantization for both operators and wavefunctions. For example, with C_3 quantization a suitable E_1 operator pair are $C_2^{(1)} + \omega C_2^{(2)} + \omega^2 C_2^{(3)}$ and $C_2^{(1)} + \omega^2 C_2^{(2)} + \omega C_2^{(3)}$, where the bracketed superscript labels the three dihedral axes.

SUMMARY

It has been pointed out that the class-sum-operator approach to group representation theory suggests the use of a modified form of the usual finite group character tables. The modified table includes all the traditional data, plus extra information which aids in the simplification of some calculations and which renders many of the group theoretical results understandable in terms of the usual operator language of quantum mechanics.

The class-sum approach has been used to demonstrate the equivalence of the direct and indirect methods of constructing projection operators for a finite group. By using the properties of the group algebra, it has been shown how a flexible method of factorizing projection operators may be achieved and also how certain tensor operators, which are the analogs of the operator equivalents of rotation group theory, may be constructed within the group.

[1] V. Heine, *Group Theory in Quantum Mechanics* (Pergamon, Oxford, 1960).
[2] G. G. Hall, *Applied Group Theory* (Longmans Green, London, 1967).
[3] J. S. Griffith, *The Irreducible Tensor Method for Molecular Symmetry Groups* (Prentice-Hall, London, 1962).
[4] M. A. Melvin, Rev. Mod. Phys. **28**, 18 (1956).
[5] M. A. Melvin, Rev. Mod. Phys. **32**, 477 (1960).
[6] B. R. Judd, Proc. Phys. Soc. **70B**, 880 (1957).
[7] K. H. Hellwege, Ann. Physik (Leipzig) **4**, 95 (1948).
[8] E. Fick and G. Joos, *Handbuch der Physik, Vol. 28: Spectroscopy II*, S. Flügge, Ed. (Springer, Berlin, 1957), p. 205.
[9] P.-O. Löwdin, Rev. Mod. Phys. **34**, 520 (1962).
[10] A. Gamba, J. Math. Phys. **9**, 186 (1968).
[11] K. W. H. Stevens, Proc. Phys. Soc. **A65**, 209 (1952).

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$O(4)$ Symmetry and the BS Equation for a Spin-1 + Spin-0 System*

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A set of vector functions analogous to the 3-dimensional vector spherical harmonics is defined in four dimensions. These functions are employed to separate the Bethe–Salpeter (BS) equation for a spin-1 + spin-0 system at vanishing total 4-momentum K, where $O(3)$ symmetry degenerates into $O(4)$ symmetry. The angular parts of the matrix elements of all possible tensor operators, symmetry conserving and otherwise, are reduced. Finally, the BS equation at small K is briefly discussed.

1. INTRODUCTION

Much work has been done in the investigation of the $O(4)$ properties of scattering amplitudes since it was first learned that these amplitudes exhibit $O(4)$ symmetry at vanishing total 4-momentum K of the interacting particles.[1–3] Besides possessing this type of symmetry, the Bethe–Salpeter (BS) model[4] is especially interesting because it exhibits several other nice properties. Hence, many attempts have been made to study the $O(4)$ properties of scattering amplitudes in the context of the BS model, and several methods have been proposed for the expansion of these amplitudes at $K = 0$ where $O(4)$ symmetry exactly holds and near $K = 0$ where it is slightly violated.[5,6]

In this work we are motivated by the 4-dimensional vector character of the BS wavefunctions for a spin-1 + spin-0 system to introduce a set of 4-dimensional vector spherical harmonics (VSH) analogous to the well-known 3-dimensional VSH.[7] Our method is, of course, good not only for the BS equation but also for any other integral or differential equations satisfied by 4-dimensional vector functions and invariant under $O(4)$ symmetry. We start by summarizing some of the results obtained by Biedenharn[8] for the 4-dimensional rotation group $R(4)$, which are necessary for defining the VSH. Having defined these functions by analogy with $O(3)$ VSH, we examine their behavior under reflection in order to define new functions which are eigenstates of reflection. The inclusion of reflection is necessary for obtaining functions that belong to $O(4)$ representations since the symmetry group of the equation we are dealing with is $O(4)$ rather than $R(4)$.

In Sec. 3, we show how to reduce the actions of various tensors on vector and scalar spherical harmonics and how to derive several useful formulas that relate these two types of functions. Then, in Sec. 4, we introduce the BS equation and use the results of the previous sections to separate this equation and discuss its solutions in the region where $O(4)$ symmetry is valid. Finally, in Sec. 5, we attack the BS equation in the region where $O(4)$ symmetry is slightly violated and put the equation in a form vulnerable to nondegenerate perturbation theory. Then we indicate how to obtain the slopes of Regge trajectories and the residues of Regge poles from the results of perturbation theory.

2. DEFINITION OF $O(4)$ VECTOR SPHERICAL HARMONICS

It is well known that the 4-dimensional rotation group $R(4)$ is locally isomorphic to $R(3) \times R(3)$ and thus homomorphic to $SU(2) \times SU(2)$. Therefore, we may find the representations of the group $R(4)$ by

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merely carrying over the already well-known results for the representations of $SU(2)$. However, we are interested in representations diagonal in the group $O(3)$ since our objective is to investigate Regge trajectories and residues of Regge poles where we have to deal explicitly with the total $O(3)$ angular momentum.

Let j_1 and j_2 be the two independent $SU(2)$ angular momenta. The states diagonal in the $O(3)$ angular momentum are $|j_1 j_2, lm\rangle \equiv |pq, lm\rangle$, where l and m stand for the total $O(3)$ angular momentum and its azimuthal component. In the future, we will label these states with the invariants $p \equiv j_1 + j_2$ and $q \equiv j_1 - j_2$, which are related to the eigenvalues of the two Casimir operators of the group $R(4)$. The states belonging to a given $O(3)$ subspace transform under a 4-dimensional rotation R in the following way:

$$R\,|pq, lm\rangle = \sum_{l'm'} D^{[p,q]}_{lm,l'm'}(R)\,|pq, l'm'\rangle. \tag{2.1}$$

The rotation matrices satisfy the following group property:

$$D^{[p,q]}_{lm,l'm'}(R) = \sum_{l''m''} D^{[p,q]}_{lm,l''m''}(RS^{-1}) D^{[p,q]}_{l''m'',l'm'}(S).$$

The well-known 4-dimensional spherical harmonics $Z^m_{nl}(\varphi, \theta, \chi)$ are defined in terms of the rotation matrices as a special case with $m' = l' = 0$. In this case the D's vanish unless $j_1 = j_2$, i.e., $p = n$, a non-negative integer, and $q = 0$. The Z^m_{nl} (normalized to unity) are expressed in terms of the D's as follows:

$$Z^m_{nl}(\varphi, \theta, \chi) = [(n+1)/\pi\sqrt{2}]\, D^{[n,0]*}_{lm,00}(\varphi, \theta, \chi). \tag{2.2}$$

The Kronecker product $R(4) \cdot R(4)$ is reduced analogously to $R(3) \cdot R(3)$:

$$\begin{aligned} &D^{[p_1,q_1]}_{l_1m_1,l_1'm_1'} D^{[p_2,q_2]}_{l_2m_2,l_2'm_2'} \\ &= \sum \langle p_1q_1l_1m_1,\, p_2q_2l_2m_2 \,|\, p_1q_1p_2q_2,\, PQLM\rangle \\ &\quad \times D^{[P,Q]}_{LM,L'M'} \langle p_1q_1p_2q_2,\, L'M' \,|\, p_1q_1l_1'm_1',\, p_2q_2l_2'm_2'\rangle. \end{aligned} \tag{2.3}$$

The reduction coefficients, however, are more involved in this case:

$$\begin{aligned} &\langle p_1q_1l_1m_1,\, p_2q_2l_2m_2 \,|\, p_1q_1p_2q_2,\, PQLM\rangle \\ &= \langle l_1m_1,\, l_2m_2 \,|\, l_1l_2,\, LM\rangle \\ &\quad \times \langle p_1q_1l_1,\, p_2q_2l_2,\, L \,|\, p_1q_1p_2q_2,\, PQL\rangle \\ &= \langle l_1m_1,\, l_2m_2 \,|\, l_1l_2,\, LM\rangle \\ &\quad \times [(2l_1+1)(2l_2+1)(P+Q+1)(P-Q+1)]^{\frac{1}{2}} \\ &\quad \times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_1-q_1) & l_1 \\ \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p_2-q_2) & l_2 \\ \frac{1}{2}(P+Q) & \frac{1}{2}(P-Q) & L \end{Bmatrix}. \end{aligned} \tag{2.4}$$

We may also write (2.4) in terms of the six $SU(2)$ angular momenta

$$\begin{aligned} j_1 &= \tfrac{1}{2}(p_1+q_1), \quad j_1' = \tfrac{1}{2}(p_1-q_1), \\ j_2 &= \tfrac{1}{2}(p_2+q_2), \quad j_2' = \tfrac{1}{2}(p_2-q_2), \\ j &= \tfrac{1}{2}(P+Q), \quad j' = \tfrac{1}{2}(P-Q) \end{aligned} \tag{2.5}$$

in the following form:

$$\begin{aligned} &\langle p_1q_1l_1m_1,\, p_2q_2l_2m_2 \,|\, p_1q_1p_2q_2,\, PQLM\rangle \\ &= \langle (j_1j_1')l_1m_1,\, (j_2j_2')l_2m_2 \,|\, (j_1j_2)j(j_1'j_2')j',\, LM\rangle \\ &= \langle l_1m_1,\, l_2m_2 \,|\, l_1l_2LM\rangle \\ &\quad \times \langle (j_1j_1')l_1(j_2j_2')l_2,\, L \,|\, (j_1j_2)j(j_1'j_2')j',\, L\rangle \\ &= \langle l_1m_1,\, l_2m_2 \,|\, l_1l_2,\, LM\rangle \\ &\quad \times [(2l_1+1)(2l_2+1)(2j+1)(2j'+1)]^{\frac{1}{2}} \\ &\quad \times \begin{Bmatrix} j_1 & j_1' & l_1 \\ j_2 & j_2' & l_2 \\ j & j' & L \end{Bmatrix}. \end{aligned} \tag{2.6}$$

The curly brackets designate the so-called Wigner 9-j symbol which characterizes the addition of four angular momenta.[7]

The reduction formula for the product of two spherical harmonics follows immediately from Eqs. (2.3) and (2.2):

$$\begin{aligned} Z^{m_1}_{n_1l_1} Z^{m_2}_{n_2l_2} &= \frac{(n_1+1)(n_2+1)}{\pi\sqrt{2}} \sum \frac{C_{Nn_1n_2}}{N+1} Z^M_{NL} \\ &\quad \times \langle n_10n_20,\, N0LM \,|\, n_10l_1m_1,\, n_20l_2m_2\rangle, \end{aligned} \tag{2.7}$$

where

$$C_{Nn_1n_2} \equiv \langle n_1000,\, n_2000 \,|\, n_10n_20,\, N000\rangle. \tag{2.8}$$

Let us now use the material developed so far to define a set of functions that separate the BS equation for a system of two particles whose spins are one and zero. These functions are found by reducing the product of the $O(4)$ orbital representation $(\frac{1}{2}n, \frac{1}{2}n)$ with the $O(4)$ spin representation $(\frac{1}{2}, \frac{1}{2})$. The $O(3)$ orbital and spin angular momenta of these representations take the values $l = 0, 1, \cdots, n$ and $s = 0, 1$, respectively. We should remark here that, in addition to the part that describes a system with total spin equal to one (the part we are interested in), a part that describes a system with total spin equal to zero is also contained in the BS equation we are attempting to investigate. To eliminate the latter part, certain subsidiary conditions must be imposed. These conditions, however, lead to a more complicated equation.

The orbital representation $(\frac{1}{2}n, \frac{1}{2}n)$ is given by the Z^m_{nl}. For the spin representation $(\frac{1}{2}, \frac{1}{2})$ we use certain

combinations of the coordinate vectors $e_1, \cdots, e_4$:

$$\begin{aligned} &\overleftarrow{e}_{00} = e_4, \qquad \overleftarrow{e}_{1-1} = (e_1 - ie_2)/\sqrt{2}, \\ &\overleftarrow{e}_{10} = e_3, \qquad \overleftarrow{e}_{11} = -(e_1 + ie_2)/\sqrt{2}, \\ &\vec{e}_{s\mu} = \overleftarrow{e}^{*}_{s\mu}, \quad \vec{e}_{s\mu}\overleftarrow{e}_{s'\mu'} = \delta_{ss'}\delta_{\mu\mu'}, \quad s\mu = 00, 1-1, 10, 11. \end{aligned} \tag{2.9}$$

The arrows indicate to which direction the vectors act. Reversing the direction of the arrow is the same as the operation of Hermitian conjugation. The arrows will often be dropped when they are not necessary. It is easy to see that, in the momentum space, the 4-momentum k is given by

$$\begin{aligned} &\overleftarrow{k} = \sum k_{s\mu}\overleftarrow{e}_{s\mu} = \vec{k} = \sum k^{*}_{s\mu}\vec{e}_{s\mu}, \\ &k_{s\mu} = \vec{e}_{s\mu}\overleftarrow{k} = (\pi k/\sqrt{2})Z^{\mu *}_{1s}(\varphi, \theta, \chi), \quad k^{*}_{s\mu} = \vec{k}\overleftarrow{e}_{s\mu}. \end{aligned} \tag{2.10}$$

Using the $e_{s\mu}$, Z^m_{nl}, and the reduction coefficients given by (2.9), (2.2), and (2.4), respectively, we define the following set of vector functions:

$$\begin{aligned} \overleftarrow{\Omega}^{J\mathcal{M}}_{N(n,Q)}(\Omega) &\equiv \sum_{\substack{l,s \\ m,\mu}} \langle n0lm, 10s\mu \mid n010, NQJ\mathcal{M}\rangle Z^m_{nl}(\Omega)\overleftarrow{e}_{s\mu} \\ &\equiv \sum_{\substack{l,s \\ m,\mu}} C^{lms\mu J\mathcal{M}}_{N(n,Q)} Z^m_{nl}\overleftarrow{e}_{s\mu}, \end{aligned} \tag{2.11}$$

$$\begin{aligned} C^{lms\mu J\mathcal{M}}_{N(n,Q)} &\equiv \langle n0lm, 10s\mu \mid n010, NQJ\mathcal{M}\rangle \\ &\equiv \langle lm, s\mu \mid ls, J\mathcal{M}\rangle C^{lsJ}_{N(n,Q)}, \end{aligned} \tag{2.12}$$

where

$$\begin{aligned} C^{lsJ}_{N(n,Q)} &= \langle n0l10s, J \mid n010, NQJ\rangle \\ &= [(2l+1)(2s+1) \\ &\quad \times (N+Q+1)(N-Q+1)]^{\frac{1}{2}} \\ &\quad \times \begin{Bmatrix} \frac{1}{2}n & \frac{1}{2}n & l \\ \frac{1}{2} & \frac{1}{2} & s \\ \frac{1}{2}(N+Q) & \frac{1}{2}(N-Q) & J \end{Bmatrix}. \end{aligned} \tag{2.13}$$

The values of Q, N, and J for which the 9-j symbol in (2.13) does not vanish are

$$\begin{aligned} &Q = \pm 1, \quad N = n, \quad 1 \le J \le N, \\ &Q = 0, \quad N = n \pm 1, \quad 0 \le J \le N. \end{aligned}$$

Thus, for given N, J, and $\mathcal{M}$, there are four possible functions with

$$(n, Q) = (N, -1), (N, 1), (N-1, 0), (N+1, 0). \tag{2.14}$$

Let us examine the behavior of these functions under the following reflection operation which leaves the BS equation invariant:

$$\hat{Q}\overleftarrow{F}(\varphi, \theta, \chi; \overleftarrow{e}_{s\mu}) = \overleftarrow{F}(\pi + \varphi, \pi - \theta, \chi; (-1)^s\overleftarrow{e}_{s\mu}). \tag{2.15}$$

It is easily found that

$$\begin{aligned} \hat{Q}\overleftarrow{\Omega}^{J\mathcal{M}}_{N(n,Q)} &= \sum_{\substack{l,s \\ m,\mu}} C^{lms\mu J\mathcal{M}}_{N(n,Q)}(-1)^l Z^m_{nl}(-1)^s\overleftarrow{e}_{s\mu} \\ &= (-1)^{N+n+J+1}\overleftarrow{\Omega}^{J\mathcal{M}}_{N(n,-Q)}. \end{aligned} \tag{2.16}$$

Thus we may define the following eigenfunctions of $\hat{Q}$:

$$\overleftarrow{\Omega}^{J\mathcal{M}}_{N(N\pm1,0)}; \overleftarrow{\Omega}^{J\mathcal{M}}_{N(N,\pm)} = 2^{-\frac{1}{2}}(\overleftarrow{\Omega}^{J\mathcal{M}}_{N(N,1)} \pm \overleftarrow{\Omega}^{J\mathcal{M}}_{N(N,-1)}), \tag{2.17}$$

where the eigenfunctions $(N \pm 1, 0)$ and $(N, -)$ belong to the eigenvalue $(-1)^J$ while $(N, +)$ belongs to $(-1)^{J+1}$. The new functions (2.17) are given explicitly by

$$\overleftarrow{\Omega}^{J\mathcal{M}}_{N(n,\epsilon)} = \sum_{\substack{l,s \\ m,\mu}} C^{lms\mu J\mathcal{M}}_{N(n,\epsilon)} Z^m_{nl}\overleftarrow{e}_{s\mu}, \quad \epsilon = 0, \pm 1, \tag{2.18}$$

where

$$C^{lms\mu J\mathcal{M}}_{N(N,\pm)} = \langle lms\mu \mid lsJ\mathcal{M}\rangle C^{lsJ\mathcal{M}}_{N(N,\pm)}, \tag{2.19}$$

$$C^{lsJ}_{N(N,\pm)} = 2^{-\frac{1}{2}}(C^{lsJ}_{N(N,1)} \pm C^{lsJ}_{N(N,-1)}). \tag{2.20}$$

We have calculated the coefficients $C^{lsJ}_{N(n,\epsilon)}$ using the recursion relations of the 9-j symbols and their symmetry properties. The results are shown in Appendix A.

It is evident that the new functions (2.18) belong to the $O(4)$ representations $(j,j') \oplus (j',j)$ [cf. (2.5)]. If we now define the quantum number $M = |Q|$, we may speak of representations belonging to $M = 0$, $\epsilon = 0$, and $M = 1$, $\epsilon = \pm$.[3]

The BS equation is invariant under the reflection operation $\hat{Q}$ in the region of $O(4)$ symmetry, i.e., when the total 4-momentum K vanishes (cf. Sec. 3). In this region the BS equation contains only the relative 4-momentum K which commutes with $\hat{Q}$, as can be seen from (2.10) and (2.15). When the total 4-momentum K differs from zero, the BS equation can again be invariant under $\hat{Q}$ provided that K is directed along the fourth axis. Thus, near $K = 0$, where $O(4)$ symmetry is slightly violated, we expect the state $\epsilon = +$ not to mix with the states $\epsilon = 0, -$ since the former state belongs to the eigenvalue $(-1)^{J+1}$ while the latter ones belong to the eigenvalue $(-1)^J$ of the reflection operation $\hat{Q}$.

3. REDUCTION OF EXPRESSIONS INVOLVING SYMMETRY-CONSERVING TENSORS

Before attempting to separate the tensor equation which will be introduced in the next section, we must learn how to reduce expressions containing Z^m_{nl} and $\Omega^{J\mathcal{M}}_{N(n,\epsilon)}$ acted upon by the various possible tensors constructed from $\overleftarrow{K}$ and $\overleftarrow{\partial}$. This may easily be achieved with the help of the material developed in the previous

section. For example, using (2.11), (2.12), (2.10), (2.7), and the unitarity of the matrix $C^{lms\mu J\mathcal{M}}_{N(n,\epsilon)}$, we may evaluate $\vec{K}\Omega^{J\mathcal{M}}_{N(n,\epsilon)}$:

$$\begin{aligned}\vec{k}\overleftarrow{\Omega}^{J\mathcal{M}}_{N(n,\epsilon)} &= \frac{\pi\ell}{\sqrt{2}}\sum_{\substack{l,s\\m,\mu}} C^{lms\mu J\mathcal{M}}_{N(n,\epsilon)} Z^{m}_{nl} Z^{\mu}_{1s} \\ &= \frac{\pi\ell}{\sqrt{2}}\sum_{\substack{l,s\\m,\mu}} C^{lms\mu J\mathcal{M}}_{N(n,\epsilon)} \frac{2(n+1)}{\pi\sqrt{2}} \\ &\quad\times \sum_{\substack{N'J'\\\mathcal{M}'}} \frac{C_{N'n1}}{N'+1} C^{lms\mu J'\mathcal{M}'}_{N'(n,0)} Z^{\mathcal{M}'}_{N'J'} \\ &= \ell\frac{n+1}{N+1} C_{Nn1}\delta_{\epsilon 0} Z^{\mathcal{M}}_{NJ}.\end{aligned}$$

If we compute C_{Nn1} from (2.8), (2.12), and Appendix A and substitute the above result, we finally obtain

$$\vec{k}\overleftarrow{\Omega}^{J\mathcal{M}}_{N(n,\epsilon)} = \delta_{\epsilon 0}\ell B_{Nn} Z^{\mathcal{M}}_{NJ}, \tag{3.1}$$

where

$$\begin{aligned}B_{Nn} &= [N/2(N+1)]^{\frac{1}{2}}, \qquad n = N-1, \\ &= [N+2/2(N+1)]^{\frac{1}{2}}, \quad n = N+1. \end{aligned}\tag{3.2}$$

We may evaluate $\overleftarrow{k}Z^{\mathcal{M}}_{NJ}$ (we will often drop the azimuthal quantum number $\mathcal{M}$ because it is irrelevant in our calculations) in a similar fashion:

$$\begin{aligned}\overleftarrow{k}Z_{NJ} &= \ell\sum_{(n,\epsilon)}\delta_{\epsilon 0} B_{Nn}\overleftarrow{\Omega}^{J}_{N(n,\epsilon)} \\ &= \ell B_{NN-1}\overleftarrow{\Omega}^{J}_{N(N-1,0)} + \ell B_{NN+1}\overleftarrow{\Omega}^{J}_{N(N+1,0)}.\end{aligned}\tag{3.3}$$

If we now combine (3.1) with (3.3), we find

$$\begin{aligned}&\overleftarrow{k}\vec{k}\overleftarrow{\Omega}^{J}_{N(n,\epsilon)} \\ &\quad= \delta_{\epsilon 0}\ell^2 B_{Nn}(B_{NN-1}\overleftarrow{\Omega}^{J}_{N(N-1,0)} + B_{NN+1}\overleftarrow{\Omega}^{J}_{N(N+1,0)}).\end{aligned}\tag{3.4}$$

To reduce expressions containing the derivative $\overleftarrow{\partial}$, we make use of the following Wigner–Eckart theorem which can be easily derived:

$$(Z^{m*}_{nl}\partial_{s\mu}Z^{\mathcal{M}}_{NJ})f(\ell) = \frac{C^{lms\mu J\mathcal{M}}_{N(n,0)}}{C_{Nn1}}(Z^{0}_{n0}\partial_{00}Z^{0}_{N0})f(\ell).$$

If we make use of this theorem and the relations

$$\begin{aligned}\partial_{00} &= \frac{\partial}{\partial x_4} = \cos\chi\frac{\partial}{\partial\ell} - \frac{1}{\ell}\sin\chi\frac{\partial}{\partial\chi}, \\ \cos\chi\, Z^{0}_{N0} &= \tfrac{1}{2}Z^{0}_{N-10} + \tfrac{1}{2}Z^{0}_{N+10}, \\ \sin\chi\frac{\partial}{\partial\chi}Z^{0}_{N0} &= -\tfrac{1}{2}(N+2)Z^{0}_{N-10} + \tfrac{1}{2}NZ^{0}_{N+10},\end{aligned}$$

we can derive the following formulas:

$$\overleftarrow{\partial}Z_{NJ}(\Omega)f(\ell) = \sum_{n}\overleftarrow{\Omega}^{J}_{N(n,0)}(\Omega)B_{Nn}D_{Nn}(\ell)f(\ell),\tag{3.5}$$

$$\vec{\partial}\overleftarrow{\Omega}^{J}_{N(n,\epsilon)}(\Omega)f(\ell) = \delta_{\epsilon 0}Z_{NJ}(\Omega)D_{Nn}(\ell)f(\ell),\tag{3.6}$$

where

$$\begin{aligned}D_{Nn}(\ell) &= B_{NN-1}\left(\frac{N+2}{\ell}+\frac{\partial}{\partial\ell}\right), \quad n = N-1, \\ &= B_{NN+1}\left(-\frac{N}{\ell}+\frac{\partial}{\partial\ell}\right), \qquad n = N+1.\end{aligned}$$

Combining (3.3) and (3.5), we obtain

$$\begin{aligned}\overleftarrow{\Omega}^{J}_{N(N-1,0)} &= -\frac{1}{[N(N+1)]^{\frac{1}{2}}}\left(\ell\overleftarrow{\partial}Z_{NJ} + \frac{N}{\ell}\overleftarrow{k}Z_{NJ}\right), \\ \overleftarrow{\Omega}^{J}_{N(N+1,0)} &= \frac{1}{[(N+1)(N+2)]^{\frac{1}{2}}} \\ &\quad\times\left(k\overleftarrow{\partial}Z_{NJ} - \frac{N-2}{\ell}\overleftarrow{k}Z_{NJ}\right).\end{aligned}$$

The formulas we have derived above provide sufficient tools for reducing the angular parts of all the symmetry-conserving tensors that may be encountered in the equation we are about to introduce.

4. SEPARATION OF THE BS EQUATION IN THE REGION OF $O(4)$ SYMMETRY

The BS equation for a bound state of two particles with spins zero and one and a total 4-momentum K is

$$\begin{aligned}&D^{-1}_{\mu\nu}(\partial_{1\alpha}, \partial_{2\alpha}, m_1, m_2)\Psi^{\nu}_{K}(x_1, x_2) \\ &\quad= \int dx_3\, dx_4[c_{\mu\nu}(\partial_{1\alpha}\cdots\partial_{4\alpha})V(x_1\cdots x_4)]\Psi^{\nu}_{K}(x_3, x_4),\end{aligned}\tag{4.1}$$

$$D^{-1}_{\mu\nu} \equiv (\Box^2_1 + m^2_1)[(\Box_2 + m^2_2)g_{\mu\nu} - \partial_{2\mu}\partial_{2\nu}],$$

where

$$\Box \equiv \partial_\mu\partial^\mu = g_{\mu\nu}\partial_\mu\partial_\nu, \quad \mu,\nu = 0,1,2,3.$$

Following Wick,[9] we rotate the time direction from the real x_0 axis to the imaginary x_4 axis. As a result of this rotation, the time component A_0 of any 4-vector A goes into iA_4, and we end up with vectors obeying the Euclidean metric. Then $D^{-1}_{\mu\nu}$ goes into

$$\begin{aligned}D^{-1}_{\mu\nu} &= (-\Box_1 + m^2_1)[(-\Box_2 + m^2_2)\delta_{\mu\nu} - \partial_{2\mu}\partial_{2\nu}], \\ \Box &\equiv \partial_\mu\partial_\mu, \quad \mu = 1,\cdots,4.\end{aligned}\tag{4.2}$$

Let us transform to momentum space where it is easier for us to work. There (4.1) and (4.2) become

$$\begin{aligned}&D^{-1}_{\mu\nu}(k_1, k_2)\Phi_{K\nu}(k_1, k_2) \\ &= \int dk_3\, dk_4 C_{\mu\nu}(k_1,\cdots,k_4)V(k_1,\cdots,k_4)\Phi_{K\nu}(k_3, k_4),\end{aligned}\tag{4.3}$$

$$D^{-1}_{\mu\nu}(k_1, k_2) = (k^2_1 + m^2_1)[(k^2_2 + m^2_2)\delta_{\mu\nu} - k_{2\mu}k_{2\nu}],$$

where

$$V(k_1, \cdots, k_4) = \frac{1}{(2\pi)^8}\int dx_1 \cdots dx_4 e^{ik_1\cdot x_1 + ik_2\cdot x_2} \times e^{-ik_3\cdot x_3 - ik_4\cdot x_4} V(x_1, \cdots, x_4),$$

$$\Phi_{K\nu}(k_1, k_2) = \frac{1}{(2\pi)^4}\int dx_1\, dx_2 e^{ik_1\cdot x_1 + ik_2\cdot x_2}\Psi_{K\nu}(x_1, x_2),$$

with $k_1 + k_2 = K$, due to translational invariance, and $k_1^2 = -m_1^2$, $k_2^2 = -m_2^2$ on the mass shell. The ladder approximation and translational invariance reduce the form of V to

$$V(x_1, \cdots, x_4) = (2\pi)^2\lambda\delta(x_1 - x_3)\delta(x_2 - x_4) \times V(x_1 - x_2). \quad (4.4)$$

If we now make the following change of variables,

$$K \equiv k_1 + k_2, \quad k \equiv ak_1 - bk_2,$$
$$K' \equiv k_3 + k_4, \quad k' \equiv ak_3 - bk_4, \quad (4.5)$$
$$X \equiv bx_1 + ax_2, \quad x \equiv x_1 - x_2, \quad a + b = 1,$$

we obtain after some algebraic manipulations the following equations for the wavefunction $\vec{\Phi}$ and its Hermitian conjugate $\overleftarrow{\Phi}$:

$$\overleftarrow{\Phi}(K, k) = \lambda\vec{D}(K, k)\int\overleftrightarrow{C}(K, k, k') \times V(k - k')\overleftarrow{\Phi}(K, k')\, dk', \quad (4.6a)$$

$$\vec{\Phi}(K, k) = \lambda\int dk'\vec{\Phi}(K, k')\overleftrightarrow{D}(K, k') \times \overleftrightarrow{C}(K, k'k)V(k - k'), \quad (4.6b)$$

where

$$D(K, k) = \frac{\overleftrightarrow{I} - (b\vec{K} - \vec{k})(b\vec{K} - \vec{k})/m_2^2}{[(aK + k)^2 + m_1^2][(bK - k)^2 + m_2^2]}, \quad (4.7a)$$

$$\overleftrightarrow{D}^{-1}(K, k) = [(aK + k)^2 + m_1^2] \times \{[(bK - k)^2 + m_2^2]\overleftrightarrow{I} - \overleftarrow{k}\overrightarrow{k}\}. \quad (4.7b)$$

Here $\overleftrightarrow{I}$ denotes the unit dyad. We have dropped the subscripts and used the more compact arrow notation introduced in Sec. 2. It is useful to note that the eigenvalue spectrum of Eqs. (4.6) is not affected by the particular choice of the parameters a and b as long as $a + b = 1$. This may easily be seen from Eqs. (4.6) and (4.7): a change of a and b into $a - c$ and $b + c$ changes k in (4.7) into $k - cK$. If we now define new variables $p = k - cK$ and $p' = k' - cK$, the eigenvalue equation will look the same as before while the function $\Phi(K, k)$ changes into $\Phi(K, p + cK) \equiv F(K, p)$. This property of the BS equation allows us to choose a and b such that the equation is simplified considerably.

At $K = 0$ the BS equation acquires $O(4)$ symmetry. In this special case Eqs. (4.6) go into

$$\overleftarrow{\varphi}(k) = \lambda\overleftrightarrow{D}_0(k)\int\overleftrightarrow{C}(k, k')V(k - k')\overleftarrow{\varphi}(k')\, dk', \quad (4.8)$$

$$\overleftrightarrow{D}_0(k) = \frac{\overleftrightarrow{I} + \overleftarrow{k}\overrightarrow{k}/m_2^2}{(k^2 + m_1^2)(k^2 + m_2^2)}. \quad (4.9)$$

The most general form of $\overleftrightarrow{C}$ at $K = 0$ is

$$\overleftrightarrow{C}(k, k') = \sum G_i(\not{k}, \not{k}', k\cdot k')\overleftrightarrow{E}_i, \quad (4.10)$$

where the $\overleftrightarrow{E}_i$, $i = 1, \cdots, 5$, denote the following symmetry-conserving tensors:

$$\overleftrightarrow{E}_i \equiv \overleftrightarrow{I}, , \overleftarrow{k}\overrightarrow{k}, \overleftarrow{k'}\overrightarrow{k'}, \overleftarrow{k}\overrightarrow{k'}, \overleftarrow{k'}\overrightarrow{k}. \quad (4.11)$$

Thus, for each term in (4.10), the BS equation (4.8) may be written in the following form:

$$\overleftarrow{\varphi}(k) = \lambda\int\overleftrightarrow{U}(k, k')\overleftarrow{\varphi}(k')\, dk', \quad (4.12)$$

$$\overleftrightarrow{U}(k, k') \equiv \overleftrightarrow{D}_0(k)\overleftrightarrow{E}G(\not{k}, \not{k}', k\cdot k')V(k - k'), \quad (4.13)$$

where $\overleftrightarrow{E}$ stands for any one of the tensors enumerated in (4.11).

To separate Eq. (4.12), we expand $\overleftarrow{\varphi}(k)$ in the set of $O(4)$ VSH defined by (2.18):

$$\overleftarrow{\varphi}(k) = \sum_{N'J'}\sum_{(n',\epsilon')}\overleftarrow{\Omega}^{J'}_{N'(n',\epsilon')}(\Omega)\gamma_{N'(n',\epsilon')}(\not{k}). \quad (4.14)$$

Since J is always conserved and since N and ϵ are good quantum numbers at $K = 0$, the matrix element of $\overleftrightarrow{U}$ with the angular functions reduces to

$$(\vec{\Omega}^J_{N(n,\epsilon)}(\Omega)\overleftrightarrow{U}(k, k')\overleftarrow{\Omega}^J_{N'(n',\epsilon')}(\Omega')) = U^{N\epsilon}_{nn'}(\not{k}, \not{k}')\delta_{JJ'}\delta_{NN'}\delta_{\epsilon\epsilon'}. \quad (4.15)$$

Thus $\overleftrightarrow{U}$ is diagonal in the $M = 1$ states ($\epsilon = \pm$) while it mixes the $M = 0$ states ($\epsilon = 0$). This result is consistent with the $O(4)$ parities and reflection eigenvalues of the states. If we now substitute (4.14) and (4.15) into (4.12), we end up with the following matrix equation (in the radial variable $\not{k}$) which consists of two 1-dimensional equations for the $M = 1$ states and a 2-dimensional matrix equation for the $M = 0$ states:

$$\begin{pmatrix} \gamma^{(\not{k})}_{N(N,+)} \\ \gamma^{(\not{k})}_{N(N,-)} \\ \gamma^{(\not{k})}_{N(N-1,0)} \\ \gamma^{(\not{k})}_{N(N+1,0)} \end{pmatrix} = \lambda_N\int\not{k}'^3\, d\not{k}' \begin{pmatrix} U^{N+}_{NN}(\not{k}, \not{k}') & & & \\ & U^{N-}_{NN}(\not{k}, \not{k}') & & \\ & & U^{N0}_{N-1N-1}(\not{k}, \not{k}')U^{N0}_{N-1N+1}(\not{k}, \not{k}') & \\ & & U^{N0}_{N+1N-1}(\not{k}, \not{k}')U^{N0}_{N+1N+1}(\not{k}, \not{k}') \end{pmatrix} \times \begin{pmatrix} \gamma^{(\not{k}')}_{N(N,+)} \\ \gamma^{(\not{k}')}_{N(N,-)} \\ \gamma^{(\not{k}')}_{N(N-1,0)} \\ \gamma^{(\not{k}')}_{N(N+1,0)} \end{pmatrix}. \quad (4.16)$$

For a given N, this equation possesses, in general, four solutions and four corresponding eigenvalues which we indicate with the subscript $r = 1, \cdots, 4$. Moreover, for given N and r there is an infinite number of eigenvalues corresponding to different potential strengths $\lambda^{\mathrm{i}}_{Nr}$. This infinity, which we indicate with the superscript i, results from solving an integral equation in the radial variable ℓ. We will find later on that $U^{N+}_{NN} = U^{N-}_{NN}$ (cf. Appendix B). Therefore, the radial wavefunctions and the eigenvalues of the $M = 1$ states are identical. Let us now write down the total wavefunctions and their eigenvalues:

$$\overleftarrow{\varphi}^{J\mathrm{i}}_{N1}(\ell) = \gamma^{\mathrm{i}}_N(\ell)\overleftarrow{\Omega}^{J\ (\Omega)}_{N(N,+)},$$

$$\overleftarrow{\varphi}^{J\mathrm{i}}_{N2}(\ell) = \gamma^{\mathrm{i}}_N(\ell)\overleftarrow{\Omega}^{J\ (\Omega)}_{N(N,-)},$$

with eigenvalue $\lambda^{\mathrm{i}}_{N1} = \lambda^{\mathrm{i}}_{N2} = \lambda^{\mathrm{i}}_N$,

$$\overleftarrow{\varphi}^{J\mathrm{i}}_{N3}(k) = \eta^{\mathrm{i}\ (\ell)}_{N(N-1,0)}\overleftarrow{\Omega}^{J\ (\Omega)}_{N(N-1,0)} + \eta^{\mathrm{i}\ (\ell)}_{N(N+1,0)}\overleftarrow{\Omega}^{J\ (\Omega)}_{N(N+1,0)}$$

with eigenvalue $\lambda^{\mathrm{i}}_{N3}$,

$$\overleftarrow{\varphi}^{J\mathrm{i}}_{N4}(k) = \zeta^{\mathrm{i}\ (\ell)}_{N(N-1,0)}\overleftarrow{\Omega}^{J\ (\Omega)}_{N(N-1,0)} + \zeta^{\mathrm{i}\ (\ell)}_{N(N+1,0)}\overleftarrow{\Omega}^{J\ (\Omega)}_{N(N+1,0)},$$

with eigenvalue $\lambda^{\mathrm{i}}_{N4}$.

It remains now to determine the explicit form of the matrix $U^{N\epsilon}_{nn}$ for the various tensors enumerated in (4.11). This may be accomplished with the help of the formulas derived in Sec. 2 and the following expansion:

$$G(\ell, \ell', k\cdot k')V(k - k') = \sum_{nlm} Z^m_{nl}(\Omega)F_n(\ell, \ell')Z^{m*}_{nl}(\Omega').$$

The results are listed in Appendix B.

5. PERTURBATION IN K; REGGE SLOPES AND RESIDUES

If we examine Eqs. (4.6) and (4.7), we find that they contain a complicated dependence on K and $\cos\chi$, where χ is the angle between the total 4-momentum K and the relative 4-momentum k (we choose a coordinate system in which K lies along the fourth axis). Thus, a rash attempt at studying Eqs. (4.6) for small values of K would result in very lengthy and complicated perturbation formulas. However, the equation will be simplified considerably if we decide to choose $a = 1$ and $b = 0$. We have already mentioned in Sec. 3 that the choice of a and b does not affect the eigenvalue spectrum as long as $a + b = 1$. The eigenfunctions, on the other hand, are dependent on the particular choice of a and b. It is possible, however, to transform among systems corresponding to different choices of a and b. (Incidentally, in the c.m. system $a = b = \frac{1}{2}$.) With $a = 1$ and $b = 0$, (4.6a) becomes

$$\left(1 + \frac{\cos\chi}{\ell^2 + m_1^2}\mathcal{K} + \frac{1}{\ell^2 + m_2^2}\mathcal{K}^2\right)\overleftarrow{\Phi}(K, k) = \lambda\int \overleftrightarrow{U}(k, k')\overleftarrow{\Phi}(K, k')\,dk' + \lambda\int \overleftrightarrow{W}(K, k, k')\Phi(K, k')\,dk', \quad (5.1)$$

where $\overleftrightarrow{U}$ is the K-independent (zeroth-order) kernel given by (4.13), while $\overleftrightarrow{W}$ is the K-dependent kernel which may be expanded in a power series in $\mathcal{K}$. In addition to the symmetry-conserving tensors listed in (4.11), $\overleftrightarrow{W}$ involves the following symmetry breaking tensors:

$$k\cdot\overleftrightarrow{KI}, \overleftrightarrow{kK}, \overleftrightarrow{Kk}, \overleftrightarrow{KK}. \quad (5.2)$$

We have calculated the matrix elements of these tensors with $O(4)$ VSH and listed them in Appendix C. Further simplifications occur if we are interested only in classes of s-independent potentials ($s = -\mathcal{K}^2$ is the square of the c.m. energy). In this case, the second term in the rhs of (5.1) drops out, and the perturbation formulas for λ and Φ assume very simple forms. These formulas may easily be found if the power series expansions in $\mathcal{K}$ of λ and Φ are substituted into (5.1). There is no need to write the formulas here, especially since we do not plan to investigate the slopes and residues.[10] However, for the sake of completeness, we will explain briefly how to extract the slopes of Regge trajectories and the residues of Regge poles from the perturbation results for λ and Φ.

To obtain the slopes of Regge trajectories, we first find the second-order corrections of λ [the first-order correction vanishes due to $O(4)$ parity considerations]:

$$\lambda^J_{Nr} = \lambda_{Nr} + \mathcal{K}^2\lambda^{J(2)}_{Nr} + \cdots, \quad r = 1, \cdots, 4.$$

Then we continue N and J to complex values keeping the difference always equal to a nonnegative integer.[5] Thus

$$N \to \nu, \quad J \to \alpha_\kappa, \quad \nu - \alpha_\kappa = \kappa = 0, 1, \cdots,$$
$$\lambda^J_{Nr} = \lambda_r(s, \alpha_\kappa), \quad \lambda_{Nr} \to \lambda_r(\alpha_0), \quad \lambda^{J(2)}_{Nr} \to \lambda^{(2)}_r(\alpha_\kappa), \quad (5.3)$$

where $s = -\mathcal{K}^2$ is the square of the c.m. energy. $\kappa = 0$ refers to what is usually called the parent trajectory, while $\kappa = 1, 2, \cdots$ refer to the daughter trajectories.[2] The equations for Regge trajectories $\alpha_\kappa = \alpha_\kappa(s)$ are found by keeping λ (the strength of

the potential) constant and varying α_κ in s, i.e., by inverting the equations $\lambda_r(s, \alpha_\kappa) = \text{const}$. Thus the slopes at zero energy are given by

$$\left.\frac{d\alpha_\kappa^r(s)}{ds}\right|_{s=0} = -\left.\frac{\partial\lambda_r(s,\alpha_\kappa)/\partial s}{\partial\lambda_r(s,\alpha_\kappa)/\partial\alpha_\kappa}\right|_{s=0}$$

$$= -\frac{\lambda_r^{(2)}(\alpha_\kappa)/\lambda_r^2(\alpha_0)}{\{\vec{\varphi}_r(k,\alpha_0)[\partial\vec{\vec{U}}(k,k')/\partial\alpha_0]\overleftarrow{\varphi}_r(k',\alpha_0)\}}, \qquad r = 1, \cdots, 4.$$

We should now be able to investigate the signs of the slopes by making use of the machinery developed in the previous sections, if we put certain general restrictions on the form of the potential.

If the kernels of Eq. (5.1) are Fredholm or may be made so by introducing suitable cutoff functions, then the resolvent kernel, which is the T matrix, is a meromorphic function of the parameter λ. Using the results for the perturbed wavefunctions, we may straightforwardly write down the residues of the poles in the λ plane if we assume these poles to be simple. Having done this, we continue N and J as prescribed in (5.3). Obviously, the residues obtained this way differ only by a factor of $(d\lambda/d\nu)^{-1}$ from the residues of the corresponding poles in the ν plane. However, these residues, which belong to what we usually call $O(4)$ poles, are not exactly the residues we are after. We are interested in Regge poles (poles in the α_κ plane) which may easily be extracted if we know how to unveil the $O(3)$ content of an $O(4)$ pole. To do this, we need to know the matrix that projects $O(4)$ VSH on $O(3)$ VSH. With the help of (2.12), (2.19), and the factorization of $Z_{nl}^m(l, \theta, \chi)$ into $\chi_n^l(\chi)Y_l^m(l, \theta)$, Eq. (2.18) can immediately be rewritten into the following form:

$$\overleftarrow{\Omega}_{N(n,\epsilon)}^{J\mathcal{M}} = \sum_{ls} C_{N(n,\epsilon)}^{lsJ}\chi_n^l(\chi)\overleftarrow{\mathcal{Y}}_{Jls}^{\mathcal{M}}(\varphi, \theta),$$

$$\overleftarrow{\mathcal{Y}}_{Jl1}^{\mathcal{M}} \equiv \sum_{m+\mu=} \langle lm, s\mu \mid ls, J\mathcal{M}\rangle Y_l^m(\varphi, \theta)\overleftarrow{e}_{1\mu},$$

$$\overleftarrow{\mathcal{Y}}_{JJ0}^{\mathcal{M}} \equiv Y_J^{\mathcal{M}}(\varphi, \theta)\overleftarrow{e}_{00}.$$

We recognize the three functions $\vec{\mathcal{Y}}_{Jl1}^{\mathcal{M}}$, $l = J, J \pm 1$, as the well-known $O(3)$ VSH.[7] They describe a system of two particles whose spins are one and zero, while the fourth function $\overleftarrow{\mathcal{Y}}_{JJ0}^{\mathcal{M}}$ describes a system with zero total spin.

ACKNOWLEDGMENT

I am grateful to Professor R. F. Sawyer for the suggestion of this problem and for many fruitful discussions.

APPENDIX A: $C_{N(n,\epsilon)}^{lsJ}$

TABLE AI.

		$M = 1$		$M = 0$	
(l, s)	(n, ϵ)	$(N, +)$	$(N, -)$	$(N-1, 0)$	$(N+1, 0)$
$(J, 0)$	0	$\left(\frac{J(J+1)}{(N+1)^2}\right)^{\frac{1}{2}}$	$\left(\frac{(N-J)(N+J+1)}{2N^2}\right)^{\frac{1}{2}}$	$\left(\frac{(N-J+1)(N+J+2)}{2(N+2)^2}\right)^{\frac{1}{2}}$	
$(J-1, 1)$	0	$-\left(\frac{(J+1)(N-J+1)(N+J+1)}{(2J+1)(N+1)^2}\right)^{\frac{1}{2}}$	$\left(\frac{J(N+J)(N+J+1)}{2(2J+1)N^2}\right)^{\frac{1}{2}}$	$\left(\frac{J(N-J+1)(N-J+2)}{2(2J+1)(N+2)^2}\right)^{\frac{1}{2}}$	
$(J, 1)$	1	0	0	0	
$(J+1, 1)$	0	$= \left(\frac{J(N-J)(N+J+2)}{2(2J+1)(N+1)^2}\right)^{\frac{1}{2}}$	$-\left(\frac{(J+1)(N-J)(N-J-1)}{2(2J+1)N^2}\right)^{\frac{1}{2}}$	$\left(\frac{(J+1)(N+J+2)(N+J+3)}{2(2J+1)(N+2)^2}\right)^{\frac{1}{2}}$	

APPENDIX B

(1) $\overleftrightarrow{E} = \overleftrightarrow{I}$,

$$(\not{k}^2 + m_1^2)(\not{k}^2 + m_2^2)\overleftrightarrow{U}^{N\epsilon}_{nn'}(\not{k}, \not{k}') = \left(\delta_{nn'} + \delta_{\epsilon 0}\frac{k^2}{m_2^2}B_{Nn}B_{Nn'}\right)F_{n'}(\not{k}, \not{k}').$$

(2) $\overleftrightarrow{E} = \overleftarrow{k}\overrightarrow{k}$,

$$m_2^2(\not{k}^2 + m_1^2)U^{N\epsilon}_{nn'}(\not{k}, \not{k}') = \delta_{\epsilon 0}B_{Nn}B_{Nn'}F_{n'}(\not{k}, \not{k}').$$

(3) $\overleftrightarrow{E} = \overleftarrow{k'}\overrightarrow{k'}$,

$$(\not{k}^2 + m_1^2)(\not{k}^2 + m_2^2)U^{N\epsilon}_{nn'}(\not{k}, \not{k}') = \delta_{\epsilon 0}\not{k}'^2 B_{Nn}B_{Nn'} \times \left(F_n(\not{k}, \not{k}') + \frac{\not{k}^2}{m_2^2}\sum_{n_1}B^2_{Nn_1}F_{n_1}(\not{k}, \not{k}')\right).$$

(4) $\overleftrightarrow{E} = \overleftarrow{k}\overrightarrow{k'}$,

$$m_2^2(\not{k}^2 + m_1^2)U^{N\epsilon}_{nn'}(\not{k}, \not{k}') = \delta_{\epsilon 0}B_{Nn}B_{Nn'}F_N(\not{k}, \not{k}').$$

APPENDIX C

$$(\vec{\Omega}^{J\,(\Omega)}_{N(n,\epsilon)}\not{k}\overleftrightarrow{K}\overrightarrow{\Omega}^{J\,(\Omega)}_{N'(n',\epsilon')}) = \not{k}\mathcal{K}\delta_{\epsilon 0}\delta_{Nn'}B_{Nn}C^{J0J}_{N'(n',\epsilon')},$$

$$(\vec{\Omega}^{J\,(\Omega)}_{N(n,\epsilon)}\overleftarrow{K}\overrightarrow{k}\overrightarrow{\Omega}^{J\,(\Omega)}_{N'(n',\epsilon')}) = \not{k}\mathcal{K}\delta_{\epsilon' 0}\delta_{nN'}B_{N'n'}C^{J0J}_{N(n,\epsilon)},$$

$$(\vec{\Omega}^{J\,(\Omega)}_{N(n,\epsilon)}\overleftarrow{K}\overrightarrow{K}\overrightarrow{\Omega}^{J\,(\Omega)}_{N'(n',\epsilon')}) = \mathcal{K}^2\delta_{nn'}C^{J0J}_{N(n,\epsilon)}C^{J0J}_{N'(n',\epsilon')},$$

$$(\vec{\Omega}^{J\,(\Omega)}_{N(n,\epsilon)}k\cdot K\overleftrightarrow{I}\overrightarrow{\Omega}^{J\,(\Omega)}_{N'(n',\epsilon')}) = \not{k}\mathcal{K}(\vec{\Omega}^{J}_{N(n,\epsilon)}\cos\chi\overrightarrow{\Omega}^{J}_{N'(n',\epsilon')}),$$

where $\cos\chi\Omega^{J\,(\Omega)}_{N(n,\epsilon)}$ is given explicitly by the following:

$$\cos\chi\,\Omega^J_{N(N,+)} = \left(\frac{(N-J)(N+J+1)}{4N(N+1)}\right)^{\frac{1}{2}}\Omega^J_{N-1(N-1,+)} + \left(\frac{(N-J+1)(N+J+2)}{4(N+1)(N+2)}\right)^{\frac{1}{2}}\Omega^J_{N+1(N+1,+)},$$

$$\cos\chi\,\Omega^J_{N(N,-)} = \left(\frac{(N-J)(N+J+1)}{4N(N+1)}\right)^{\frac{1}{2}}\Omega^J_{N-1(N-1,-)} - \left(\frac{J(J+1)}{2N(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N(N-1,0)} + \left(\frac{J(J+1)}{2(N+2)(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N(N+1,0)} + \left(\frac{(N-J+1)(N+J+2)}{4(N+1)(N+2)}\right)^{\frac{1}{2}}\Omega^J_{N+1(N+1,-)},$$

$$\cos\chi\,\Omega_{N(N-1,0)} = \left(\frac{(N-1)(N-J)(N+J+1)}{4N^3}\right)^{\frac{1}{2}}\Omega^J_{N-1(N-2,-)} + \left(\frac{(N-J)(N+J+1)}{4N^3(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N-1(N,0)} - \left(\frac{J(J+1)}{2N(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N(N,-)} + \left(\frac{N(N-J+1)(N+J+2)}{4(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N+1(N,0)},$$

$$\cos\chi\,\Omega_{N(N+1,0)} = \left(\frac{(N-J)(N+J+1)}{4(N+2)(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N-1(N,0)} + \left(\frac{J(J+1)}{2(N+2)(N+1)^3}\right)^{\frac{1}{2}}\Omega^J_{N(N,-)} + \left(\frac{(N-J+1)(N+J+2)}{4(N+1)^3(N+2)^3}\right)^{\frac{1}{2}}\Omega^J_{N+1(N,0)} + \left(\frac{(N-J+1)(N+J+2)}{4(N+3)(N+2)^3}\right)^{\frac{1}{2}}\Omega^J_{N+1(N+2,0)}.$$

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[1] G. Domokos and P. Suranyi, Nucl. Phys. **54**, 529 (1964).

[2] D. Z. Freedman and J. M. Wang, Phys. Rev. Letters **17**, 569 (1966); Phys. Rev. **153**, 1596 (1967).

[3] M. Toller, Nuovo Cimento **53**, 671 (1968). Toller works directly with the homogeneous Lorentz group $O(3, 1)$ which is related to $O(4)$ through analytic continuation.

[4] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper & Row, New York, 1962).

[5] G. Domokos, Phys. Rev. **159**, 1387 (1967).

[6] W. R. Frazer, F. R. Halpern, H. M. Lipinski, and D. R. Snider, Phys. Rev. **176**, 2047 (1968).

[7] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, N.J., 1957).

[8] L. C. Biedenharn, J. Math. Phys. **2**, 433 (1961).

[9] G.-C. Wick, Phys. Rev. **96**, 1124 (1954).

[10] We have done some investigations of the slopes and residues elsewhere [Phys. Rev. (to be published)].

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Block Diagrams and the Extension of Timelike Two-Surfaces

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The work of Finkelstein, Kruskal, Graves and Brill, Carter, and Boyer and Lindquist on the extension and schematic representation of 2-dimensional metrics is systematized and generalized. As a result, a number of extensions may be found by inspection. Some well-known examples are given, and the technique is applied to the "soluzioni oblique" of Levi-Civita.

INTRODUCTION

An exhaustive global analysis of a solution[1] of Einstein's gravitational-field equations is usually a formidable task. In certain special cases however, there are intrinsically singled-out 2-dimensional submanifolds of the 4-dimensional space–times which can be simply analyzed. Examples are the symmetry axis of an axially symmetric static or stationary solution or the 2-surfaces containing the repeated principal null directions in a type [22] solution. In many cases, the analysis of such a 2-surface has provided valuable clues to the global structure of the space–time.[2] The first applications of a 2-dimensional approach were Finkelstein's[3] and Kruskal's[4] maximal extensions of the Schwarzschild solution. Subsequently, analogous techniques were employed by Graves and Brill[5] and Carter[6] for the Reissner–Nordstrøm solution and by Carter[2] and Boyer and Lindquist[7] for the Kerr solution.

In this paper, we systematize and generalize the techniques of the above authors. A result is that all of the well-known 2-dimensional extensions, together with their schematic representations, can be found by inspection.

TIMELIKE TWO-SURFACES

We work with a static, totally geodesic,[8] timelike 2-surface T. Because of the static, totally geodesic requirement, the metric on T can always be put in the form

$$ds^2 = F\,dt^2 - dr^2/F, \tag{1}$$

where F is the norm of the timelike Killing vector in T. F is a function of r and possibly of other coordinates on the 4-dimensional space–time, but by the totally geodesic property the other coordinates can be chosen constant on T.

Let

$$t^a = \left(\frac{dt}{d\lambda}, \frac{dr}{d\lambda}\right)$$

be the tangent vector to an affinely parametrized geodesic γ in T, with affine parameter λ. Then t^a satisfies $t^c\nabla_c t^a = 0$ (where ∇_c is covariant derivative) which, in the coordinates of (1), can be integrated once to give

$$\frac{dt}{d\lambda} = \frac{A}{F},$$

$$\frac{dr}{d\lambda} = (A^2 - \epsilon F)^{\frac{1}{2}}. \tag{2}$$

A is a constant and $t_c t^c = \epsilon = 0, +1$, or -1 according as γ is null, timelike, or spacelike. r is seen to be an affine parameter along null geodesics in T and is therefore an almost invariant coordinate. When $F = 0$, there are incomplete geodesics of all three types, and, to the extent to which the incompleteness is due to a bad choice of coordinates, the fault lies with the coordinate t.

The only invariant of the curvature of T is the intrinsic Gaussian curvature $K = \frac{1}{2}d^2F/dr^2$. We show that, if F and K are finite for all r in the range $-\infty < r < \infty$, then every geodesic in T can be extended until it is complete. If, on the other hand, F or K becomes unbounded for some value r_0 of r, then only those geodesics along which $r = r_0$ within a finite affine distance from some point of T are incomplete and inextendible. In the latter case, T, and the space–time in which T is imbedded, are intrinsically singular. The extensions obtained are accordingly maximal.

Let the zeros of F be given by $r = a_i$, $i = 1, 2, \cdots, n$ (n finite), with $-\infty < a_1 < a_2 < \cdots < a_n < \infty$. If F approaches a constant finite value as $r \to \infty$ (so that $K \to 0$), then we can rescale the coordinates if necessary so that $\lim F = \pm 1$, as $r \to \infty$. For such an F, T is asymptotically flat, and conformal infinity[9] $\mathscr{I}$ can be represented by a pair of finite null lines. A similar remark applies in the case $r \to -\infty$.

BLOCKS

When F vanishes, the orbits of the timelike Killing vector become null, so that we can think of the $r = a_i$ as dividing T into $n + 1$ distinct regions. Each such region is bounded by the null Killing vector orbits

(or horizons), by one such orbit and $\mathscr{I}$, or by a null orbit and a singular line at $r = r_0$. Each region $a_i \leq r \leq a_{i+1}$ will be called a *block*. The maximal extension of T is found by "gluing" the blocks together along their boundaries (called *seams*) according to a well-defined scheme. Those seams along which $F = 0$ and K is finite are called *nonsingular*, while those along which F or K is unbounded are *singular*. Blocks can only be glued together along nonsingular seams across which K is smooth (C^∞, say).

In each region

$$T_i = \{(t, r) \mid -\infty < t < \infty, a_i \leq r \leq a_{i+1}\},$$

fix some r_i between a_i and a_{i+1} and define new coordinates[10]

$$u_i = t + \int_{r_i}^{r} \frac{dw}{F(w)}$$

and

$$v_i = t - \int_{r_i}^{r} \frac{dw}{F(w)}. \tag{3}$$

Then

$$u_i + v_i = 2t \quad \text{and} \quad u_i - v_i = 2\int_{r_i}^{r} \frac{dw}{F(w)}.$$

T_i has metric $ds^2 = F\,du_i\,dv_i$ which, for $C^\infty F$, is C^∞ for $-\infty < u_i < \infty$ and $-\infty < v_i < \infty$ except when T_i is singular. (In the singular case, put $r_i = r_0$.)

In the nonsingular case, with $F > 0$ in T_i, we have the following implications:

$$r \to a_{i+1} \text{ implies } \begin{cases} v_i \text{ finite: } u_i \to \infty, t \to \infty, \\ u_i \text{ finite: } v_i \to -\infty, t \to -\infty, \end{cases}$$

$$r \to a_i \text{ implies } \begin{cases} v_i \text{ finite: } u_i \to -\infty, t \to -\infty, \\ u_i \text{ finite: } v_i \to \infty, t \to \infty. \end{cases}$$

Defining $\varphi_i = \tan^{-1} u_i$ and $\psi_i = \tan^{-1} v_i$, we can represent T_i schematically by means of the block in Fig. 1.

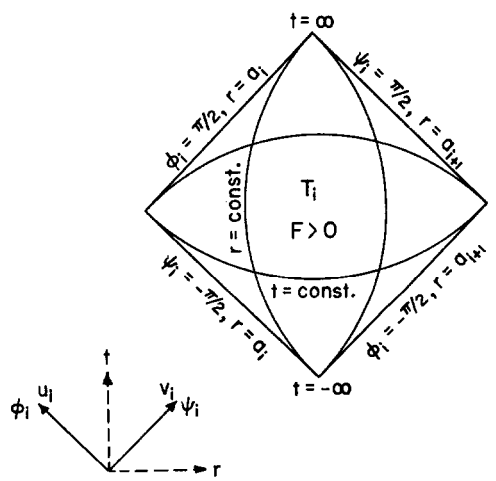

FIG. 1. A nonsingular block. The figure in the lower left shows the axis orientation.

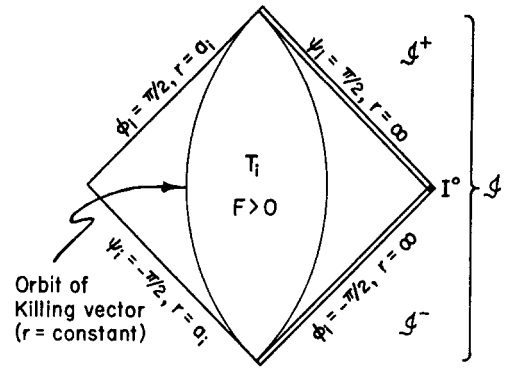

FIG. 2. A nonsingular block with conformal infinity $\mathscr{I}$ represented by double lines.

If $a_i \leq r < \infty$ and T_i is asymptotically flat, we represent conformal infinity $\mathscr{I}$ by double lines as in Fig. 2.

We discuss the exceptional points at the corners of the blocks later. The "point" labeled I^0 in Fig. 2 is not included in $\mathscr{I}$.

If $r_0 < r \leq a_{i+1}$ and T_i is singular, we have the situation represented schematically in Fig. 3, where the serrated line represents the singularity as $K \to \infty$. The singular "points" ($r = r_0$, $-\infty < t < \infty$) are not in T_i.

If F were negative in T_i, all of the above would hold in the same way except that u_i and v_i (and, hence, φ_i and ψ_i) would be replaced by their negatives. The Killing vector orbits in such a block are spacelike.

Note that each block may be flipped about $r = r_i$ by interchanging the roles of u_i and v_i and that the discrete isometry $t \to -t$ turns the block upside down. These flips are shown in Fig. 4.

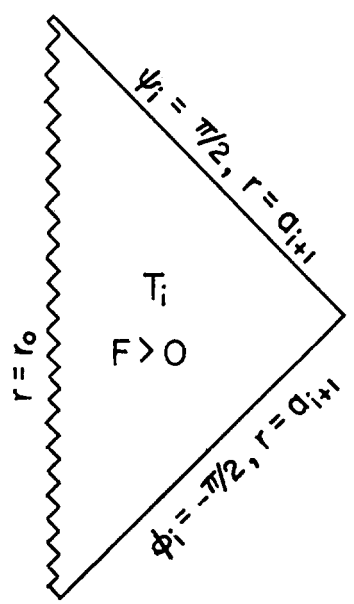

FIG. 3. A singular block. The serrated line $r = r_0$ shows where the intrinsic curvature K of T_i is infinite.

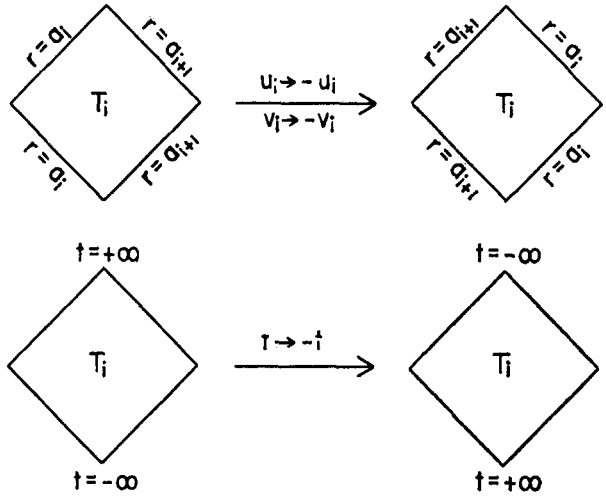

FIG. 4. The flipping of blocks.

GLUING BLOCKS TOGETHER

We now turn to the problem of extending geodesics which are incomplete in one block, or, equivalently, of gluing the blocks together along their nonsingular seams. [We have seen from Eq. (2) that all geodesics along which $r = a_i$ are incomplete.] Our convention for the resulting diagram is that the timelike coordinate in each block (t if $F > 0$, r if $F < 0$) change vertically. Consider the case of gluing T_{i+1} with $F > 0$ to T_i with $F < 0$. According to the convention, the blocks are as shown in Fig. 5.

Intuitively, by making use of the discrete isometry $t \to -t$, the blocks can be glued together in the two ways indicated by the arrows in Fig. 5. Since the intrinsic curvature is assumed to be a smooth function of r at $r = a_{i+1}$, showing that the blocks can be so glued reduces to showing that the null "cones" are continuous across the seams, i.e., that their exists a coordinate system covering both blocks in a neighborhood of $r = a_{i+1}$ in a smooth way. To do this, we use a patching technique discovered by Finkelstein.[3] Taking configuration 1 of Fig. 5 first, define $du = dt + dr/F$. Then $2\,du\,dr = 2\,dt\,dr + 2\,dr^2/F$ and

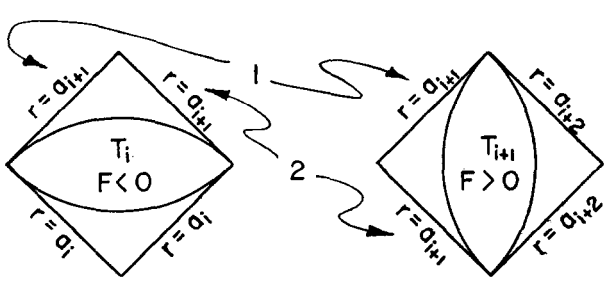

FIG. 5. Gluing blocks together: 1 and 2 indicate the two ways in which T_i may be glued to T_{i+1}, as discussed in the text. A representative pair of Killing vector orbits r = const is shown.

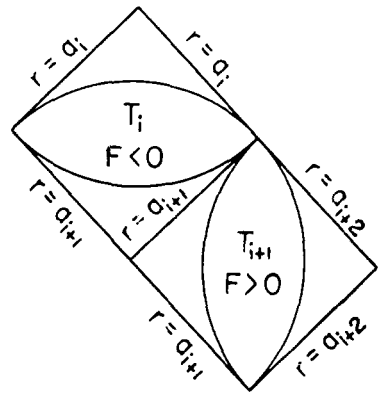

FIG. 6. T_i glued to T_{i+1} in configuration 1 of Fig. 5.

$F\,du^2 = F\,dt + 2\,dr\,dt + dr^2/F$, so that

$$ds^2 = F\,dt^2 - dr^2/F = F\,du^2 - 2\,du\,dr. \qquad (4)$$

Allowing r the range $a_i \leq r \leq a_{i+2}$,[11] we see that the coordinates (u, r) cover both blocks in configuration 1 of Fig. 6. The coordinate u is finite at $r = a_{i+1}$ and the metric (4) is C^∞ in the region $a_i < r < a_{i+2}$.

Defining in a similar way $dv = dt - dr/F$ so that

$$ds^2 = F\,dv^2 + 2\,dv\,dr, \qquad (5)$$

where v is finite at $r = a_{i+1}$, we see that metric (5) is C^∞ in the region $a_i < r < a_{i+2}$ also, but now the blocks have been glued together in configuration 2 of Fig. 7.

Performing both gluing operations simultaneously, we obtain Fig. 8. Because of the flip mentioned earlier, obtained by interchanging the roles of u_{i+1} and v_{i+1} in T_{i+1}, we can also glue in the dotted T_{i+1} of Fig. 8. The point labeled p in Fig. 8 is covered neither by the coordinates of Eq. (4) nor by those of Eq. (5). By making a further restriction on the function F, we are nevertheless able to include p by defining a coordinate system (originally found by Kruskal[4] in the case of the Schwarzschild solution) which covers all four blocks of Fig. 8 at once.

We ask for coordinates U and V such that $ds^2 = F\,dt^2 - dr^2/F = G\,dU\,dV$, where G is a function that

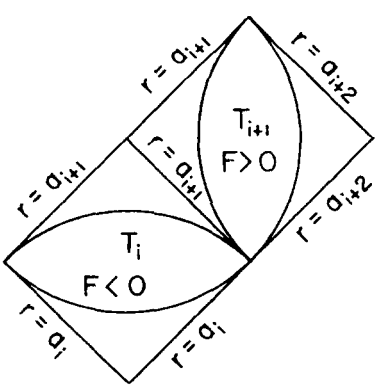

FIG. 7. T_i glued to T_{i+1} in configuration 2 of Fig. 5.

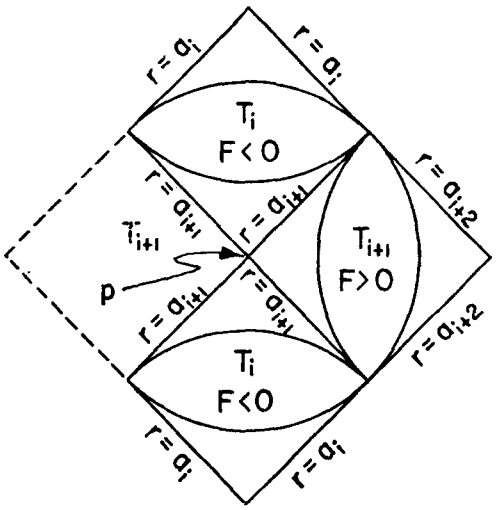

FIG. 8. Both gluing operations performed simultaneously. The point p is not covered by either coordinate system.

is finite and nonzero at $r = a_{i+1}$. Since $U = U(r, t)$ and $V = V(r, t)$, we must solve the equations

$$\begin{aligned} G\frac{\partial U}{\partial t}\frac{\partial V}{\partial t} &= F, \\ \frac{\partial U}{\partial r}\frac{\partial V}{\partial t} + \frac{\partial U}{\partial t}\frac{\partial V}{\partial r} &= 0, \\ G\frac{\partial U}{\partial r}\frac{\partial V}{\partial r} &= -\frac{1}{F}. \end{aligned} \tag{6}$$

Letting $U = R(r)T(t)$ and $V = \rho(r)\tau(t)$, we see that Eq. (6) separates with separation constants

$$\frac{dT}{dt}\frac{d\tau}{dt} = a \quad \text{and} \quad FG\frac{dR}{dr}\frac{d\rho}{dr} = \frac{1}{b}.$$

For later convenience, rescale the coordinates so that $b = 1$. Then with $a = c^2$ we find

$$\frac{1}{T}\frac{dT}{dt} = -\frac{1}{\tau}\frac{d\tau}{dt} = c \quad \text{and} \quad \frac{1}{R}\frac{dR}{dr} = \frac{1}{\rho}\frac{d\rho}{dr} = \frac{c}{F},$$

so that

$$R = \rho = \exp\left(c\int\frac{dr}{F}\right) \quad \text{and} \quad T = -\frac{1}{\tau} = \alpha e^{ct},$$

where α is a constant of integration. Hence, coordinates U and V and a function G satisfying (6) are given by

$$\begin{aligned} U &= \alpha e^{ct}\exp\left(c\int\frac{dr}{F}\right), \\ V &= -\frac{1}{\alpha}e^{-ct}\exp\left(c\int\frac{dr}{F}\right), \\ G &= \frac{F}{a}\exp\left(-2c\int\frac{dr}{F}\right). \end{aligned} \tag{7}$$

The problem therefore reduces to that of finding a suitable value for the constant c (by rescaling the coordinates) so that G is finite and nonzero at $r = a_{i+1}$. We show that this can indeed be done, provided F is of the form $H^{-1}(r - a_1)(r - a_2)\cdots(r - a_n)$, where H is a polynomial in r of degree n whose zeros (if any) are distinct from those of F. We write

$$\frac{1}{F} = H\left(\frac{\alpha_1}{r - a_1} + \frac{\alpha_2}{r - a_2} + \cdots + \frac{\alpha_n}{r - a_n}\right),$$

where

$$\alpha_j = (r - a_1)\cdots(r - a_{j-1}) \times (r - a_{j+1})\cdots(r - a_n)\big|_{r=a_j}.$$

Integrating by parts once, we obtain

$$\int\frac{dr}{F} = \ln(r - a_1)^{\alpha_1 H}(r - a_2)^{\alpha_2 H}\cdots(r - a_n)^{\alpha_n H} - \int\ln\left[(r - a_1)^{\alpha_1}(r - a_2)^{\alpha_2}\cdots(r - a_n)^{\alpha_n}\right]\frac{dH}{dr}\,dr.$$

Each subsequent integration by parts produces a higher derivative of H, so that after n such integrations by parts we find

$$dr/F = \ln\left[h(r - a_{i+1})^f + g\right],$$

where h, f, and g are polynomials in the $(r - a_j)$ and h and f do not have $(r - a_{i+1})$ as a factor. Hence,

$$G = a^{-1}(r - a_1)\cdots(r - a_i)(r - a_{i+1})^{(1-2cf)} \times (r - a_{i+2})\cdots(r - a_n)h^{-2c}e^{-2cg}$$

and, by choosing $c = [2f(a_{i+1})]^{-1}$, we obtain

$$G = a^{-1}(r - a_1)\cdots(r - a_i) \times (r - a_{i+2})\cdots(r - a_n)h^{-2c}e^{-2cg},$$

which is finite and nonzero for $r = a_{i+1}$ as required. In all of the cases which we consider, F will have the above polynomial form, so that the exceptional point p of Fig. 8 will be a regular point of the extensions constructed. Note, however, that the Kruskal technique for covering four blocks at once cannot be generalized in a simple way to give coordinates regularly covering more than four blocks, because of the way we had to choose the constant c of Eq. (7).

THE GENERAL CASE

Given the function F, the rules for constructing the maximal extension of T starting from any r value are now very simple:

(1) The timelike coordinate in each block changes vertically;

(2) The blocks are combined in all possible ways by joining them along nonsingular seams;

(3) The Gaussian curvature K must be smooth across the seam between any two blocks. Thus, a

block cannot be simply flipped and joined to itself, for example.

EXAMPLES

We illustrate the technique with three well-known examples and one which has not been given hitherto.

In the usual coordinates, the metric of the timelike 2-surfaces containing the repeated principal null directions in the Schwarzschild solution is

$$ds^2 = (1 - 2m/r)\,dt^2 - (1 - 2m/r)^{-1}\,dr^2$$

so that $F = 1 - 2m/r$ and $K = 2m/r^3$, $n = 1$, and $a_1 = 2m$; thus there are two blocks: T_1, bounded by $r = 2m$ and the singular seam at $r = 0$, and T_2, bounded by $r = 2m$ and null infinity (Fig. 9). Combining T_1 and T_2 according to the above rules, we obtain the Kruskal[4] diagram, with conformal infinity $\mathscr{I}$ represented by four finite null lines $\mathscr{I}_1^{\pm}$ and $\mathscr{I}_2^{\pm}$ (Fig. 10).

In the charged Schwarzschild or Reissner–Nordstrøm solution, the corresponding 2-surface T has metric

$$ds^2 = \left(1 - \frac{2m}{r} + \frac{e^2}{r^2}\right)dt - \left(1 - \frac{2m}{r} + \frac{e^2}{r^2}\right)^{-1} dr^2,$$

where e is the charge parameter. Suppose $m > e$; then $F = 1 - 2m/r + e^2/r^2$ has two real zeros at $r = m \pm (m^2 - e^2)^{\frac{1}{2}}$. The Gaussian curvature $K = (2mr - 3e^2)/r^4$, and there are three blocks. Combining them according to the rules, we obtain the usual diagram (Carter[6]) shown in Fig. 11.

Our third example is one in which T is nonsingular, namely, the symmetry axis of the Kerr solution which was analyzed by Carter.[2] Every geodesic in the maximally extended T is complete. In the coordinates used by Carter, we have $F = 1 - 2mr/(r^2 + a^2)$ and $K = 2mr(r^2 - 3a^2)(r^2 + a^2)^{-3}$, where a is the angular-momentum parameter. F has two zeros, provided $m > a$, at $r = m \pm (m^2 - a^2)^{\frac{1}{2}}$, so that there are three blocks. Combining them according to the rules, we obtain Fig. 12. F and K are plotted against r in Fig. 13.

Finally, we discuss briefly the "soluzioni oblique" of Levi-Civita,[12] which has been rediscovered by a number of authors[13] and is perhaps best known as the C metric of Ehlers and Kundt.[14] The C metric has been given in a coordinate system which lends

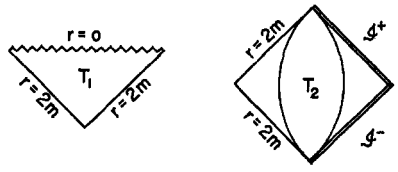

FIG. 9. The blocks for the Schwarzschild solution.

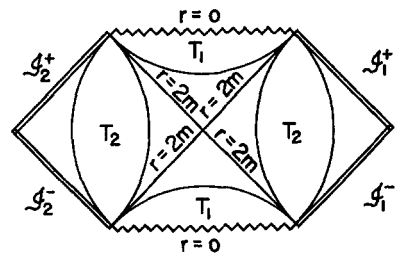

FIG. 10. The Kruskal diagram for the Schwarzschild solution with conformal infinity represented.

itself to the most straightforward analysis by Kinnersley[15]:

$$ds^2 = F\,du^2 + 2\,du\,dr + 2r^2\,du\,dx - dx^2/G - G\,dz^2.$$

Here, u is a null coordinate and r is an affine parameter along the repeated principal null rays, $G = mx^3 - ax - b$, and $F = m/r - Gr^2 + (dG/dx)r - 3mx$ where m, a, and b are constants. In order to ensure that spacelike cross sections of the null cone in the tangent space at each point are topologically 2-spheres, it is necessary to have $\frac{1}{4}b^2 < \frac{1}{27}a^3$ and also to restrict the range of x to $x_0 \leq x \leq x_1$ say, where x_0 and x_1 are determined by m, a, and b. This restriction on the range of x, together with the fact that a curvature singularity at $r = 0$ restricts r to $0 < r < \infty$, means that F has only one zero for each (fixed) value of x with $x_0 < x \leq x_1$. When $x = x_0$, F has no zeros.

The timelike 2-surface T containing the repeated principal null rays has metric $ds^2 = F\,du^2 + 2\,du\,dr$ and Gaussian curvature $K = 2m/r^3 - 2G$. T is

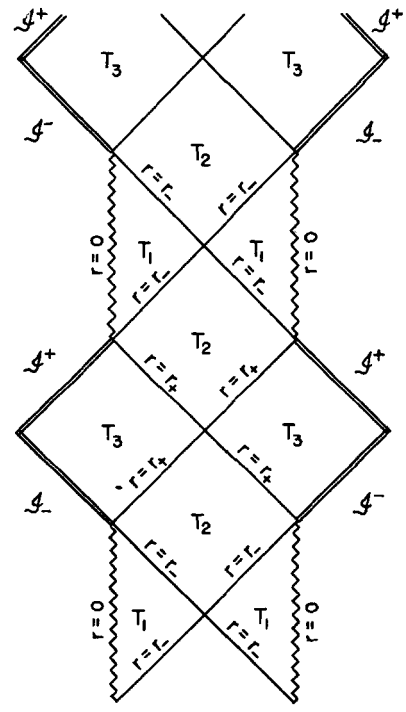

FIG. 11. The Reissner–Nordstrøm solution.

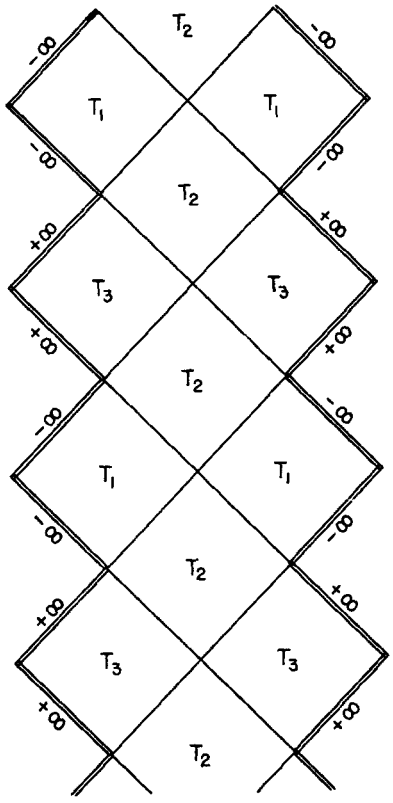

FIG. 12. The symmetry axis of the Kerr solution. Conformal infinities are labeled by $\pm\infty$ according to the value of r there.

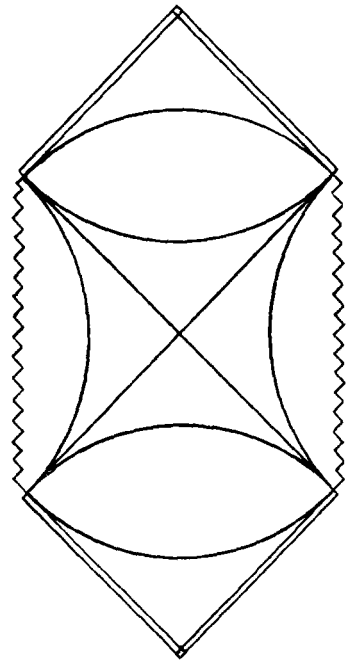

FIG. 14. The C metric.

totally geodesic only for null geodesics, and its asymptotic Gaussian curvature (as $r \to \infty$) depends on x. For these reasons, as well as for the reason that F has no zeros on the "south pole" of S at $x = x_0$, the block diagram for T must be interpreted with care; the diagram is given in Fig. 14. A complete account of the peculiar properties of the C metric will be given elsewhere.[16]

CONCLUSION

In conclusion, we remark briefly on the applicability of the extension technique for timelike 2-surfaces given here to the analysis of the global structure of the corresponding 4-dimensional space–times. Since T is totally geodesic, the topology of the inextendible space–time is $T \times S$ where S is the spacelike 2-surface orthogonal to T. Thus, in the Schwarzschild and Reissner–Nordstrøm solution, the space–time has topology $R^2 \times S^2$ because of the spherical symmetry, and we can think of each point of T as representing a 2-sphere whose radius is the r value at that point. In these two cases, the global properties of T exactly mirror those of the full space–time.

In the Kerr solution, however, this is not the case. There are incomplete, inextendible geodesics in the Kerr solution which do not lie in any totally geodesic timelike 2-surface. Nevertheless, it was by studying the symmetry axis that Carter[6] was able to guess at the complete global structure of the Kerr solution, and his guesses were borne out by the independent investigations of Boyer and Lindquist.[7]

The block diagrams are most useful in that they give a sound basis from which to begin a more detailed investigation of the space–time.

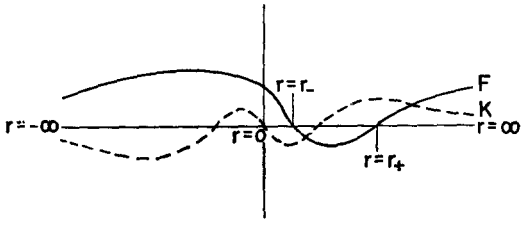

FIG. 13. F and K plotted against r for the Kerr solution; not to scale.

ACKNOWLEDGMENTS

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[1] By a solution of Einstein's equations we understand a Lorentz metric of appropriate signature defined (in general) on some open submanifold of an inextendible space–time. Global analysis is largely concerned with finding the inextendible space–time given only the metric components in some coordinate system. See R. P. Geroch, J. Math. Phys. **9**, 450 (1968).

[2] B. Carter, Phys. Rev. **141**, 1242 (1966).

[3] D. Finkelstein, Phys. Rev. **110**, 965 (1958).
[4] M. D. Kruskal, Phys. Rev. **119**, 1743 (1960).
[5] J. C. Graves and D. R. Brill, Phys. Rev. **120**, 1507 (1960).
[6] B. Carter, Phys. Letters **21**, 423 (1966).
[7] R. H. Boyer and R. W. Lindquist, J. Math. Phys. **8**, 265 (1967).
[8] A hypersurface in a space–time is totally geodesic if any geodesic tangent to the surface at a point lies in the surface.
[9] R. Penrose, Proc. Roy. Soc. (London) **A284**, 159 (1965).
[10] u_i and v_i are sometimes called advanced and retarded null coordinates, respectively.
[11] We could equally well let r take on its full range in Eq. (4), but it is more convenient for our purposes to restrict r to $a_i \leq r \leq a_{i+2}$.
[12] T. Levi-Civita, Atti Accad. Nazl. Lincei, Rend.,**27**(2), 343 (1918).
[13] E. T. Newman and L. A. Tamburino, J. Math. Phys. **2**, 667 (1961); P. Jordan, J. Ehlers, and W. Kundt, Akad. Wiss. Lit. (Mainz), Abhandl Math. Nat. Kl., No. 2 (1960).
[14] J. Ehlers and W. Kundt, *Gravitation, an Introduction to Current Research*, L. Witten, Ed. (Wiley, New York, 1963), p. 49.
[15] W. Kinnersley, J. Math. Phys. **10**, 1195 (1969).
[16] W. Kinnersley and M. Walker, submitted to Phys. Rev., 1970.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 11, NUMBER 8 AUGUST 1970

Classical and Quantum Mechanical Correlation Functions of Fields in Thermal Equilibrium*

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(Received 26 September 1969; Revised Manuscript Received 10 February 1970)

The two-point, two-time correlation functions of classical and quantum mechanical fields in thermal equilibrium in an arbitrary domain are considered. For classical fields that satisfy linear equations of motion, the correlation functions are expressed in terms of certain Green's functions of the domain. It is also shown, by evaluating the characteristic functional of the field, that a classical field is Gaussian distributed, so that all higher-order correlations can be expressed in terms of the second-order correlations. Then the second-order correlations are evaluated in various cases, and the classical and quantum mechanical results are compared. They are found to agree except within layers, about a thermal wavelength wide, near the boundaries of the domain and near the characteristic surface or light cone emanating from either of the two points. Thus the quantum mechanical correlation function can be approximated by the classical one with quantum-mechanical boundary-layer corrections.

1. INTRODUCTION

Classical statistical mechanics yields the Rayleigh–Jeans law for the power spectrum of a linear field in thermal equilibrium. This law differs from the Planck distribution of quantum statistical mechanics at high frequencies and yields an infinite energy density. As a result, classical statistical mechanics has not been used to calculate other properties of fields. But the Rayleigh–Jeans law agrees with the Planck law at low frequencies. Therefore, we should expect that classical and quantum statistical mechanics will yield approximately the same results for any property of a field which does not depend appreciably on the high-frequency components. Since the classical result is usually easier to calculate, it can be used as an approximation to the quantum result. In addition, the statistical properties of classical fields are of interest in themselves.

For these reasons, we calculate the classical characteristic functional of any field in thermal equilibrium satisfying linear equations of motion in an arbitrary domain. This functional is just the function-space Fourier transform of the Gibbs distribution. As is to be expected, it is a Gaussian functional, just as in the quantum mechanical case. Therefore, all the higher-order correlation functions of the field $u_i(\mathbf{x}, t)$ can be expressed in terms of the second-order or two-point, two-time correlation function $\langle u_i(\mathbf{x}, t)u_j(\mathbf{x}', t')\rangle$.

The second-order correlation can be expressed as a sum or integral over the modes of the field with amplitudes determined by the Rayleigh–Jeans law in the classical case and by the Planck law in the quantum case. In the classical case it also solves an initial-boundary-value problem and, therefore, it can be expressed in terms of two Green's functions. This representation exhibits the structure of the second-order correlation and also facilitates its calculation. We shall see that the quantum mechanical second-order correlation function satisfies a difference equation involving one of the same Green's functions.

To illustrate our results, we shall use them to calculate the second-order correlation function of a scalar field in various domains with different boundary conditions. The illustration applies to sound waves in three dimensions and to vibrating strings, sound waves, and electromagnetic waves in one dimension. For comparison we shall also calculate the correlation of the corresponding quantized boson field. We shall see that the two correlations are in close agreement except within layers about a thermal wavelength wide

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1. INTRODUCTION

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For these reasons, we calculate the classical characteristic functional of any field in thermal equilibrium satisfying linear equations of motion in an arbitrary domain. This functional is just the function-space Fourier transform of the Gibbs distribution. As is to be expected, it is a Gaussian functional, just as in the quantum mechanical case. Therefore, all the higher-order correlation functions of the field $u_i(\mathbf{x}, t)$ can be expressed in terms of the second-order or two-point, two-time correlation function $\langle u_i(\mathbf{x}, t)u_j(\mathbf{x}', t')\rangle$.

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To illustrate our results, we shall use them to calculate the second-order correlation function of a scalar field in various domains with different boundary conditions. The illustration applies to sound waves in three dimensions and to vibrating strings, sound waves, and electromagnetic waves in one dimension. For comparison we shall also calculate the correlation of the corresponding quantized boson field. We shall see that the two correlations are in close agreement except within layers about a thermal wavelength wide

near the boundaries of the domain and near the characteristic surface or light cone emanating from either of the two points at which the correlation is calculated. Therefore, we can approximate the quantum correlation function by the classical one with quantum mechanical boundary-layer corrections in these places.

For the quantized electromagnetic field in an unbounded domain, the second-order correlations have been found by Bourret,[1] Sarfatt,[2] Mehta and Wolf,[3] and others. Glauber[4] and Holliday[5] showed that this field is Gaussian. For the electromagnetic field in an arbitrary domain and for a scalar meson field obeying the Klein–Gordon equation, the quantum mechanical characteristic functionals were found by E. F. Keller[6] and also found to be Gaussian.

For a classical field satisfying nonlinear equations of motion, the characteristic functional and the second-order correlation have not been evaluated. The present results can be used to obtain a low-temperature expansion of them by means of Laplace's method applied to function-space integrals. E. A. Spiegel and I tried to use this idea to treat turbulence in an inviscid incompressible fluid, using Clebsch potentials to write the equations of fluid motion in Hamiltonian form. The Hamiltonian is homogeneous of degree four in the potentials, so Laplace's method is not applicable.

In Sec. 2 we express the characteristic functional of a classical linear field in thermal equilibrium in terms of the second-order correlation $\langle u_i u_j \rangle$. In Sec. 3 we obtain three different expressions for $\langle u_i u_j \rangle$ in the classical case. In Sec. 4 we give a representation for $\langle u_i u_j \rangle$ in the quantum case and also a difference equation for it. In Secs. 5–7 we apply our results to find $\langle u_i u_j \rangle$ in various special cases.

2. CHARACTERISTIC FUNCTIONAL OF A CLASSICAL FIELD

Let

$$q(\mathbf{x}, t) = [q_1(\mathbf{x}, t), \cdots, q_n(\mathbf{x}, t)]$$

and

$$p(\mathbf{x}, t) = [p_1(\mathbf{x}, t), \cdots, p_n(\mathbf{x}, t)]$$

be the coordinates and conjugate momenta of a classical field with Hamiltonian $H(q, p)$ defined in a domain D. Hamilton's equations of motion for the field are

$$q_{it} = \frac{\delta H}{\delta p_i}(\mathbf{x}, t), \quad p_{it} = -\frac{\delta H}{\delta q_i}(\mathbf{x}, t), \quad i = 1, \cdots, n. \tag{2.1}$$

We require that the field satisfy homogeneous boundary conditions on the boundary of D, which we shall not write explicitly, and the initial conditions

$$q(\mathbf{x}, 0) = q_0(\mathbf{x}), \quad p(\mathbf{x}, 0) = p_0(\mathbf{x}). \tag{2.2}$$

Now we suppose that (2.1), (2.2), and the boundary conditions determine q and p uniquely in terms of the initial data q_0 and p_0. It is convenient to introduce the $2n$-component vector $u(x, t) = [q(x, t), p(x, t)]$ and to write $H(q, p) = H(u)$ and $u_0 = [q_0, p_0]$.

If the field is in thermal equilibrium at temperature T, then its statistical properties are determined by the Gibbs distribution $e^{-\beta H(u_0)}(\int e^{-\beta H(u_0)} du_0)^{-1}$. Here $\beta = 1/kT$, where k is Boltzmann's constant. We now introduce the characteristic functional $F(\lambda)$, which is the function-space Fourier transform of the Gibbs distribution, defined by

$$F(\lambda) = \int \exp\left(i \int_{-\infty}^{\infty} \int_D \lambda(\mathbf{x}, t) \cdot u(\mathbf{x}, t)\, d\mathbf{x}\, dt - \beta H(u_0)\right) du_0 \times \left(\int e^{-\beta H(u_0)}\, du_0\right)^{-1}. \tag{2.3}$$

Here λ is a $2n$-component vector. One virtue of F is that, except for a power of i, its functional derivatives at $\lambda = 0$ are the correlation functions of the field, as we see from the following consequence of (2.3):

$$\frac{\delta^j F}{\delta\lambda_{i_1}(\mathbf{x}_1, t_1) \cdots \delta\lambda_{i_j}(\mathbf{x}_j, t_j)}\bigg|_{\lambda=0} = i^j \int u_{i_1}(\mathbf{x}_1, t_1) \cdots u_{i_j}(\mathbf{x}_j, t_j) e^{-\beta H(u_0)}\, du_0 \times \left(\int e^{-\beta H(u_0)}\, du_0\right)^{-1} \equiv i^j \langle u_{i_1}(\mathbf{x}_1, t_1) \cdots u_{i_j}(\mathbf{x}_j, t_j) \rangle. \tag{2.4}$$

The last equality in (2.4) defines the angular-bracket notation for the thermal average.

In general, it is difficult to determine F, but, for a field with a quadratic Hamiltonian, F can be obtained readily from (2.3), as we shall now show. First we write H in the form

$$H(u) = \tfrac{1}{2} \int_D uMu\, dx. \tag{2.5}$$

Here M is a self-adjoint operator with its domain defined to include only fields which satisfy the boundary conditions. Then $F(\lambda)$ is given by the following theorem, in which the summation convention is used.

Theorem 1: The characteristic functional (2.3) of a field with the quadratic Hamiltonian (2.5) is given by

$$F(\lambda) = \exp\left(-\tfrac{1}{2} \int_{-\infty}^{\infty} \int_D \int_{-\infty}^{\infty} \int_D \lambda_i(\mathbf{x}, t) \langle u_i(\mathbf{x}, t) u_j(\mathbf{x}', t') \rangle \lambda_j(\mathbf{x}', t')\, d\mathbf{x}'\, dt'\, d\mathbf{x}\, dt\right)$$

This result shows that the field is a Gaussian random function and that all its correlation functions are expressible in terms of its second-order or two-point, two-time correlation functions.

Theorem 1 can be proved by using the normal-mode representation of the field to evaluate the integrals in (2.3). However, we shall give a different proof which also yields an interesting expression for the two-point, two-time correlation function. First, by using (2.5) in (2.1), we find that the field satisfies the linear equations of motion

$$u_t = Lu. \tag{2.6}$$

Here L is defined by

$$L = JM, \tag{2.7}$$

where J is given in terms of the nth-order identity matrix I by

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{2.8}$$

The solution of the initial-value problem (2.6) and (2.2) can be written as

$$u = e^{tL}u_0. \tag{2.9}$$

By using (2.9), we can rewrite the exponent α of the numerator in (2.3). Then we replace e^{tL} acting on u_0 by its adjoint e^{tL^+} acting on λ to obtain

$$\begin{aligned}\alpha &\equiv i\int_{-\infty}^{\infty}\int_D \lambda \cdot e^{tL}u_0\, d\mathbf{x}\, dt - \beta H(u_0) \\ &= i\int_{-\infty}^{\infty}\int_D e^{-tL}\lambda \cdot u_0\, d\mathbf{x}\, dt - \beta H(u_0).\end{aligned} \tag{2.10}$$

We now change from the integration variable u_0 in the numerator of (2.3) to the new integration variable u^0 defined by $u_0(\mathbf{x}) = u^0(\mathbf{x}) + \mu(\mathbf{x})$, where $\mu(\mathbf{x})$ is a function to be chosen. Then (2.10) becomes

$$\begin{aligned}\alpha = i\int_D\int_{-\infty}^{\infty} e^{tL^+}\lambda \cdot (u^0 + \mu)\, dt\, d\mathbf{x} \\ - \beta\int_D u^0 M\mu\, d\mathbf{x} - \beta H(u^0) - \beta H(\mu).\end{aligned} \tag{2.11}$$

To complete the square in (2.11) by eliminating the terms linear in u^0, we choose for $\mu(\mathbf{x})$ the value

$$\mu(\mathbf{x}) = \frac{i}{\beta} M^{-1}\int_{-\infty}^{\infty} e^{tL^+}\lambda(\mathbf{x}, t)\, dt. \tag{2.12}$$

Now (2.11) becomes

$$\begin{aligned}\alpha = -\frac{1}{\beta}\int_D\int_{-\infty}^{\infty} e^{tL^+}\lambda(\mathbf{x}, t)\, dt \\ \times M^{-1}\int_{-\infty}^{\infty} e^{t'L^+}\lambda(\mathbf{x}, t')\, dt'\, d\mathbf{x} - \beta H(u^0) - \beta H(\mu).\end{aligned} \tag{2.13}$$

The first term on the right side of (2.13) is just $2\beta H(\mu)$, as we see from (2.12) and (2.5). Therefore, (2.13) can be written

$$\alpha = \beta H(\mu) - \beta H(u^0). \tag{2.14}$$

When (2.14) is used for the exponent in the numerator of (2.3), the integrals in the numerator and denominator become identical except for the factor $e^{\beta H(\mu)}$. Therefore, they cancel, leaving the result

$$F(\lambda) = e^{\beta H(\mu)}. \tag{2.15}$$

By using (2.12) in (2.5) and replacing e^{tL^+} acting on $\lambda(\mathbf{x}, t)$ by its adjoint acting on $\lambda(\mathbf{x}, t')$, we can write $\beta H(\mu)$ as

$$\begin{aligned}&\beta H(\mu) \\ &= -\frac{1}{2\beta}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_D \lambda(\mathbf{x}, t)e^{tL}M^{-1}e^{t'L^+}\lambda(\mathbf{x}, t')\, d\mathbf{x}\, dt\, dt' \\ &= -\frac{1}{2\beta}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_D \lambda(\mathbf{x}, t)e^{(t-t')L}M^{-1}\lambda(\mathbf{x}, t')\, d\mathbf{x}\, dt\, dt'.\end{aligned} \tag{2.16}$$

The last form of (2.16) results from the following sequence of identities:

$$\begin{aligned}e^{tL}M^{-1}e^{t'L^+} &= e^{tL}L^{-1}Je^{-t'MJ} = e^{tL}L^{-1}e^{-t'JM}J \\ &= e^{tL}e^{-t'L}L^{-1}J = e^{(t-t')L}M^{-1}.\end{aligned} \tag{2.17}$$

The second equality follows from the power series for the exponential.

We shall now represent the operator $e^{(t-t')L}M^{-1}$ in (2.16) as an integral operator with kernel $\beta R(\mathbf{x}, \mathbf{x}', t - t')$,

$$e^{(t-t')L}M^{-1}f(x) = \beta\int_D R(\mathbf{x}, \mathbf{x}', t - t')f(\mathbf{x}')\, d\mathbf{x}'. \tag{2.18}$$

Then by using (2.18) in (2.16) and (2.16) in (2.15), we obtain

$$\begin{aligned}F(\lambda) = \exp\Big(-\tfrac{1}{2}\int_{-\infty}^{\infty}\int_D\int_{-\infty}^{\infty}\int_D \lambda(\mathbf{x}, t)R(\mathbf{x}, \mathbf{x}', t - t') \\ \times \lambda(\mathbf{x}', t')\, d\mathbf{x}'\, dt'\, d\mathbf{x}\, dt\Big).\end{aligned} \tag{2.19}$$

Differentiating (2.19) with respect to $\lambda_i(\mathbf{x}, t)$ and $\lambda_j(\mathbf{x}', t')$ and then setting $\lambda = 0$ and using (2.4) yield

$$\begin{aligned}&\langle u_i(\mathbf{x}, t)u_j(\mathbf{x}', t')\rangle \\ &\quad = \tfrac{1}{2}[R_{ij}(\mathbf{x}, \mathbf{x}', t - t') + R_{ji}(\mathbf{x}', \mathbf{x}, t' - t)].\end{aligned} \tag{2.20}$$

Since only the symmetric part of R on the right side of (2.20) occurs in (2.19), we can use (2.20) to eliminate R from (2.19). In this way we obtain Theorem 1.

3. TWO-POINT, TWO-TIME CORRELATIONS OF A CLASSICAL FIELD

The two-point, two-time correlation function $u\langle_i(\mathbf{x}, t)u_j(\mathbf{x}', t')\rangle$ is given by (2.20) in terms of the

matrix R defined by (2.18). From (2.18) it follows that R can be written explicitly in the form

$$R(\mathbf{x}, \mathbf{x}', t - t') = \frac{1}{\beta} \int_D \Gamma(\mathbf{x}, \mathbf{y}, t - t') G(\mathbf{y}, \mathbf{x}')\, d\mathbf{y}. \tag{3.1}$$

Here G and Γ are the Green's matrices defined by

$$MG(\mathbf{x}, \mathbf{x}') = I\delta(\mathbf{x} - \mathbf{x}'), \tag{3.2}$$

$$\Gamma_t(\mathbf{x}, \mathbf{x}', t) = L\Gamma(\mathbf{x}, \mathbf{x}', t), \quad \Gamma(\mathbf{x}, \mathbf{x}', 0) = I\delta(\mathbf{x} - \mathbf{x}'). \tag{3.3}$$

To obtain another expression for R, we first set $t - t' = 0$ in (3.1) and use (3.3) to get

$$R(\mathbf{x}, \mathbf{x}', 0) = \beta^{-1} G(\mathbf{x}, \mathbf{x}'). \tag{3.4}$$

From (3.2) and the fact that $M^+ = M$, it follows that

$$G^{\mathrm{T}}(\mathbf{x}', \mathbf{x}) = G(\mathbf{x}, \mathbf{x}'). \tag{3.5}$$

Here the superscript T denotes the transposed matrix. Similarly from (3.3) we find after a little calculation that

$$\Gamma^{\mathrm{T}}(\mathbf{x}, \mathbf{x}', t) = -J\Gamma(\mathbf{x}', \mathbf{x}, -t)J. \tag{3.6}$$

Now we differentiate (3.6) with respect to t and use (3.3) and (2.7) to obtain

$$\begin{aligned} \Gamma_t^{\mathrm{T}}(\mathbf{x}, \mathbf{y}, t) &= J\Gamma_t(\mathbf{y}, \mathbf{x}, -t)J = JL\Gamma(\mathbf{y}, \mathbf{x}, -t)J \\ &= -M\Gamma(\mathbf{y}, \mathbf{x}, -t)J. \end{aligned} \tag{3.7}$$

We note that, in (3.7), L and M operate on the variable $\mathbf{y}$. Next we differentiate (3.1) with respect to t, use (3.7), replace M acting on Γ by $M^+ = M$ acting on G, and use (3.2) and (3.7) to obtain

$$\begin{aligned} R_t(\mathbf{x}, \mathbf{x}', t) &= \frac{1}{\beta} \int_D \Gamma_t(\mathbf{x}, \mathbf{y}, t) G(\mathbf{y}, \mathbf{x}')\, d\mathbf{y} \\ &= \frac{J}{\beta} \int_D [M\Gamma(\mathbf{y}, \mathbf{x}, -t)]^{\mathrm{T}} G(\mathbf{y}, \mathbf{x}')\, d\mathbf{y} \\ &= \frac{J}{\beta} \int_D \Gamma^{\mathrm{T}}(\mathbf{y}, \mathbf{x}, -t) MG(\mathbf{y}, \mathbf{x}')\, d\mathbf{y} \\ &= \beta^{-1} J\Gamma^{\mathrm{T}}(\mathbf{x}', \mathbf{x}, -t) \\ &= \beta\Gamma(\mathbf{x}, \mathbf{x}', t)J. \end{aligned} \tag{3.8}$$

Finally, we integrate (3.8) with respect to t and use (3.5) to get

$$R(\mathbf{x}, \mathbf{x}', t - t') = \beta^{-1} G(\mathbf{x}, \mathbf{x}') + \beta^{-1} \int_0^{t-t'} \Gamma(\mathbf{x}, \mathbf{x}', s)\, ds\, J. \tag{3.9}$$

From (3.9) we find, by using (3.5) and (3.6), that

$$R^{\mathrm{T}}(\mathbf{x}', \mathbf{x}, t' - t) = R(\mathbf{x}, \mathbf{x}', t - t'). \tag{3.10}$$

This fact and (2.20) show that

$$\langle u_i(\mathbf{x}, t) u_j(\mathbf{x}', t') \rangle = R_{ij}(\mathbf{x}, \mathbf{x}', t - t'). \tag{3.11}$$

Another expression for R can be obtained by using the normal modes of the field. To obtain it, we assume that $p(\mathbf{x}, t)$ can be calculated from $q(\mathbf{x}, t)$, and we shall deal only with q. Then we introduce the complete set of complex normal modes $v_s(\mathbf{x})$, which are n-component vectors and the corresponding eigenfrequencies ω_s, $s = 1, 2, \cdots$. In terms of them the field $q(x, t)$ can be written

$$\begin{aligned} q(\mathbf{x}, t) = \tfrac{1}{2} \sum_{s=1}^{\infty} \omega_s^{-\frac{1}{2}} \{ &[P_s(t) + iQ_s(t)] v_s(\mathbf{x}) \\ &+ [P_s(t) - iQ_s(t)] v_s^*(\mathbf{x}) \}. \end{aligned} \tag{3.12}$$

Here Q_s and P_s are the coordinate and momentum of mode s. The modes are assumed to be orthogonal with respect to M and so normalized that the Hamiltonian (2.5) takes the form

$$H = \tfrac{1}{2} \sum_{s=1}^{\infty} \omega_s (P_s^2 + Q_s^2). \tag{3.13}$$

Then the equations of motion for P_s and Q_s are $P_{st} = \omega_s Q_s$ and $Q_{st} = -\omega_s P_s$, which yield

$$P_s(t) + iQ_s(t) = [P_s(0) + iQ_s(0)] e^{i\omega_s t}. \tag{3.14}$$

We now use (3.12)–(3.14) in the integral in (2.4) which defines $\langle u_i(\mathbf{x}, t) u_j(\mathbf{x}', t') \rangle$. The integration is taken over $P_s(0)$ and $Q_s(0)$, and it can be performed explicitly with the result

$$\begin{aligned} R_{ij}(\mathbf{x}, \mathbf{x}', t - t') &= \langle q_i(\mathbf{x}, t) q_j(\mathbf{x}', t') \rangle \\ &= \frac{1}{\beta} \sum_{s=1}^{\infty} \omega_s^{-2} \operatorname{Re} [v_{si}(\mathbf{x}) v_{sj}^*(\mathbf{x}') e^{i\omega_s(t-t')}], \\ &\qquad i, j = 1, \cdots, n. \end{aligned} \tag{3.15}$$

Here v_{si} denotes component i of v_s and * denotes the complex conjugate.

We shall state the results of this section as a theorem.

Theorem 2: The second-order correlation matrix $R(\mathbf{x}, \mathbf{x}', t - t') = \langle u(\mathbf{x}, t) u(\mathbf{x}', t') \rangle$ is given by (3.1) or (3.9). It is the solution of the initial-value problem $R_t = LR$, $R(\mathbf{x}, \mathbf{x}', 0) = \beta^{-1} G(\mathbf{x}, \mathbf{x}')$. The correlation matrix $\langle q_i q_j \rangle$ is also given by (3.15).

4. TWO-POINT, TWO-TIME CORRELATIONS OF A QUANTUM MECHANICAL FIELD

Theorem 1 also applies to a quantum mechanical boson field. [See Ref. 6, Eq. (22).] However, the two-point, two-time correlation function differs from the classical one. In the quantum mechanical case, $q_i(\mathbf{x}, t)$ and $q_j(\mathbf{x}', t')$ are possibly noncommuting operators, and the expectation value of their product may

not be real. Therefore, we define the correlation function $R_{ij}^{\text{q.m.}}$ to be the thermal expectation of one-half the anticommutator of the two operators, which is real. Then we use Eq. (20) of Ref. 6, with q instead of A, with $c = 1$, and with v_i replaced by $v_{si}e^{i\omega_s t}$, to obtain in our notation

$$R_{ij}^{\text{q.m.}}(\mathbf{x}, \mathbf{x}', t - t')$$
$$\equiv \tfrac{1}{2}\langle q_i(\mathbf{x}, t)q_j(\mathbf{x}', t') + q_j(\mathbf{x}', t')q_i(\mathbf{x}, t)\rangle$$
$$= \hbar\sum_{s=1}^{\infty}[(e^{\beta\hbar\omega_s} - 1)^{-1} + \tfrac{1}{2}]\omega_s^{-1}\,\text{Re}\,[v_{si}(\mathbf{x})v_{sj}^*(\mathbf{x}')e^{i\omega_s(t-t')}],$$
$$i = 1, \cdots, n. \quad (4.1)$$

In view of the symmetric form of the integral defining $F(\lambda)$ in Eq. (22) of Ref. 6, only this anticommutator occurs in it. We see from (4.1) that, as $\hbar$ tends to zero, the limit of $R_{ij}^{\text{q.m.}}$ is R_{ij} given by (3.15).

We shall now obtain an interesting alternative characterization of $R^{\text{q.m.}}$ for a boson or a fermion field. First we write

$$R^{\text{q.m.}}(\mathbf{x}, t, \mathbf{x}', t')$$
$$= \tfrac{1}{2}[\rho(\mathbf{x}, \mathbf{x}', t - t') \pm \rho^{\text{T}}(\mathbf{x}', \mathbf{x}, t' - t)]. \quad (4.2)$$

Here and below the upper sign applies to bosons and the lower sign to fermions, ρ^{T} denotes the transpose of the matrix ρ, and ρ is defined in terms of the operator u by

$$\rho(\mathbf{x}, \mathbf{x}', t - t') = \text{Tr}\,[e^{-\beta H}u(\mathbf{x}, t)u(\mathbf{x}', t')]/\text{Tr}\,e^{-\beta H}. \quad (4.3)$$

The operator H is the Hamiltonian, which is a scalar. The fact that ρ depends on $t - t'$ can be proved from (4.3) by rewriting the numerator of (4.3) as follows and using the invariance of the trace under cyclic permutation:

$$\text{Tr}\,[e^{-\beta H}e^{i\hbar^{-1}tH}u(\mathbf{x}, 0)e^{-i\hbar^{-1}tH}e^{i\hbar^{-1}t'H}u(x', 0)e^{-\hbar^{-1}t'H}$$
$$= \text{Tr}\,[e^{-\beta H}e^{i\hbar^{-1}(t-t')H}u(\mathbf{x}, 0)e^{-i\hbar^{-1}(t-t')}u(\mathbf{x}', 0)]. \quad (4.4)$$

The commutation relations for the field operators can be written succinctly in the form

$$u(\mathbf{x}, t)u(\mathbf{x}', t') \mp [u(\mathbf{x}, t)u(\mathbf{x}', t')]^{\text{T}} = i\hbar\Gamma(\mathbf{x}, \mathbf{x}', t - t')J. \quad (4.5)$$

It is clear that (4.5) holds when $t = t'$, and it can be proved for $t \neq t'$ by applying $\partial/\partial t - L$ to both sides and noting that both sides vanish because of (2.6) and (3.3). Upon taking the thermal average of (4.5), we obtain

$$\rho(\mathbf{x}, \mathbf{x}', t - t') \mp \rho^{\text{T}}(\mathbf{x}', \mathbf{x}, t' - t) = i\hbar\Gamma(\mathbf{x}, \mathbf{x}', t - t')J. \quad (4.6)$$

Another relation satisfied by ρ can be obtained by writing (4.3) in the form

$$\rho^{\text{T}}(\mathbf{x}, \mathbf{x}', t - t')$$
$$= \text{Tr}\,[e^{-\beta H}e^{\beta H}u(\mathbf{x}', t')e^{-\beta H}u(\mathbf{x}, t)]/\text{Tr}\,e^{-\beta H}$$
$$= \text{Tr}\,[e^{-\beta H}u(\mathbf{x}', t' - i\beta\hbar)u(\mathbf{x}, t)]/\text{Tr}\,e^{-\beta H}$$
$$= \rho(\mathbf{x}', \mathbf{x}, t' - t - i\beta\hbar). \quad (4.7)$$

By combining (4.6) and (4.7) we obtain the following result:

Theorem 3: The quantum mechanical second-order correlation $R^{\text{q.m.}}(\mathbf{x}, t, \mathbf{x}', t')$ of a boson or fermion field with the quadratic Hamiltonian (2.5) is given by (4.2) with ρ determined by the difference equation

$$\rho(\mathbf{x}, \mathbf{x}', t - t') \mp \rho(\mathbf{x}, \mathbf{x}', t - t' - i\beta\hbar) = i\hbar\Gamma(\mathbf{x}, \mathbf{x}', t - t')J. \quad (4.8)$$

If we take the upper sign, divide both sides of (4.8) by $-i\beta\hbar$, and let $\hbar$ tend to zero, we obtain the classical result (3.8), since R is the limit of ρ in the boson case.

5. CORRELATION OF A SCALAR WAVE IN THREE DIMENSIONS

We shall now apply Theorem 2 to obtain the two-point, two-time correlation function of a scalar field q satisfying the wave equation in an unbounded 3-dimensional domain

$$\Delta q - c^{-2}q_{tt} = 0. \quad (5.1)$$

The field q could be the velocity potential of an acoustic wave or could have various other interpretations. In this case $p = c^{-1}q_t$, and so it suffices to determine the two-point correlation of q. By symmetry it depends only upon the distance $r = |\mathbf{x} - \mathbf{x}'|$ and the time difference $\tau = c\,|t - t'|$; thus we write

$$R(r, \tau) = \langle q(\mathbf{x}, t)q(\mathbf{x}', t')\rangle. \quad (5.2)$$

In Appendix A we show, by using Theorem 2, that

$$R(r, \tau) = 1/4\pi\beta r, \quad \tau < r,$$
$$= 0, \quad \tau > r. \quad (5.3)$$

The corresponding result for a quantum mechanical scalar boson field, omitting a vacuum fluctuation term which is singular when $r = \tau$, is given by Eq. (5.6) of Ref. 6. When a factor 16 is corrected to be 8, the result is

$$R^{\text{q.m.}}(r, \tau) = \frac{1}{8\pi\beta r}\left[L\left(\frac{\pi}{\hbar\beta c}(r + \tau)\right) + L\left(\frac{\pi}{\hbar\beta c}(r - \tau)\right)\right]. \quad (5.4)$$

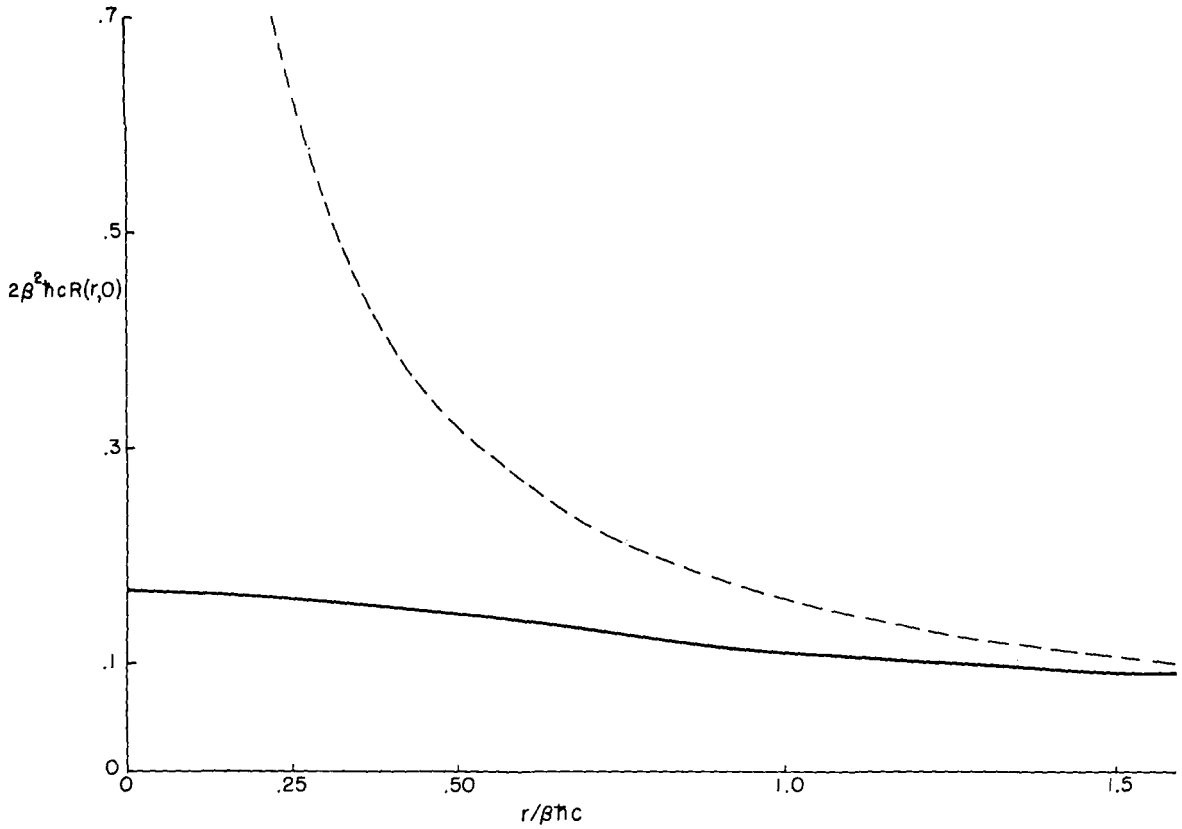

FIG. 1. Comparison between the simultaneous two-point correlation functions of a 3-dimensional scalar classical field and a scalar quantum mechanical boson field both satisfying the wave equation (5.1). The classical correlation $R(r, 0)$ (dashed line) is given by (5.3) and the quantum mechanical correlation $R^{q.m.}(r, 0)$ (solid line) is given by (5.4) with $\tau = 0$. The abscissa is $r/\beta\hbar c$ where r is the distance between the two points.

Here L is the Langevin function

$$L(s) = \coth s - s^{-1}. \tag{5.5}$$

When $\pi(r + \tau)/\hbar\beta c$ and $\pi(r - \tau)/\hbar\beta c$ are both large and positive, both L's are approximately unity and $R^{q.m.}$ is approximately R given by (5.3). When $\pi(r - \tau)/\hbar\beta c$ is large and negative, the second L is nearly -1 and $R^{q.m.}$ is nearly zero, in agreement with (5.3). The difference between $R^{q.m.}$ and R is appreciable only within a thermal wavelength $\beta\hbar c$ or so of the light cone $r = \tau$, and it decreases exponentially with distance from the cone. Therefore, $R^{q.m.}$ can be approximated by R except in this layer (see Fig. 1).

6. CLASSICAL CORRELATION OF A SCALAR WAVE IN ONE DIMENSION

If q satisfies (5.1) in one dimension, an analysis similar to the foregoing yields

$$R(r, \tau) = R(0, 0) - r/2\beta, \quad \tau < r, \tag{6.1}$$

$$R(r, t) = R(0, 0) - \tau/2\beta, \quad \tau > r. \tag{6.2}$$

The constant $R(0, 0)$ is undetermined because G is determined only within an additive constant. These results (6.1) and (6.2) apply to a transverse component of the vector potential of an electromagnetic field, to the velocity potential of an acoustic wave, etc. In these cases the physical quantities are first derivatives of the potentials and the correlation of two physical quantities is a second derivative of R. Therefore, it is a δ function, vanishing except on the light cone $r = \tau$, where it is singular, and the arbitrariness of $R(0, 0)$ is of no significance. However, if q represents the transverse or longitudinal displacement of an elastic string, R itself is meaningful. But since the string is not tied down anywhere, it is not surprising that $R(0, 0)$ is undetermined.

To eliminate the arbitrariness of $R(0, 0)$, let us consider a semi-infinite string fixed at its end point $x = 0$. Thus we assume that $q(x, t)$ satisfies (5.1) for $x > 0$ and that $q(0, t) = 0$. Then $G(x, x')$ satisfies $G_{xx} = -\delta(x - x')$ and $G(0, x') = 0$. Therefore,

$$G(x, x') = x$$

for $0 \leq x \leq x'$ and $G(x, x') = x'$ for $x \geq x'$, assuming that G is bounded. We now solve the wave equation for R with the initial value $\beta^{-1}G$, where $R_\tau = 0$

initially because R is even in τ and where $R = 0$ at $x = 0$. We readily find that

$$\begin{aligned} R(x, x', \tau) &= x/\beta, \quad 0 \le x \le x' - \tau, && \text{(I)} \\ &= x'/\beta, \quad x \ge x' + \tau, && \text{(I')} \\ &= 0, \quad 0 \le x \le \tau - x', && \text{(III)} \\ &= (x + x' - \tau)/2\beta, \\ &\quad |x' - \tau| \le x \le x' + \tau. && \text{(II)} \end{aligned} \tag{6.3}$$

The numbered regions are shown in Fig. 2.

From (6.3) we see that $R(x, x, 0) = x/\beta$; thus, the mean-square value of $q(x, t)$ increases linearly with the distance from the end point $x = 0$. The two-point correlation at one time $R(x, x', 0)$ is given by x/β for $0 \le x \le x'$ and by x'/β for $x \ge x'$. The two-time correlation at one point $R(x, x, \tau)$ is given by $(2x - \tau)/2\beta$ for $\tau \le 2x$ and by zero for $\tau \ge 2x$. The remarks above, about the vanishing of correlations of physical quantities which are derivatives of q, also apply here since R is piecewise linear.

Next we shall consider a solution of (5.1) in the 1-dimensional finite interval of length L with the boundary conditions

$$q(0, t) = q(L, t) = 0. \tag{6.4}$$

To illustrate the use of (3.15), we shall use it to find R. The normalized modes and eigenfrequencies of (5.1) and (6.4) are

$$\begin{aligned} v_s(x) &= (2/L)^{\frac{1}{2}} \sin(s\pi x/L), \\ \omega_s &= s\pi c/L, \quad s = 1, 2, \cdots. \end{aligned} \tag{6.5}$$

When (6.5) is used in (3.15), the result is

$$\begin{aligned} &R(x, x', \tau) \\ &= \frac{2L}{\pi^2\beta} \sum_{s=1}^{\infty} s^{-2} \sin\left(\frac{s\pi x}{L}\right) \sin\left(\frac{s\pi x'}{L}\right) \cos\left(\frac{s\pi\tau}{L}\right) \\ &= \frac{L}{2\pi^2\beta} \sum_{s=1}^{\infty} s^{-2} \left[\cos\left(\frac{s\pi(x - x' + \tau)}{L}\right)\right. \\ &\quad + \cos\left(\frac{s\pi(x - x' - \tau)}{L}\right) \\ &\quad \left. - \cos\left(\frac{s\pi(x + x' + \tau)}{L}\right) - \cos\left(\frac{s\pi(x + x' - \tau)}{L}\right)\right]. \end{aligned} \tag{6.6}$$

We see that R is periodic in τ with period $2L$, so that it suffices to determine it in one period.

To evaluate the sum in (6.6), we use the identity

$$\begin{aligned} \sum_{s=1}^{\infty} s^{-2} \cos sz' &= \tfrac{1}{6}\pi^2 - \tfrac{1}{2}\pi z + \tfrac{1}{4}z^2, \\ z &= z' \bmod 2\pi, \quad 0 \le z \le 2\pi. \end{aligned} \tag{6.7}$$

When we use (6.7), we obtain different analytic expressions for R in different regions of (x, x', τ) space. In Fig. 3, six numbered regions of the (x, τ) plane are shown. The value of R in each region is given in the following list:

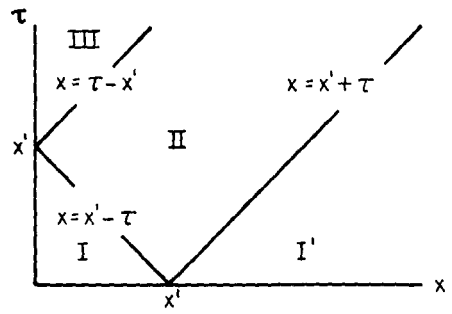

FIG. 2. Three numbered regions of the positive quadrant of the (x, τ) plane are shown for a fixed value of x'. The inequalities defining these regions are given in (6.3).

$$\begin{aligned} R(x, x', \tau) &= x(L - x')/\beta L, \quad \text{in I}, \\ &= x'(L - x)/\beta L, \quad \text{in I}', \\ &= -xx'/\beta L, \quad \text{in III}, \\ &= -(L - x)(L - x')/\beta L, \quad \text{in III}', \\ &= [x(L - x') + x'(L - x) - L\tau]/2\beta L, \\ &\qquad \text{in II}, \\ &= [x(L - x') + x'(L - x) \\ &\quad - L(2L - 2\tau)]/2\beta L, \quad \text{in IV}. \end{aligned} \tag{6.8}$$

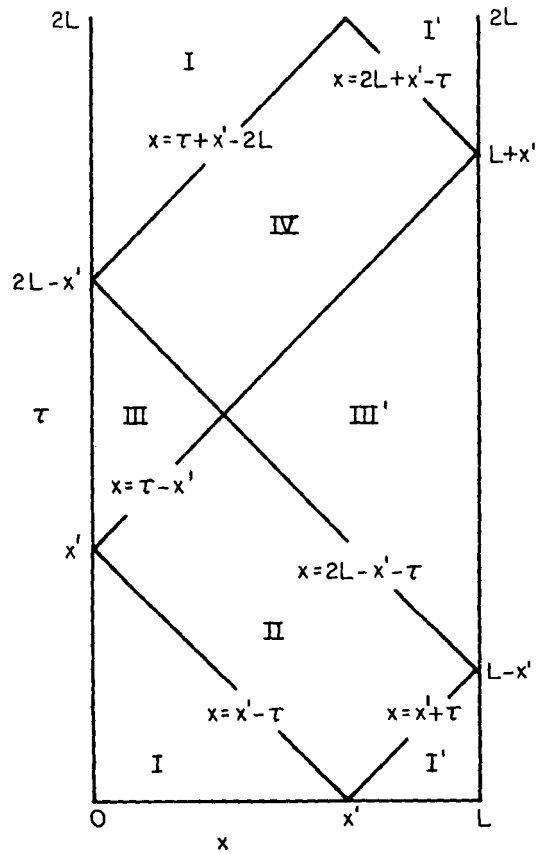

FIG. 3. Six numbered regions of the strip $0 \le x \le L, 0 \le \tau < 2L$ in the (x, τ) plane are shown for a fixed value of x'. The slanting lines bounding these regions are characteristics with slope $+1$ or -1.

This function is continuous and has discontinuities in its first derivatives on the characteristics separating the various regions. The result (6.3) for the semi-infinite domain and the results (6.1) and (6.2) for the infinite domain can be obtained from (6.8) by letting L become infinite, with one or no end points fixed. The mean-square value of $q(x, t)$ is, from (6.8),

$$R(x, x, 0) = x(L - x)/\beta L. \tag{6.9}$$

Thus it varies quadratically from zero at the end points to a maximum of $L/4\beta$ at the midpoint. This result is of interest for the thermal oscillation of a string of length L fixed at its end points.

The case $q_x = 0$ at the end points is treated in Appendix B.

7. QUANTUM MECHANICAL CORRELATION OF A SCALAR WAVE IN ONE DIMENSION

Let us repeat the preceding calculations for a quantum mechanical scalar boson field satisfying (5.1) and (6.4). Then the eigenfunctions and eigenvalues are again given by (6.5), and (4.1) becomes

$$R^{\text{q.m.}}(x, x', \tau) = \frac{2c\hbar}{\pi}\sum_{k=1}^{\infty}[(e^{k\beta\hbar\pi c/L} - 1)^{-1} + \tfrac{1}{2}]k^{-1} \times \sin\left(\frac{k\pi x}{L}\right)\sin\left(\frac{k\pi x'}{L}\right)\cos\left(\frac{k\pi\tau}{L}\right). \tag{7.1}$$

From (7.1) we see that $R^{\text{q.m.}}$ is symmetric in x and x' and even and periodic in τ.

The most essential features of $R_{\text{q.m.}}$ will be retained, and the analysis will be simplified, if we let L become infinite in (7.1). In this case the interval becomes semi-infinite. Then the sum in (7.1) becomes an integral, and we obtain

$$R^{\text{q.m.}}(x, x', \tau) = \frac{2c\hbar}{\pi}\int_0^{\infty}[(e^{\alpha\beta\hbar c} - 1)^{-1} + \tfrac{1}{2}]\alpha^{-1}\sin\alpha x\sin\alpha x'\cos\alpha\tau\, d\alpha. \tag{7.2}$$

The integral (7.2) is the sum of a vacuum fluctuation term $R_1^{\text{q.m.}}$, which has just $\frac{1}{2}$ in the bracket, and the main part $R_0^{\text{q.m.}}$ in which the $\frac{1}{2}$ is omitted. In Appendix C we evaluate $R_0^{\text{q.m.}}$ and $R_1^{\text{q.m.}}$ with the result

$$R^{\text{q.m.}} = R_0^{\text{q.m.}} + R_1^{\text{q.m.}} = \frac{\hbar c}{4\pi}\log\left|\frac{\sinh(\pi|x + x' + \tau|/\beta\hbar c)\sinh(\pi|x + x' - \tau|/\beta\hbar c)}{\sinh(\pi|x - x' + \tau|/\beta\hbar c)\sinh(\pi|x - x' - \tau|/\beta\hbar c)}\right|. \tag{7.3}$$

Since $R_1^{\text{q.m.}}$ becomes infinite when any of the four absolute values in (7.3) vanishes, (7.3) is not then valid. This occurs on the light cones shown in Fig. 2, which separate the various regions.

The mean-square value of $q(x, t)$ is given by setting $x' = x$ and $\tau = 0$ in $R^{\text{q.m.}}(x, x', \tau)$. From (C4) we find

$$R_0^{\text{q.m.}}(x, x, 0) = \frac{\hbar c}{2\pi}\log\left|\frac{\sinh(2\pi x/\beta\hbar c)}{2\pi x/\beta\hbar c}\right|. \tag{7.4}$$

The vacuum fluctuation term $R_1^{\text{q.m.}}(x, x', \tau)$ is singular at $x = x'$ and $\tau = 0$. For $2\pi x/\beta\hbar c$ large, (7.4) yields

$$R_0^{\text{q.m.}}(x, x, 0) \sim \frac{x}{\beta} - \frac{\hbar c}{2\pi}\log\frac{4\pi x}{\beta\hbar c} + \cdots. \tag{7.5}$$

Since $R(x, x, 0) = x/\beta$, Eq. (7.5) shows that the classical and quantum mechanical results agree, except for a term of order $\hbar$, as $2\pi x/\beta\hbar c$ increases. Since the coefficient of this $\hbar$ term increases as x increases, the difference is not uniformly small for all x, although it is a small fraction of the leading term. This is shown clearly in Fig. 4.

The case $q_x = 0$ at the end points is treated in Appendix C.

ACKNOWLEDGMENTS

I wish to thank Dr. K. Symanzik and Dr. D. Ludwig for their suggestions, which simplified some of the calculations.

APPENDIX A: DETERMINATION OF R FOR A SCALAR FIELD

From (5.1) and (5.2), R satisfies the wave equation; thus it is of the form

$$R(r, \tau) = r^{-1}[f(r - \tau) + g(r + \tau)]. \tag{A1}$$

Since R is even in τ, $g = f + b$, where b is a constant which can be set equal to zero without loss of generality.

To use Theorem 2, we note that in the present case

$$H(u) = \tfrac{1}{2}\int_D [(\nabla q)^2 + c^{-2}q_t^2]\, d\mathbf{x} = \tfrac{1}{2}\int_D (-q\Delta q + p^2)\, d\mathbf{x}. \tag{A2}$$

Therefore, $M = \text{diag}\,(-\Delta, 1)$ and $G = \text{diag}\,[1/4\pi r, \delta(\mathbf{x} - \mathbf{x}')]$, so that

$$R(r, 0) = 1/4\pi\beta r. \tag{A3}$$

Now (A1) and (A3) yield $2f(r) = 1/4\pi\beta$ for $r > 0$.

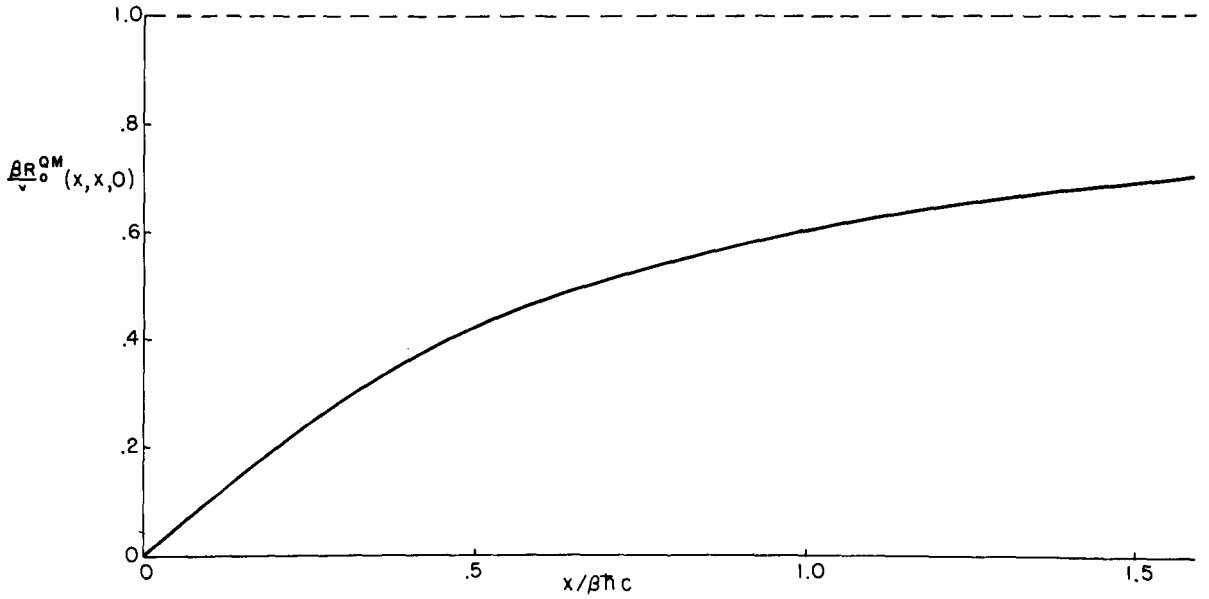

FIG. 4. The mean-square value of a 1-dimensional scalar field satisfying the wave equation (5.1) in a semi-infinite region, as a function of the distance x from the boundary. The classical value $R(x, x, 0)$ (dashed line) is given by (6.3) and the quantum mechanical value for a boson field, $R_0^{q\cdot m\cdot}(x, x, 0)$ (solid line), is given by (7.4). The ordinate is $\beta R_0^{q\cdot m\cdot}(x, x, 0)/x$ which is unity in the classical case, and the abscissa is $x/\beta\hbar c$.

Then (A1) can be written

$$R(r, \tau) = 1/4\pi\beta r, \quad \tau < r. \tag{A4}$$

For $|\tau| \neq 0$, we require that R be finite. By using this condition in (A1), we obtain

$$f(-\tau) + g(\tau) = 0, \quad \tau > 0. \tag{A5}$$

Since, for $\tau > 0$, $g = f = 1/8\pi\beta$, (A5) yields $f(-\tau) = -1/8\pi\beta$ for $\tau > 0$. Then (A1) gives

$$R(r, \tau) = 0, \quad \tau > r. \tag{A6}$$

Equations (A3) and (A6) determine $R(r, \tau)$ completely and yield (5.3).

APPENDIX B: R FOR A SCALAR FIELD WITH $q_x = 0$ AT THE END POINTS

Now we shall consider (5.1) again, but with the boundary conditions

$$q_x(0, t) = q_x(L, t) = 0. \tag{B1}$$

In this case the normalized eigenfunctions and eigenvalues are

$$v_0 = L^{-\frac{1}{2}}, \quad \omega_0 = 0, \quad v_s = (2/L)^{\frac{1}{2}} \cos(s\pi x/L),$$
$$\omega_s = s\pi c/L, \quad s = 1, 2, \cdots. \tag{B2}$$

In the derivation of (3.15), it was assumed that $\omega_s \neq 0$, for otherwise the integral diverges. Therefore, we shall omit the mode v_0 with frequency zero. Then (3.15) becomes

$$\begin{aligned} R(x, x', \tau) &= \frac{2L}{\pi^2\beta} \sum_{s=1}^{\infty} s^{-2} \cos\left(\frac{s\pi x}{L}\right) \cos\left(\frac{s\pi x'}{L}\right) \cos\left(\frac{s\pi\tau}{L}\right) \\ &= \frac{L}{2\pi^2\beta} \sum_{s=1}^{\infty} s^{-2} \left[\cos\left(\frac{s\pi(x + x' + \tau)}{L}\right)\right. \\ &\quad + \cos\left(\frac{s\pi(x - x' + \tau)}{L}\right) \\ &\quad \left. + \cos\left(\frac{s\pi(x - x' - \tau)}{L}\right) + \cos\left(\frac{s\pi(x + x' - \tau)}{L}\right)\right]. \end{aligned} \tag{B3}$$

Proceeding as before, we find the following, with the regions shown in Fig. 3:

$$\begin{aligned} R(x, x', \tau) &= \left(\frac{1}{3} - \frac{x'}{L} + \frac{x^2 + (x')^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, && \text{in I,} \\ &= \left(\frac{1}{3} - \frac{x}{L} + \frac{x^2 + (x')^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, && \text{in I',} \\ &= \left(\frac{1}{3} - \frac{\tau}{L} + \frac{x^2 + (x')^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, && \text{in III,} \\ &= \left(\frac{4}{3} - \frac{x + x' + \tau}{L} + \frac{x^2 + (x')^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, && \text{in III',} \\ &= \left(\frac{1}{3} - \frac{x + x' + \tau}{2L} + \frac{x^2 + (x')^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, && \text{in II,} \\ &= \left(\frac{4}{3} - \frac{x + x' + 3\tau}{2L} + \frac{x^2 + (x')^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, && \text{in IV.} \end{aligned} \tag{B4}$$

As before, R is continuous with discontinuous first derivatives on those characteristics of the wave equation separating the various regions.

The mean-square value of $q(x, t)$ is, from (B4) in region I,

$$R(x, x, 0) = \left(\frac{1}{3} - \frac{x}{L} + \frac{x^2}{L^2}\right)\frac{L}{\beta}. \tag{B5}$$

We see that this function has its maximum at the end points and its minimum at the midpoint. The two-point correlation at equal times, $R(x, x', 0)$, is found to be

$$\begin{aligned} R(x, x', 0) &= \left(\frac{1}{3} - \frac{x}{L} + \frac{x^2 + (x')^2}{2L^2}\right)\frac{L}{\beta}, \quad x \geq x', \\ &= \left(\frac{1}{3} - \frac{x'}{L} + \frac{x^2 + (x')^2}{2L^2}\right)\frac{L}{\beta}, \quad x \leq x'. \end{aligned} \tag{B6}$$

The two-time correlation at one point, $R(x, x, \tau)$ is, for $x \geq \frac{1}{2}L$,

$$\begin{aligned} R(x, x, \tau) &= \left(\frac{1}{3} - \frac{2x + \tau}{L} + \frac{2x^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, \\ &\qquad 0 \leq \tau \leq 2(L - x), \\ &= \left(\frac{4}{3} - \frac{2x + \tau}{L} + \frac{2x^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, \\ &\qquad 2(L - x) \leq \tau \leq 2x, \\ &= \left(\frac{4}{3} - \frac{2x + 3\tau}{2L} + \frac{2x^2 + \tau^2}{2L^2}\right)\frac{L}{\beta}, \\ &\qquad 2x \leq \tau \leq 2L. \end{aligned} \tag{B7}$$

For $0 \leq x \leq \frac{1}{2}L$, (B7) holds with x replaced by $L - x$ in the inequalities.

To obtain the correlation function for the semi-infinite region $x \geq 0$, we may try to let L become infinite in (B4); but then R diverges like $L/3\beta$. Therefore, we first subtract $L/3\beta = R(0, 0, 0)$ from R and then let L become infinite. In this way, we obtain

$$\begin{aligned} R(x, x', \tau) - R(0, 0, 0) &= -x'/\beta, && \text{in I,} \\ &= -x/\beta, && \text{in I',} \\ &= -\tau/\beta, && \text{in III,} \\ &= -(x + x' + \tau)/2\beta, && \text{in II.} \end{aligned} \tag{B8}$$

From (6.17) we find that

$$R(x, x, 0) - R(0, 0, 0) = -x/\beta, \tag{B9}$$

$$\begin{aligned} R(x, x, \tau) - R(0, 0, 0) &= -(2x + \tau)/2\beta, \\ &\qquad 0 \leq \tau \leq 2x, \\ &= -\tau/\beta, \quad \tau \geq 2x. \end{aligned} \tag{B10}$$

APPENDIX C: EVALUATION OF $R^{\text{q.m.}}$

By using trigonometric identities, we can rewrite (7.2) as

$$\begin{aligned} R^{\text{q.m.}} = \frac{c\hbar}{2\pi}\int_0^\infty &[(e^{\alpha b} - 1)^{-1} + \tfrac{1}{2}]\alpha^{-1}[\cos\alpha(x - x' + \tau) \\ &+ \cos\alpha(x - x' - \tau) - \cos\alpha(x + x' + \tau) \\ &- \cos\alpha(x + x' - \tau)]\, d\alpha. \end{aligned} \tag{C1}$$

Here $b = \beta\hbar c$. To evaluate the integral in (B2), let us consider the integral

$$-\int_0^\infty \frac{\sin\alpha z}{e^{\alpha b} - 1}\, d\alpha = -\frac{\pi}{2b}\left(\coth\frac{\pi z}{b} - \frac{b}{\pi z}\right), \quad b > 0. \tag{C2}$$

Integration of (C2) with respect to z, from z_1 to z_2, yields

$$\begin{aligned} &\int_0^\infty \frac{\cos\alpha z_2 - \cos\alpha z_1}{\alpha(e^{\alpha b} - 1)}\, d\alpha \\ &= \tfrac{1}{2}\log\left(\frac{\sinh(\pi z_1/b)}{\pi z_1/b}\right) - \tfrac{1}{2}\log\left(\frac{\sinh(\pi z_2/b)}{\pi z_2/b}\right). \end{aligned} \tag{C3}$$

We can use the result (C3) to evaluate that part of the integral in (C1) containing $(e^{\alpha b} - 1)^{-1}$ as a factor. We shall denote it by $R_0^{\text{q.m.}}$. It is given by

$$\begin{aligned} R_0^{\text{q.m.}} = \frac{c\hbar}{4\pi}\log\Bigg(&\frac{\sinh[\pi(x + x' + \tau)/\beta\hbar c]}{(x + x' + \tau)} \\ &\times \frac{\sinh[\pi(x + x' - \tau)/\beta\hbar c]}{(x + x' - \tau)} \\ &\times \frac{(x - x' + \tau)}{\sinh[\pi(x - x' + \tau)/\beta\hbar c]} \\ &\times \frac{(x - x' - \tau)}{\sinh[\pi(x - x' - \tau)/\beta\hbar c]}\Bigg). \end{aligned} \tag{C4}$$

The remaining integral, containing $\frac{1}{2}$ as a factor in the integrand, is associated with vacuum fluctuations. We shall denote it by $R_1^{\text{q.m.}}$. It can be evaluated by utilizing the following integral, in which z_1 and z_2 are both positive:

$$\begin{aligned} \int_0^a (\cos\alpha z_2 - \cos\alpha z_1)\alpha^{-1}\, d\alpha &= \int_0^a\int_{z_1}^{z_2} (-\sin\alpha z)\, dz\, d\alpha \\ &= \int_{z_1}^{z_2} (\cos az - 1)z^{-1}\, dz \\ &= \log\frac{z_1}{z_2} + \int_{az_1}^{az_2}\frac{\cos x}{x}\, dx. \end{aligned} \tag{C5}$$

Upon taking the limit as a becomes infinite in (C5), the left side assumes the form of the integral in $R_1^{\text{q.m.}}$,

while the integral on the right vanishes. By using this result in (C1), we obtain

$$R_1^{\text{q.m.}} = \frac{\hbar c}{4\pi} \log\left(\frac{|x - x' + \tau|\,|x - x' - \tau|}{|x + x' + \tau|\,|x + x' - \tau|}\right). \quad \text{(C6)}$$

The absolute signs occur in (C6) because all the cosines in (7.3) are even functions. The result (C6) is not valid if any one of the four absolute values vanishes, since then the limit of the last integral in (7.7) is not zero. Instead it leads to δ functions of these absolute values. By combining (C6) and (C4), we obtain (7.3).

In case $q_x = 0$ at the end points, the modes and eigenfrequencies are given by (B2), and $R^{\text{q.m.}}$ is given by using them in (4.1). As in the classical case, we omit the mode v_0 with eigenfrequency zero. By letting L become infinite, we convert the sum representing $R^{\text{q.m.}}$ into an integral. It is the same as (7.2) with $\sin \alpha x \sin \alpha x'$ replaced by $\cos \alpha x \cos \alpha x'$. Trigonometric identities enable us to reduce the integral to the form (C1), with plus signs in front of all four cosines.

Before evaluating the integral, we observe that it diverges at the lower end point. Therefore, we consider the difference

$$R^{\text{q.m.}}(x, x', \tau) - R^{\text{q.m.}}(0, 0, 0),$$

which is finite. We denote the difference between the integrals containing $(e^{ab} - 1)^{-1}$ as a factor by

$$R_0^{\text{q.m.}}(x, x', \tau) - R_0^{\text{q.m.}}(0, 0, 0).$$

By using (C3) with $z_1 = 0$, we can write it as

$$\begin{aligned} R_0^{\text{q.m.}}(x, x', \tau) &- R_0^{\text{q.m.}}(0, 0, 0) \\ &= -\frac{c\hbar}{4\pi} \log\left(\frac{\sinh \pi b^{-1}(x - x' + \tau)}{\pi b^{-1}(x - x' + \tau)}\right. \\ &\quad \times \frac{\sinh \pi b^{-1}(x - x' - \tau)}{\pi b^{-1}(x - x' - \tau)} \frac{\sinh \pi b^{-1}(x + x' + \tau)}{\pi b^{-1}(x + x' + \tau)} \\ &\quad \left. \times \frac{\sinh \pi b^{-1}(x + x' - \tau)}{\pi b^{-1}(x + x' - \tau)}\right). \end{aligned} \quad \text{(C7)}$$

The difference between the integrals containing $\frac{1}{2}$ as a factor is the vacuum fluctuation term, which is divergent.

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[1] R. C. Bourret, Nuovo Cimento **18**, 347 (1960).
[2] J. Sarfatt, Nuovo Cimento **27**, 1119 (1963).
[3] C. L. Mehta and E. Wolf, Phys. Rev. **134**, A1143, A1149 (1964).
[4] R. J. Glauber, Phys. Rev. **131**, 2766 (1963).
[5] D. Holliday, Phys. Letters **8**, 250 (1964).
[6] E. F. Keller, Phys. Rev. **139**, B202 (1965).

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Relation of the Inhomogeneous de Sitter Group to the Quantum Mechanics of Elementary Particles*

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A relativistic dynamical group recently introduced by Aghassi, Roman, and Santilli for the quantum mechanics of elementary particles is briefly reviewed. It is shown in detail that the algebra of this group can be obtained by contracting the Lie algebra of the inhomogeneous de Sitter group $ISO(3, 2)$. Some crucial concepts of the proposed new group are shown to appear in a new light when viewed in the context of a de Sitter world. The emergence of proper time as an additional kinematical variable is discussed in some detail.

1. INTRODUCTION

Recently[1] we proposed a new relativistic group (denoted by $\mathfrak{G}_5$) as the symmetry group of dynamics. The carrier space of $\mathfrak{G}_5$ is the Cartesian product space $E_{3,1} \times E_1$, where $E_{3,1}$ is the Minkowski space and E_1 a 1-dimensional manifold, with

$$x = (x^0, x^1, x^2, x^3) \in E_{3,1}$$

and $u \in E_1$. The defining transformations of $\mathfrak{G}_5$ are

$$x^\mu \to x'^\mu = \Lambda^\mu_\nu x^\nu + a^\mu + b^\mu u,$$
$$u \to u' = u + \sigma. \tag{1.1}$$

Here Λ^μ_ν is a restricted Lorentz matrix, a^μ a constant translation vector, b^μ another constant vector, and σ a scalar. Since we choose all x^μ and u to have the dimension of length, b^μ is dimensionless and σ has the dimension of length. Clearly, the 15-parameter group $\mathfrak{G}_5$ contains the restricted Poincaré group as a subgroup. The subset of transformations $x^\mu \to x^\mu + b^\mu u$ we call zest transformations. They are analogous to the boost transformations of the nonrelativistic Galilei group. Actually, it is easy to see that $\mathfrak{G}_5$ contains the nonrelativistic Galilei group $\mathfrak{G}_4$ as a subgroup. The detailed structure of $\mathfrak{G}_5$ can be written as

$$\mathfrak{G}_5 = \{T_4^a \circledS T_1^\sigma\} \times \{T_4^b \circledS SO_0(3, 1)\}. \tag{1.2}$$

Here T_4^a is the space–time translation group, T_1^σ the u translation group, T_4^b the zest group, and $SO_0(3, 1)$ the restricted Lorentz group. Equation (1.2) reveals that $\mathfrak{G}_5$ is a group extension[2] of the restricted Lorentz group.[3] Since the restricted Poincaré group is also an extension of $SO_0(3, 1)$, our suggested group $\mathfrak{G}_5$ can be looked upon as a natural generalization of the Poincaré group. Both "grow out" from the metric-determining Lorentz group in an analogous manner. We recall at this point that the nonrelativistic Galilei group $\mathfrak{G}_4$ is a group extension of the rotation group $SO(3)$ which, in turn, is the metric-determining group of the Euclidean space[4] E_3. Furthermore, $\mathfrak{G}_4$ contains the inhomogeneous Euclidean group $ISO(3)$ as a subgroup. All these considerations show that our proposed group $\mathfrak{G}_5$ is a natural generalization of the Galilei group $\mathfrak{G}_4$, but it is a group for relativistic phenomena. The main heuristic point of our argument in Ref. 1 was that the Poincaré group should be looked upon simply as a geometrical, *kinematical* group, just as $ISO(3)$ is only a (nonrelativistic) kinematical group. In order to have a relativistic *dynamical* group, the Poincaré group should be augmented in a manner analogous to the enlargement of $ISO(3)$ to $\mathfrak{G}_4$, which is known to be the (nonrelativistic) dynamical group. Our discussion above shows that this enlargement of the Poincaré group leads precisely to our group $\mathfrak{G}_5$.

As was discussed in detail in Ref. 1, for the use in relativistic *quantum* mechanics a further extension must be made.[5] The new relativistic quantum mechanical group will be denoted by $\tilde{\mathfrak{G}}_5$ and its structure is

$$\mathfrak{G}_5 = \{T_1^\theta \times (T_4^a \times T_1^\sigma)\} \circledS \{T_4^b \circledS SL(2, C)\}. \tag{1.3}$$

Here T_1^θ denotes a 1-dimensional Abelian phase group and $SL(2, C)$ is the covering group of $SO_0(3, 1)$. Thus, our $\tilde{\mathfrak{G}}_5$ is the scalar extension[2] of the covering group of $\mathfrak{G}_5$ by a phase group.

By denoting the generators of $SL(2, C)$, T_4^a, T_4^b, and T_1^σ by $J_{\mu\nu}$, P_μ, Q_μ, S, respectively, the Lie algebra of $\tilde{\mathfrak{G}}_5$ was found to be as follows[6]:

$$[J_{\mu\nu}, J_{\rho\sigma}] = i(g_{\nu\rho}J_{\mu\sigma} - g_{\mu\rho}J_{\nu\sigma} - g_{\mu\sigma}J_{\rho\nu} + g_{\nu\sigma}J_{\rho\mu}), \tag{1.4a}$$
$$[P_\mu, J_{\rho\sigma}] = i(g_{\mu\rho}P_\sigma - g_{\mu\sigma}P_\rho), \tag{1.4b}$$
$$[P_\mu, P_\nu] = 0, \tag{1.4c}$$
$$[J_{\mu\nu}, S] = 0, \tag{1.4d}$$
$$[P_\mu, S] = 0, \tag{1.4e}$$
$$[Q_\mu, Q_\nu] = 0, \tag{1.4f}$$
$$[P_\mu, Q_\nu] = -ig_{\mu\nu}l^{-1}, \tag{1.4g}$$
$$[J_{\mu\nu}, Q_\rho] = i(g_{\nu\rho}Q_\mu - g_{\mu\rho}Q_\nu), \tag{1.4h}$$
$$[S, Q_\mu] = iP_\mu. \tag{1.4i}$$

The constant l in (1.4g) has the dimension of length and its appearance is connected with the phase group T_1^9. We interpret l as a covariant fundamental length, and, clearly, we have a superselection rule.

The Casimir operators of $\tilde{\mathfrak{G}}_5$ were found to be

$$\mathfrak{D} = P_\mu P^\mu + 2l^{-1}S, \tag{1.5a}$$

$$\mathfrak{I} = \tfrac{1}{2}T_{\mu\nu}T^{\mu\nu}, \tag{1.5b}$$

$$\mathfrak{K} = \tfrac{1}{4}\epsilon_{\mu\nu\rho\sigma}T^{\mu\nu}T^{\rho\sigma}, \tag{1.5c}$$

where

$$T_{\mu\nu} \equiv J_{\mu\nu} - lM_{\mu\nu}, \tag{1.6}$$

with

$$M_{\mu\nu} \equiv P_\mu Q_\nu - P_\nu Q_\mu. \tag{1.6'}$$

In Ref. 1 we discussed the immediate physical implications of $\tilde{\mathfrak{G}}_5$. We showed that $X_\mu \equiv -lQ_\mu$ is a perfectly acceptable relativistic space–time position operator. Furthermore,

$$\mathcal{M}^2 \equiv -2l^{-1}S \tag{1.7}$$

was shown to act as a nontrivial relativistic mass operator. Note that both X_μ and $\mathcal{M}^2$ are operators in the *Lie algebra* of $\tilde{\mathfrak{G}}_5$. We also pointed out that S plays a further role: It acts as an evolution operator in the sense that

$$\frac{d\Omega}{du} = i[S, \Omega] \tag{1.8}$$

for any operator Ω which is a function of $X_\mu(u)$ and $P_\mu(u)$. In addition to these basic observations, we studied briefly the projective irreducible unitary representations of $\tilde{\mathfrak{G}}_5$ and pointed out that we obtain towers of states with increasing spin. Using the realization of the operators, we also gave simple models where the mass spectrum was calculated.

At this point we note that the carrier space $E_{3,1} \times E_1$ of $\tilde{\mathfrak{G}}_5$ is not endowed with metric.[7] We may therefore ask whether there exists some metric space with a group of motions which, by a well-defined limiting procedure, reduces to our $\tilde{\mathfrak{G}}_5$. It is well known that the standard procedure for performing limiting procedures on groups is that of contraction.[8] In particular, it has been shown[9] that the nonrelativistic quantum mechanical Galilei group arises as the contraction of the covering of the connected Poincaré group. The main purpose of the present paper is to show that *our relativistic quantum mechanical group $\tilde{\mathfrak{G}}_5$ is the contracted limit of the covering of the connected component of the inhomogeneous de Sitter group $ISO(3, 2)$.*

There are several reasons why our present study merits some interest. First, the representation of quantities belonging to $\tilde{\mathfrak{G}}_5$ in terms of limits of quantities that belong to $ISO(3, 2)$ sheds further light on to the nature of important physical entities, such as the mass (and evolution) operator S and the zest (or position) operators Q_μ. Secondly, the formulation of a theory in de Sitter space, of which our $\tilde{\mathfrak{G}}_5$ theory is a limiting case, opens up the possibility of studying directly quantum dynamics in the de Sitter world. As is well known, the de Sitter world merits special attention because it is the embedding of the simplest nonflat Riemannian spaces, viz., the spaces of constant curvature. Thirdly, the study of the contraction of $ISO(3, 2)$ is interesting from the purely mathematical point of view as well.

In connection with the second and third item listed above, we note that even though much work has been done in exploring the possibility of a particle theory in a de Sitter world,[10] these investigations centered on the use of the *homogeneous* group $SO(4, 1)$ or $SO(3, 2)$. As far as we know, there is only one attempt[11] to utilize the framework of $ISO(4, 1)$.

There is one more bibliographical remark we wish to make. While we were preparing the present work, we became aware of a paper by Castell[12] in which he endeavors to construct Lie algebras that contain a relativistic position operator. One of his algebras is isomorphic to the Lie algebra of our group $\tilde{\mathfrak{G}}_5$, and another of his algebras is isomorphic to the $ISO(3, 2)$ Lie algebra. He also mentions that the former can be obtained by contracting the latter. However, the detailed properties of these algebras and the actual process of the contraction have not been considered in Ref. 12.

2. THE $ISO(3, 2)$ GROUP AND ITS CONTRACTION

Let us start with the carrier space $E_{3,1} \times E_1$ of our group $\tilde{\mathfrak{G}}_5$ and change it to the geometrical manifold $E_{3,2}$ by introducing a metric. We denote the points[13] of $E_{3,2}$ by x^a, so that for $a = 0, 1, 2, 3$ we have our previous x^μ coordinates, while we set

$$x^4 = u. \tag{2.1}$$

The metric in $E_{3,2}$ is defined by the line element[14]

$$d\rho^2 = g_{ab}\, dx^a\, dx^b, \tag{2.2}$$

where

$$\begin{gathered} g_{ab} = 0, \quad \text{if} \quad a \neq b, \\ g_{00} = +1, \\ g_{11} = g_{22} = g_{33} = -1, \\ g_{44} = +k^2. \end{gathered} \tag{2.2'}$$

For the actual $E_{3,2}$ space, k^2 can be taken to be the constant $+1$; however, since it will be our contraction

parameter, we prefer to use right from the beginning the notation k^2.

As usual, we define g^{ab} through the relation

$$g^{ac}g_{cb} = \delta^a_b. \tag{2.2''}$$

This implies, in particular, that

$$g^{44} = 1/k^2. \tag{2.2'''}$$

To avoid confusion, we also note that

$$x_4 = g_{44}x^4 = k^2u. \tag{2.3}$$

The space $E_{3,2}$ equipped with the metric (2.2) is the embedding of the so-called closed de Sitter world. The group of isometries (group of rigid motions) of $E_{3,2}$ is the inhomogeneous de Sitter group $ISO(3, 2)$. The transformations of this group are defined by

$$x^a \to x'^a = \Omega^a_b x^b + B^a, \tag{2.4}$$

where B^a is a constant 5-vector and

$$\Omega^a_c\Omega^c_b = \delta^a_b. \tag{2.4'}$$

In the present paper we are interested only in the Lie algebra of the (covering group) of the connected component of $ISO(3, 2)$. This algebra has the fifteen generators $J_{ab} = -J_{ba}$ and P_a. The algebra is given by

$$[J_{ab}, J_{cd}] = i(g_{bc}J_{ad} - g_{ac}J_{bd} - g_{ad}J_{cb} + g_{bd}J_{ca}), \tag{2.5}$$

$$[P_a, J_{bc}] = i(g_{ab}P_c - g_{ac}P_b), \tag{2.6}$$

$$[P_a, P_b] = 0. \tag{2.7}$$

It will be convenient to rewrite these relations in a more detailed form. We then have the algebra

$$[J_{\mu\nu}, J_{\rho\sigma}] = i(g_{\nu\rho}J_{\mu\sigma} - g_{\mu\rho}J_{\nu\sigma} - g_{\mu\sigma}J_{\rho\nu} + g_{\nu\sigma}J_{\rho\mu}), \tag{2.8a}$$

$$[P_\mu, J_{\rho\sigma}] = i(g_{\mu\rho}P_\sigma - g_{\mu\sigma}P_\rho), \tag{2.8b}$$

$$[P_\mu, P_\nu] = 0, \tag{2.8c}$$

$$[J_{\mu\nu}, P_4] = 0, \tag{2.8d}$$

$$[P_\mu, P_4] = 0, \tag{2.8e}$$

$$[J_{4\mu}, J_{4\nu}] = ik^2J_{\mu\nu}, \tag{2.8f}$$

$$[P_\mu, J_{4\nu}] = -ig_{\mu\nu}P_4, \tag{2.8g}$$

$$[J_{\mu\nu}, J_{4\rho}] = i(g_{\nu\rho}J_{4\mu} - g_{\mu\rho}J_{4\nu}), \tag{2.8h}$$

$$[P_4, J_{4\mu}] = ik^2P_\mu. \tag{2.8i}$$

The Casimir operators of $ISO(3, 2)$ are constructed in the standard manner. We have at our disposal the vector P_a, the tensor J_{ab}, and form the pseudotensor

$$W_{ab} \equiv \epsilon_{abcde}J^{cd}P^e. \tag{2.9}$$

We then easily verify that the Casimir operators are

$$I_2 = P_aP^a, \tag{2.10a}$$

$$I_4 = \tfrac{1}{2}W_{ab}W^{ab}, \tag{2.10b}$$

$$I_3 = \tfrac{1}{4}W_{ab}J^{ab}. \tag{2.10c}$$

It will be convenient to rewrite these expressions in 4-dimensional notation. With some trivial labor, we get

$$I_2 = P_\mu P^\mu + P_4P^4, \tag{2.11a}$$

$$I_4 = (1/2k^2)W_\mu W^\mu + \tfrac{1}{2}H_{\mu\nu}H^{\mu\nu}, \tag{2.11b}$$

$$I_3 = \tfrac{1}{4}\epsilon^{\mu\nu\sigma\tau}(J_{\mu\nu}J_{\sigma\tau}P_4 + k^2J_{\mu\nu}M_{\sigma\tau} + k^2M_{\mu\nu}J_{\sigma\tau}). \tag{2.11c}$$

Here W_μ is the Pauli–Lubanski vector

$$W_\mu \equiv \epsilon_{\mu\nu\sigma\tau}J^{\nu\sigma}P^\tau, \tag{2.12}$$

$H^{\mu\nu}$ is the abbreviation

$$H^{\mu\nu} = \epsilon^{\mu\nu\sigma\tau}(J_{\sigma\tau}P_4/k^2 + M_{\sigma\tau}), \tag{2.13}$$

and $M_{\sigma\tau}$ is defined by (1.6′).

We are now ready to perform the *contraction of the $ISO(3, 2)$ algebra with respect to the Poincaré algebra $ISO(3, 1)$*. This means that we will let $J_{\mu\nu}$ and P_ν go to zero *relative to* $J_{4\mu}$ and P_4. However, prior to this limiting, we first make a redefinition of the latter operators, viz., perform the transformations

$$P_4 = k^2/l + S, \tag{2.14}$$

$$J_{4\mu} = k^2Q_\mu. \tag{2.15}$$

In (2.17), l is an *arbitrary* nonzero constant of the dimension of length. It is now clear that the above defined *contraction amounts to letting* $k^2 \to \infty$.

Trivial inspection of Eqs. (2.8) now reveals that *under the contraction the $ISO(3, 2)$ algebra goes over into our $\tilde{\mathfrak{G}}_5$ algebra* (1.4). QED

Concerning the contraction of the Casimir operators, we note the following. From (2.14) we get

$$P_4P^4 \equiv g^{44}P_4P_4 = k^2/l^2 + 2S/l + S^2/k^2. \tag{2.16}$$

Thus, redefining the invariant I_2 of $ISO(3, 2)$ to be

$$I_2' = I_2 - k^2/l^2 = P_aP^a - k^2/l^2, \tag{2.17}$$

we see that under contraction

$$I_2' \to \mathfrak{D}, \tag{2.18}$$

with $\mathfrak{D}$ being the Casimir operator of $\tilde{\mathfrak{G}}_5$ as given by Eq. (1.5a).

Next, we consider (2.13) and observe that, owing to (2.14) and (1.6), we have

$$H^{\mu\nu} \to l^{-1}\epsilon^{\mu\nu\sigma\tau}T_{\sigma\tau}. \tag{2.19}$$

Hence, redefining I_4 to be

$$I_4' = l^2 I_4, \tag{2.20}$$

we obtain easily from (2.11b) that under contraction

$$I_4' \to \mathfrak{Z}, \tag{2.21}$$

where $\mathfrak{Z}$ is given by (1.5b).

Finally, concerning the contraction of I_3, we first redefine it to be

$$I_3' = lI_3/k^2. \tag{2.22}$$

Then we note that we may add to the right-hand side of (2.11c) an arbitrary multiple of

$$B \equiv \epsilon^{\mu\nu\sigma\tau} M_{\mu\nu} M_{\sigma\tau},$$

because, on account of (1.6'), this expression is identically zero. After these trivial manipulations we then readily see that under contraction

$$I_3' \to \mathfrak{K}, \tag{2.23}$$

with $\mathfrak{K}$ given by (1.5c).

3. DISCUSSION

The major insight that we gained from the present work is that, if desired, our proposed relativistic quantum dynamics can be formulated in the framework of $ISO(3,2)$ rather than of $\tilde{\mathfrak{G}}_5$. This has the advantage that we are more familiar with groups of isometries than with the rather complicated group structure (1.3). For example, it will be easier to find equations describing particles of arbitrary spin in the $ISO(3,2)$ framework than it would be in the $\tilde{\mathfrak{G}}_5$ framework. The corresponding $\tilde{\mathfrak{G}}_5$ equation will then be obtained by contraction.[15] In spite of these formal advantages we maintain that the theory to be pursued further is the $\tilde{\mathfrak{G}}_5$ dynamics discussed in Ref. 1. This does not demand the description of phenomena in a 5-dimensional world: The metric space–time structure is still the Minkowski world, even though an additional kinematical parameter must be added so as to obtain the carrier space of the dynamical group.[16] The zest operators Q_μ (or equivalently, the relativistic position operators X_μ) have a much more direct meaning than the rotation operators $J_{4\mu}$ from which they arise by contraction, cf. (2.15).

One further insight we obtained in our calculations is that, as seen from (2.14), our operator S [connected, via Eq. (1.7), with the mass] is essentially the finite part of the P_4 translation operator of the de Sitter world. This observation also sheds further light on our previous knowledge [see Eq. (1.8)] that S in some sense serves as an evolution operator. Actually, we can now directly show that *this evolution is with respect to proper time*. To see this, let us define the proper time τ of the de Sitter world by setting

$$d\rho = k\, d\tau. \tag{3.1}$$

Then, from Eq. (2.2) we have

$$d\tau^2 = (1/k^2)\, dx_\mu\, dx^\mu + (dx^4)^2, \tag{3.2}$$

so that after the contraction $k^2 \to \infty$ we obtain

$$d\tau \to dx^4 \equiv du. \tag{3.3}$$

This tells us that in the $\tilde{\mathfrak{G}}_5$ framework *the additional kinematical variable u is nothing else than the proper time.*

We can go somewhat further and define in the de Sitter world the 5-velocity

$$U^a = \frac{dx^a}{d\tau}. \tag{3.4}$$

Upon contraction we then get

$$U^\mu \to \frac{dx^\mu}{du}, \tag{3.5a}$$

confirming the interpretation of u, and we also find

$$U^4 \to 1. \tag{3.5b}$$

From (3.2) it follows that

$$U_\mu U^\mu = k^2[1 - (U^4)^2]. \tag{3.6}$$

In view of (3.5b), the contraction of $U_\mu U^\mu$ is an *indefinite expression*, and, clearly, it is not invariant under $\tilde{\mathfrak{G}}_5$. However, it is invariant not only under the Poincaré group $\mathfrak{P}$ but also under $\mathfrak{P} \circledS T_1^\sigma$ (where T_1^σ is the u-translation group).

A definite numerical value for $U_\mu U^\mu$ in the $\tilde{\mathfrak{G}}_5$ framework can be obtained if we set

$$P^a = mU^a, \tag{3.7}$$

with m being the mass eigenvalue. An elementary calculation then tells us that, after contraction,[17]

$$U_\mu U^\mu + (2S/lm^2) = \mathfrak{D}/m^2. \tag{3.8}$$

Since (3.8) together with (3.7) is consistent with (1.5a), the relating of U^a and P^a by (3.7) is justified. Then, as a consequence, in the $\tilde{\mathfrak{G}}_5$ theory we have $P^\mu = mU^\mu$, as already conjectured in Ref. 1.

APPENDIX

We wish to illustrate here the obtaining of dynamical equations and Lagrangians in the $\tilde{\mathfrak{G}}_5$ framework via contracting $ISO(3,2)$ results.

The simplest dynamical equation in the $ISO(3,2)$ framework is $I_2' = 0$. Realizing the P_a by the differential operators $i\partial_a$, we have, from (2.17),

$$(\partial_a\partial^a + k^2/l^2)\psi(x^a) = 0. \tag{A1}$$

Assuming that ψ is complex, we have that the corresponding action integral is

$$W = \int \mathfrak{L}(\psi, \partial_a\psi)\, dx = \int \left(\partial_a\psi^*\partial^a\psi - \frac{k^2}{l^2}\,\psi^*\psi\right) dx, \tag{A2}$$

where

$$dx = dx^0\, dx^4\, dx^1\, dx^2\, dx^3. \tag{A2'}$$

Using (2.14), we easily find that, upon contraction,

$$W \to \int \left(\partial_\mu\psi^*\partial^\mu\psi + \frac{2i}{l}\,\psi^*\partial_u\psi\right) dx^0\, dx^1\, dx^2\, dx^3\, du. \tag{A3}$$

(Here we used the realization of S by $i\partial_u$, cf. Ref. 1.) The corresponding equation of motion is

$$(\Box - 2l^{-1}i\partial_u)\psi(x^\mu; u) = 0. \tag{A4}$$

This, naturally, coincides[18] with what one obtains directly from contracting (A1). However, there is some new insight, inasmuch as we know now that the action integral in the $\tilde{\mathfrak{G}}_5$ framework must be an integral not only over the Minkowski coordinate space, but must also involve integration over the proper time u. In other words, the Lagrangian density in the Poincaré framework may be looked upon as

$$L(x^0, x^1, x^2, x^3) = \int \mathfrak{L}(x^\mu; u)\, du. \tag{A5}$$

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[1] J. J. Aghassi, P. Roman, and R. M. Santilli, Phys. Rev. D **1**, 2753 (1970).

[2] For a brief review of the notion of group extensions, see, for example, Appendix A of Ref. 1 or G. C. Hegerfeldt and J. Hennig, Fortschr. Physik **16**, 491 (1968), Sec. I.6.

[3] On the other hand, $\tilde{\mathfrak{G}}_5$ is *not* a group extension of the Poincaré group.

[4] Let us recall that the carrier space of the Galilei group is $E_3 \times E_1$, with $x = (x_1, x_2, x_3) \in E_3$ and $t \in E_1$.

[5] This procedure is also analogous to the one followed in nonrelativistic quantum dynamics, see E. Inönü and E. P. Wigner, Nuovo Cimento **9**, 705 (1952).

[6] Here and in the following $g_{\mu\nu}$ is the metric tensor of $E_{3,1}$, viz., $g_{\mu\nu} = 0$ if $\mu \neq \nu$, $g_{00} = 1$, $g_{kk} = -1$.

[7] This is analogous to the situation for the nonrelativistic Galilei group: $E_3 \times E_1$ is not endowed with metric.

[8] E. Inönü and E. P. Wigner, Proc. Natl. Acad. Sci. U.S. **39**, 510 (1953). Also, E. Inönü, in *Group Theoretical Concepts and Methods in Elementary Particle Physics*, F. Gürsey, Ed. (Gordon & Breach, New York, 1964), p. 365; J. Rosen, Nuovo Cimento **35**, 1234 (1965); T. O. Philips and E. P. Wigner, in *Group Theory and its Applications*, M. Loebl, Ed. (Academic, New York, 1968), p. 631.

[9] E. Inönü and E. P. Wigner, Ref. 8; E. J. Saletan, J. Math. Phys. **2**, 1 (1961).

[10] From the vast literature on this subject, we can mention only a few representative papers. Each of them contains further references. Our partial list is: P. A. M. Dirac, Ann. Math. **36**, 657 (1935); K. Goto, Progr. Theoret. Phys. (Kyoto) **12**, 311 (1954); F. Gürsey, in *Group Theoretical Concepts and Methods in Elementary Particle Physics*, F. Gürsey, Ed. (Gordon and Breach, New York, 1964), p. 365; J. B. Ehrman, Proc. Cambridge Phil. Soc. **53**, 290 (1957); T. U. Philips and E. P. Wigner, Ref. 8; A. Böhm, Phys. Rev. **145**, 1212 (1965); O. Nachtman, Commun. Math. Phys. **6**, 1 (1967); C. Fronsdal, Rev. Mod. Phys. **37**, 221 (1965); P. Roman and J. J. Aghassi, Phys. Letters **14**, 68 (1965); P. Roman and J. J. Aghassi, J. Math. Phys. **7**, 1273 (1966); P. Roman and J. J. Aghassi, Nuovo Cimento **42A**, 193 (1966); P. Roman and C. J. Koh, *ibid.* **45A**, 268 (1966); G. Börner and H. P. Dürr, *ibid.* (to be published).

[11] I. Fushchich and I. Yu. Krivsky, Nucl. Phys. **B7**, 79 (1968); Preprint ITF-69-1, Kiev, 1969.

[12] L. Castell, Nuovo Cimento **49**, 285 (1967). See also the recent paper by J. E. Johnson, Phys. Rev. **181**, 1755 (1969).

[13] Latin labels a, b, etc., run through values 0, 4, 1, 2, and 3. Greek labels μ, ν, etc., will be reserved to run through 0, 1, 2, and 3. We use natural units, $\hbar = c = 1$, so that all x^a have dimension of length.

[14] All the g_{ab} are *dimensionless*.

[15] We shall discuss these questions in a later publication. A trivial example will be given in our present Appendix.

[16] The physical interpretation of u will be discussed below.

[17] Use was made of (2.17) and (2.18).

[18] Eq. (A4) was also obtained directly within the $\tilde{\mathfrak{G}}_5$ framework in Ref. 1.

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Summability of the Many-Fermion Perturbation Series with Attractive Forces*

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The summability of the many-fermion perturbation series in the presence of attractive forces is considered. We find that, although it is an asymptotic series, the potential-strength perturbation series is summable. We find that some rearrangements to handle the hard-core potentials also lead to the correct sum; however, the "hole-line" summation procedure using Brandow's choice for intermediate state energies is either wrong or deceptive in its convergence.

1. INTRODUCTION

Insofar as we can discover, the problem of the summability of the many-fermion perturbation series in the presence of attractive forces has not yet been treated in any detail. Negative results, showing that it cannot be summable for a purely attractive potential due to "nuclear collapse", have been known for a long time.[1] We have investigated summability for a purely repulsive potential[2] and found, in the case where some physically plausible estimates are valid, that summability by appropriate methods is possible. The reason that the question of summability arises is that the many-fermion perturbation series for the usual type of potentials with a strong central repulsion can be at best asymptotic[2] and not convergent. Hence, the usual procedure of adding up the terms in a power series, or even a rearrangement power series, cannot *a priori* be supposed to yield a satisfactory answer.

In Sec. 2, we give an example which illustrates one of the problems which can arise, even for a convergent series beyond its radius of convergence. We then argue that, at least for weak enough attraction, the ordinary perturbation series in powers of the potential strength is summable, in the same way that the series for a purely repulsive potential was.[2] We next consider the rearrangement problem. We have in mind those rearrangements which are used to handle the hard-core potentials and also to improve generally the accuracy of the early terms in the series. We conclude that many of the commonly used procedures are satisfactory. One notable exception was found, that is, the hole-line resummation procedure[3,4] using the Brandow choice[5] for the intermediate state energies. We discuss this procedure in Sec. 3 and show by means of a counterexample that it is either wrong (possible though a formally correct resummation of a divergent series) or deceptive in its convergence properties.

2. ACCEPTIBILITY OF RESUMMATIONS OF THE POTENTIAL-STRENGTH PERTURBATION SERIES

As has been previously pointed out,[2] the perturbation series in the potential strength for the many-fermion ground-state energy problem is divergent for potentials of the type commonly employed. As is well known, due care must be exercised in manipulations with such series. The problem of even defining the answer which corresponds to the physical problem at hand is not one which is always completely obvious. As an example of a purely mathematical nature, consider[6]

$$1 + 2x^2 + 2x^4 + 2x^6 + 2x^8 + \cdots, \tag{2.1}$$

which can be summed for small x as

$$(1 + x^2)/(1 - x^2). \tag{2.2}$$

However, by rearranging (2.1) as

$$1 + \frac{1}{2}\left(\frac{2x}{1+x^2}\right)^2 + \frac{1\cdot 3}{2\cdot 4}\left(\frac{2x}{1+x^2}\right)^4 + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\left(\frac{2x}{1+x^2}\right)^6 + \cdots, \tag{2.3}$$

we obtain a series which is now also convergent for large x. Summing up directly, we get, for large x,

$$(x^2 + 1)/(x^2 - 1). \tag{2.4}$$

Since (2.2) is a meromorphic function, it represents the unique analytic continuation of the series (2.1) throughout the whole complex plane. The result (2.4), seemingly valid for large x, is the negative of (2.2) and thus incorrect. Nevertheless (2.3) gives the correct sum for small x. This example illustrates that some care is necessary in rearrangement of series. In the many-fermion problem, we have a procedure for defining the physical sum of the series. We want that sum which is the limit as N tends to infinity of the energy of a system of N particles (density held constant in this limiting process).

We have previously discussed in detail[2] the convergence problem for finite repulsive potentials. We made it very plausible that the rate of divergence of the perturbation series is no faster than

$$\Gamma n!\,(\tilde{\Lambda})^n, \tag{2.5}$$

where Γ and $\tilde{\Lambda}$ are potential-dependent constants and n is the order in the perturbation series. In this estimate, it was essential that the "self-energy" insertions on occupied lines and hole lines be taken together since, in higher order, they separately diverge.[2,7] The only property of the potential used in this proof was that

$$|v(x)| \leq A/(1 + Bx^2), \tag{2.6}$$

where $v(x)$ is the momentum representation of the potential interaction. This form is clearly as suitable for potentials of two signs as for purely repulsive potentials. Hence, we conclude that, for bounded, nonsingular potentials of the usual sort, Eq. (2.5) forms a valid bound for the perturbation series. The next step in assigning a meaning to the perturbation series comes from a theorem of Carleman.[6] He proved that a necessary and sufficient condition for

$$|g(z)| \leq \alpha_n^n |z|^n, \quad |z| \leq r_0 < \infty, \quad |\arg z| \leq \tfrac{1}{2}\pi \tag{2.7}$$

to imply $g(z) = 0$ is that $\sum \alpha_n^{-1}$ diverge (for suitably regular α). If the many-fermion perturbation series is asymptotic in the angular sector $|\arg V| \leq \frac{1}{2}\pi$, then this theorem means, since $(n!)^{1/n} \propto n$ implies $\sum \alpha_n^{-1}$ diverges, that there exists at most one function which is regular for positive real V in the neighborhood of $V = 0$ and asymptotically equal to the perturbation series. Consider those potentials in which there is a strong but finite central repulsion so that no collapsed state is possible.We feel that for such potentials ($V \approx 0$) the behavior should be essentially that of the central repulsion. That case was analyzed in detail and the location of the singularities nearest the origin estimated.[2] It was found that they approach the origin from the direction of the negative real axis. The closest one is at a distance of the order $N^{-\frac{1}{3}}$ to N^{-1} from the origin and makes an angle with the negative real axis of at most $\ln N/N^{\frac{1}{3}}$. The physical reason for this singularity is the well-known collapse phenomenon in (for V negative) an attractive short-range potential well. Thus it is, we feel, physically reasonable to suppose that, for very weak potentials, at least, the ground-state energy is asymptotic in the closed right half-plane. Let us specifically mention that the type of singularities found in superconductivity

$$Ae^{-B/V} \tag{2.8}$$

are excluded here since they do not satisfy (2.7) for V pure imaginary. We have argued in a previous paper[8] that, for the usual sort of potential with a central repulsion plus short-range attraction, superconductivity should not be a problem. We also remark that the nearest singularity of course sets a limit on the radius of convergence so that, while $V = 0$ is a regular point for a system of finite size N, the radius of convergence tends to zero as N tends to infinity.

In order to deal with the hard-core potential, a number of resummation procedures have been proposed.[3,4,8-10] Let us now consider under what conditions these resummations correctly define the proper physical function. Let the energy per particle in the N-fermion problem with pair interaction $V\varphi(r)$ be

$$E_N(V) = \sum_{n=0}^{\infty} {}_N e_n V^n. \tag{2.9}$$

This series has a nonzero radius of convergence as mentioned above, and hence, by analytic continuation, defines $E_N(V)$ everywhere in the complex V plane except at singular points or on branch cuts. This analytic continuation is conveniently given by the Mittag-Leffler method.[6] We define

$$E_N(V, \delta) = \sum_{n=0}^{\infty} \frac{{}_N e_n V^n}{\Gamma(\delta n + 1)}. \tag{2.10}$$

For every $\delta > 0$, $E_N(V, \delta)$ is an entire function of V as $E_N(V)$ is analytic at $V = 0$. Also, as shown by Hardy[6] (Theorem 135), the relation

$$\lim_{\delta \to 0} E_N(V, \delta) = E_N(V) \tag{2.11}$$

holds uniformly in any closed and bounded region in the Mittag-Leffler star of $E_N(V)$. The Mittag-Leffler star is defined by cutting the complex V plane from every singularity to infinity along rays. As we have pointed out above, $E_N(V)$ is regular for positive real V (at least V small), and hence the positive real axis in the neighborhood of $V = 0$ is interior to the Mittag-Leffler star for all N. The meaning we wish to assign to the sum of the perturbation series for infinitely many fermions is

$$\lim_{N \to \infty} E_N(V) = \lim_{N \to \infty} \lim_{\delta \to 0} E_N(V, \delta). \tag{2.12}$$

With this prescription as a guide, we shall show that a wide class of rearrangements, including many of the usual ones, are frequently satisfactory. We now introduce the Mittag-Leffler function

$$\varphi_\delta(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1 + \delta n)} \xrightarrow[|z| \to \infty]{} (1 - z)^{-1}, \qquad \tfrac{1}{2}\pi\delta \leq |\arg z| \leq \pi. \tag{2.13}$$

For V less than the radius of convergence we have, by Cauchy's theorem for regular functions of a complex variable,

$$E_N(V, \delta) = \frac{1}{2\pi i} \oint \varphi_\delta\left(\frac{V}{u}\right) E_N(u) \frac{du}{u}, \quad (2.14)$$

where the contour is a circle about the origin inside the circle of convergence. Again using Cauchy's theorem, we may deform the contour as shown in Fig. 1, provided we cross no singular points of $E_N(u)$. If we now restrict $\pi\delta < 2\psi$, then, for

$$\psi \leq |\arg (V/u)| \leq \pi,$$

we find that

$$u^{-1}\varphi_\delta(V/u) \to (u - V)^{-1} \quad (2.15)$$

as V/u tends to infinity. Thus $\varphi_\delta(V/u)$ is bounded on the contour of Fig. 1. We may now shrink the circular arc part of the contour to the origin. Since $E_N(u)$ is bounded and the length of the arc goes to zero, the contribution from this part of the contour goes to zero. Hence, we can replace the contour of Fig. 1 by that of Fig. 2 which is now independent of N. However, $E_N(u)$ tends to a finite limit at every point on this contour and hence does so uniformly. Thus, for all $\pi\delta < 2\psi$, when we take the limit of (2.14), we have that $E_N(V, \delta)$ tends uniformly to

$$E(V, \delta) = \frac{1}{2\pi i} \oint \varphi_\delta\left(\frac{V}{u}\right) E(u) \frac{du}{u}. \quad (2.16)$$

By the properties of $\varphi_\delta(x)$, we deduce that

$$E(V) = \lim_{\delta \to 0} E(V, \delta) = \lim_{\delta \to 0} \lim_{N \to \infty} E_N(V, \delta). \quad (2.17)$$

That is to say, we may obtain $E(V)$ correctly from the V series by first taking the limit as system size increases indefinitely and then summing the series. We can see roughly how the Carleman restriction comes into play by noting that we can get $E(V, \delta)$ by simple series summation only when $\delta > 1$, and we can only prove analyticity in δ for $0 < \delta < 2\psi/\pi$. Thus, if $2\psi/\pi > 1$,

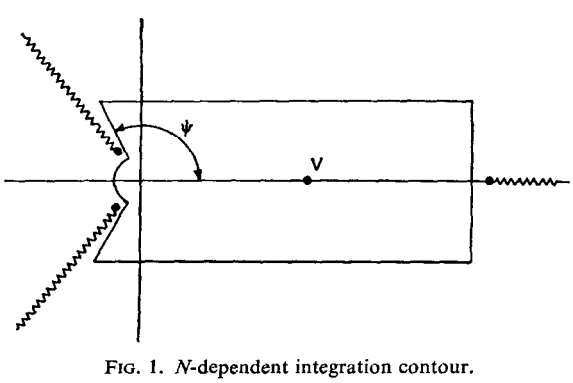

FIG. 1. N-dependent integration contour.

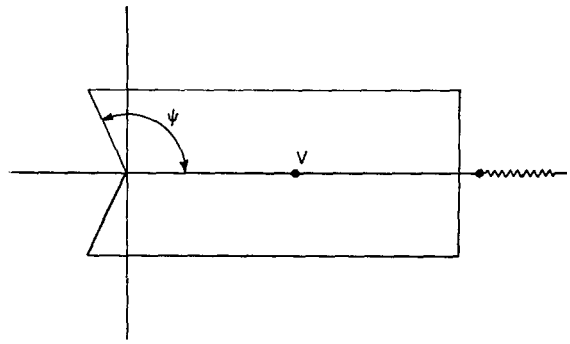

FIG. 2. N-independent integration contour.

we can establish $E(V, \delta)$ over a range of δ and hence analytically continue it uniquely to $\delta = 0$, whereas, if $2\psi/\pi < 1$, we cannot make contact and sum in this manner. In the latter case, Carleman's theorem assures us that indeed there is not a unique analytic continuation, but in the former case, which obtains for the problem at hand, we do have a unique analytic continuation and hence a well-defined sum for the energy series.

We will now formally rearrange the series as

$$\mathcal{E}_N(V) = \sum_{n=0}^{\infty} {}_N a_n \left(V^n \sum_{j=0}^{\infty} {}_N b_{n,j} V^j \right). \quad (2.18)$$

We require that

$${}_N e_m = \sum_{n=0}^{m} ({}_N a_n)({}_N b_{n,m-n}), \quad (2.19)$$

in order that this be a formal rearrangement of the energy. In order to facilitate our development, we will introduce the auxiliary function

$$\mathcal{E}_N(V, \lambda) = \sum_{n=0}^{\infty} {}_N a_n \lambda^n V^n \left(\sum_{j=0}^{\infty} {}_N b_{n,j} V^j \right). \quad (2.20)$$

We will assume that the rearrangement has preserved the bounds for the original series in the sense that

$$\sum_{n=0}^{m} |({}_N a_n)({}_N b_{n,m-n})| \leq A(BN^\nu)^m \quad \text{and} \quad \Gamma'(\Lambda')^m m!, \quad (2.21)$$

the second bound holding uniformly in N. Under this assumption, there exists a circle $|V| \leq \rho(N)$, for which the double series converges uniformly and absolutely, provided $|\lambda| \leq R > 1$. It follows, then, by standard arguments that for V in this circle

$$\mathcal{E}_N(V, 1) = E_N(V). \quad (2.22)$$

We now wish to extend $\mathcal{E}_N(V, \lambda)$ by analytic continuation to a wider domain. This may be done, again by the Mittag-Leffler method. To this end, we

introduce

$$\mathcal{E}_N(V, \lambda, \delta, \eta) = \sum_{n=0}^{\infty} \frac{{}_N a_n \lambda^n V^n}{\Gamma(\eta n + 1)} \left(\sum_{j=0}^{\infty} \frac{{}_N b_{n,j} V^j}{\Gamma((j+n)\delta + 1)} \right). \tag{2.23}$$

The analytic continuation is then given by

$$\mathcal{E}_N(V, \lambda) = \lim_{\delta \to 0} \lim_{\eta \to 0} \mathcal{E}_N(V, \lambda, \delta, \eta) \tag{2.24}$$

throughout the Mittag–Leffler star. If there exists a path, interior to the Mittag–Leffler star, connecting $(V = 0, \lambda = 1)$ with $(V = \tilde{V}, \lambda = 1)$ for all N, then by analytic continuation from (2.22) we have (2.22) also valid for $(V = \tilde{V}, \lambda = 1)$. Now, since this path is a closed and bounded set and since, from our discussion of the V series, $E_N(V)$ tends to a finite limit at every point of such a path, it does so uniformly in N; thus, we conclude that under these assumptions

$$E(V) = \mathcal{E}(V, 1) = \sum_{n=0}^{\infty} a_n \left(V^n \sum_{j=0}^{\infty} b_{n,j} V^j \right). \tag{2.25}$$

We have established that this series is summable to the correct value provided the rearrangement satisfies (2.21) and there exists a path in the Mittag–Leffler star joining $(V = 0, \lambda = 1)$ and the point of interest. The imposition of the second part of (2.21) is necessary to insure that the limiting analytic continuation be unique.

We remark that, when (2.25) is known to be summable and the terms in parentheses are at least asymptotic in an angular wedge $0 \leq |\arg V| \leq \psi \geq \frac{1}{2}\pi$ in the sense of (2.7), then Carleman's theorem assures us that it sums to the correct result in any connected region of summability. To see this, we need only note that a finite number of terms from the n and j sums in (2.25) will suffice to give any finite-order coefficient. These restrictions on the quantities in parentheses are certainly valid for resummation of the ladder diagrams into a K matrix when the potential is purely repulsive. This result follows since the series is closely related to a series of Stieltjes.[11] The R-matrix procedure,[8] also, satisfies these restrictions because $R(V)$ is convergent when V is bounded and of finite range, and, for usual potentials, $R(V)$ is nonsingular in the neighborhood of the positive real V axis.[8]

It is worth noting that the example at the beginning of this section violates one of our conditions. To see that this is so, rewrite (2.3) as

$$1 + \frac{1}{2}\left(\frac{2x}{1+x^2}\right)^2 \lambda + \frac{1}{2} \cdot \frac{3}{4}\left(\frac{2x}{1+x^2}\right)^4 \lambda^2 + \cdots = \left[1 - \left(\frac{2x}{1+x^2}\right)^2 \lambda\right]^{-\frac{1}{2}}. \tag{2.26}$$

Now, it is not possible to pass from small x to large x without crossing the unit circle in the complex x plane by the Jordan curve theorem. For x on the unit circle, we find that

$$1 \leq [2x/(1+x^2)]^2 \leq \infty$$

and hence points on the unit circle in the x plane lie on the branch cut introduced by Mittag–Leffler summation of the λ series when $\lambda = 1$. Hence, there is no path within the Mittag–Leffler star which connects large and small values of x and thus no necessity for the sum of (2.3) to be the same function in the two regions.

We remark that the "hole-line" expansion method, using the Brandow choice[5] for the energy denominators, as used by Kallio and Day,[12] for example, is not analyzable by this method. It violates the inequalities (2.21), as we will see. Besides this mathematical infelicity, there is a physical reason to believe that the "hole-line" expansion method, under Brandow choice, may suffer from the problem that our example (2.3) does. That is to say, there is doubt as to whether, if carried out, it would in principle lead to the correct sum. The situation can be studied by considering the first, or two "hole-line," contributions. The energy-contribution calculations here follow the usual procedures of the Brueckner method.[13,14] The difference comes only in the definition of the Green's function, which is defined as

$$G_{k,l}(r, r') = \int_0^{\infty} k''^2 \, dk'' \, \frac{j_l(k''r) j_l(k''r')}{2[H(k'') - \Delta(k)]} F(\bar{p}, k'', k). \tag{2.27}$$

The Brandow choice[5] is

$$H(k'') = \tfrac{1}{2}k''^2, \qquad \Delta(k) = E(k), \tag{2.28}$$

which uses the unperturbed energies for the occupied states and makes the hole-state energies self-consistent. This procedure sums[9] all the self-energy insertions on the hole lines but leaves the occupied state lines bare. The V expansion of E_b for this procedure does not exist on account of infinities in the coefficients for higher powers of V as we have shown previously.[2] In the rearranged series, these are canceled exactly by compensating contributions on the occupied state lines.

For normal nuclear-type potentials, the Brandow choice results in a large energy gap at the Fermi surface so that the convergence of the integral (2.27) is greatly improved. However, as we weaken the strength, the short-range repulsion becomes dominant and the energy gap becomes *negative*. This unhappy

circumstance makes the integral in (2.27) divergent! The consequence is that E_b from the two "hole-line" terms is not an analytic function on the positive real V axis. This trouble persists to arbitrarily small potential strengths with usual potentials for $N = \infty$. Furthermore, it also occurs for the analogous finite-N result. For N finite, we still have the first of inequalities (2.21) but not the second. We can, perhaps, therefore still establish an analytic continuation to V's of interest; however, with singularities in the right half-plane it is difficult to know whether we are on the right Riemann sheet of the resummation or, as in example (2.3), we have the incorrect answer for large x.

3. EXAMPLE OF THE HOLE-LINE RESUMMATION PROCEDURE

In this section, we shall give in some detail the results of applying the "hole-line" resummation procedures, using the Brandow choice (2.28) to two simple potentials which resemble the nucleon–nucleon potential to some extent. For simplicity, we choose them to be of the following form. First, for states of even relative angular momentum,

$$\begin{aligned} &V_T(r) = V_1, \quad V_S(r) = V_2, \quad 0 < r < c, \\ &V_T(r) = V_3, \quad V_S(r) = V_4, \quad c < r < d, \\ &V_T(r) = V_S(r) = 0, \qquad\quad d < r, \end{aligned} \tag{3.1}$$

where V_S is the singlet potential and V_T is the triplet potential. For states of odd relative angular momentum, we choose

$$\begin{aligned} &V_T(r) = V_5, \quad V_S(r) = V_6, \quad 0 < r < c, \\ &V_T(r) = V_S(r) = 0, \qquad\quad c < r. \end{aligned} \tag{3.2}$$

For the first potential, we have picked

$$\begin{aligned} &c = 0.4 \text{ F}, \quad d = \tfrac{29}{7}c, \\ &V_1 = V_2 = V_5 = V_6 = 10^5\hbar^2/Mc^2, \\ &V_3 = 1.25\left(\frac{7\pi}{44}\right)^2 \frac{\hbar^2}{Mc^2}, \quad V_4 = 0.96\left(\frac{7\pi}{44}\right)^2 \frac{\hbar^2}{Mc^2}. \end{aligned} \tag{3.3}$$

This potential has the 2-body data

$$\begin{aligned} a_T = 5.39 \text{ F}, \quad r_{0T} = 1.71 \text{ F}, \quad E_T = -2.20 \text{ MeV}, \\ a_S = -23.7 \text{ F}, \quad r_{0S} = 2.14 \text{ F}. \end{aligned} \tag{3.4}$$

All these values except E_T and r_{0S} were fitted. The singlet effective range should have been about 2.6 F. The singlet phase shift $\delta_0 = 0$ for k around 150 MeV instead of 200 MeV which serves to illustrate the well-known fact that the simple square-well shape is inadequate for nuclear forces.

Next, we note that according to the variational principle we can give a rigorous upper bound on the many-fermion binding energy by use of the first V-series term.[9] If we denote the momentum transform of the potential by $v(\mathbf{q}, \mathbf{q}_{\text{exch}})$, then we easily compute that

$$\begin{aligned} \frac{E}{N} \le \frac{3}{2^7\pi^4 k_F^3} \int d\mathbf{m}\, d\mathbf{n} [&4v_S(0, (\mathbf{m} - \mathbf{n})) + 2v_S(\mathbf{m} - \mathbf{n}, 0) \\ &+ 12v_T(0, \mathbf{m} - \mathbf{n}) - 6v_T(\mathbf{m} - \mathbf{n}, 0)], \end{aligned} \tag{3.5}$$

where $\mathbf{q}$ is the momentum transfer and $\mathbf{q}_{\text{exch}}$ is the exchanged momentum transfer and the range of integration is $|\mathbf{m}|$ and $|\mathbf{n}| \le k_F$. For this potential, the momentum representation can be expressed in terms of that for the simple square-well of various arguments. In this case, (3.5) can be evaluated exactly.[11] When this is done and the collapse limit $k_F \to \infty$ is taken, we obtain for our shape of potential

$$\begin{aligned} &\lim_{k_F \to \infty} \frac{E}{(k_F^3 N)} \\ &\le \frac{3}{2^5\pi^3}\left(\int_0^c (3V_1 + 9V_5) r^2\, dr + 3\int_c^d V_3 r^2\, dr \right. \\ &\quad \left. + \int_0^c (3V_2 + V_6) r^2\, dr + 3\int_c^d V_4 r^2\, dr\right) \\ &= \frac{3c^3}{2^5\pi^3} [3V_1 + 3V_2 + 9V_5 + V_6 + 100.36(V_3 + V_4)], \end{aligned} \tag{3.6}$$

where the last line has been evaluated for $d = \frac{29}{9}c$. We have increased the core radius to 0.51 F to roughly maintain its effective radius in the face of the weaker core repulsion anticipated. For our second potential, we have picked a Serber force, i.e., $V_5 = V_6 = 0$. In addition, we will choose

$$\begin{aligned} V_1 &= -(5.6)^2 V_3, \\ V_2 &= -(5.6)^2 V_4, \end{aligned} \tag{3.7}$$

and with this choice, by virtue of (3.6), the system will collapse (tend to infinity density) for any real negative V_3, V_4. (It will also collapse for real positive V_3, V_4 by a modification of the standard arguments.[1]) We have selected, in the same units as (3.3) where 1 = 259.2 MeV,

$$V_3 = -0.3318, \quad V_4 = -0.2290 \tag{3.8}$$

which values reproduce the deutron binding energy and the singlet scattering length. The triplet core is about 2.7 BeV.

We have adapted the numerical procedures of Baker, Gammel, and Hill [11] to compute the hole-line 2-particle energy contributions. The numerical details

are explained therein, except that we have used a 29-point mesh for r with 7 points in the core for the first potential. This procedure is closely parallel to that of Kallio and Day.[12] For the hard-core potential (non-collapsing), using $0 \leq l \leq 3$ at a density of $k_F c = 0.625$—the apparent saturation density for this potential (nuclear saturation density[3] is $k_F c = 0.544$)—we obtain the following results:

$$E_b = -8.38 \text{ MeV},$$
$$E(k) \simeq -122 \text{ MeV} + \tfrac{1}{2}k^2/m^*, \qquad (3.9)$$
$$m^* = 0.54,$$

where E_b is the binding energy and $E(k)$ is the converged single-particle energy for k less than the Fermi momentum k_F. The formula for $E(k)$ is only a fit to the final results and was not used in the determination. Four iterations were necessary for four-figure convergence. We used a new guess for the function $\Delta(k)$ which was $\frac{3}{4}$ of the way from the old to the new single-particle energy. Our results with this fairly crude potential are generally similar to those of Kallio and Day using a more realistic potential. Their binding energy was less, and the single-particle energy was about -81 MeV at $k = 0$ and had a larger $m^* \approx 0.6$ which yielded a similar but shallower, flatter curve.

The results for the second potential are qualitatively similar to those of the first potential. The main difference at $k_F c = 0.625$ comes from a more negative value of $E(0)$. The results are

$$E_b = -27.55 \text{ MeV},$$
$$E(k) \simeq -141 \text{ MeV} + \tfrac{1}{2}k^2/m^*, \qquad (3.10)$$
$$m^* = 0.56.$$

Of the change in binding energy, about 2 MeV of the 11-MeV shift are due to dropping the odd-state repulsions in going to Serber-type forces. The rest of the shift would roughly be expected,[4,15] in going to a soft core from a hard one. This result also accords with our results[16] on the velocity dependent force which exactly simulates a hard core in 2-body scattering. There, it was found to be less repulsive for the many-fermion problem than an ordinary hard core.

In Fig. 3, we have plotted both the two "hole-line" approximation to the binding energy using the Brandow choice for the energy denominators and the ladder approximation. It will be noted that the former shows the usual saturation minimum (although at higher density) even though the potential is known

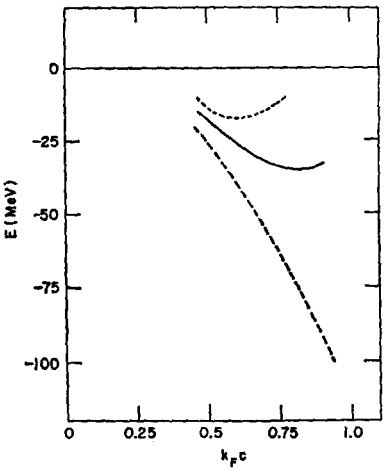

FIG. 3. Binding energy vs $k_F c$ for the soft-core, collapsing potential. The solid curve is the two "hole-line" approximation using the Brandow choice for the energy denominators. The dashed curve is the usual ladder approximation. For comparison, we have included the two "hole-line" approximation using the Brandow choice for the energy denominators for the binding energy curve for our hard-core potential (dotted curve).

to cause nuclear collapse. Following the usual procedures of that approximation, we would be led to the fallacious conclusion that a many-body system interacting under these forces would saturate at about $k_F c = 0.82$, with an energy of $E_b \approx -35$ MeV. The ladder approximation, on the other hand, not only has no minimum but curves downward.

Estimates of the relative importance of higher-order corrections to be expected can be given when we compare the first potential (hard core) with the second (soft core): "It should also be remembered that, for a soft-core potential, the 3-body interaction should not be so important," according to Rajaraman and Bethe.[17] They give an extensive discussion to justify this statement. This effect should, we feel, compensate for the increase in the size of the corrections due to a larger saturation density. Therefore, as far as we can tell, it is in line with current thinking on this subject to conclude that the next few terms (four-hole-line contributions have been considered recently by Day[18]) in the hole-line rearrangement using the Brandow choice, will converge about as well for our soft-core potential as for the hard-core one.

We are therefore left with only two alternatives: (i) that the sum given by the hole-line resummation procedure is incorrect; or (ii) that it is deceptive in low order. No matter which of these is the true state of affairs, we think it is therefore not satisfactory as a numerical method.

* This work performed under the auspices of the U.S. Atomic Energy Commission.

[1] J. M. Blatt and V. F. Weisskoff, *Theoretical Nuclear Physics* (Wiley, New York, 1952).
[2] G. A. Baker, Jr., Phys. Rev. **131**, 1869 (1963).
[3] B. D. Day, Rev. Mod. Phys. **39**, 719 (1967).
[4] R. Rajaraman and H. A. Bethe, Rev. Mod. Phys. **39**, 745 (1967).

[5] B. H. Brandow, Phys. Rev. **152**, 863 (1966).
[6] G. H. Hardy, *Divergent Series* (Oxford U.P., New York, 1956).
[7] V. V. Tolmachev, Dokl. Akad. Nauk. S.S.S.R. **141**, 582 (1961) [Sov. Phys. Dokl. **6**, 976 (1962)].
[8] G. A. Baker, Jr. and J. Kahane, J. Math. Phys. **10**, 1647 (1969).
[9] K. A. Brueckner, *The Many Body Problem*, C. de Witt, Ed. (Wiley, New York, 1959).
[10] G. A. Baker, Jr., Phys. Rev. **140**, B9 (1965).
[11] G. A. Baker, Jr., J. L. Gammel, and B. J. Hill, Phys. Rev. **132**, 1373 (1963).
[12] A. Kallio and B. D. Day, Nucl. Phys. **A124**, 177 (1969).
[13] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).
[14] K. A. Brueckner and K. S. Masterson, Phys. Rev. **128**, 2267 (1962).
[15] C. W. Wong, Nucl. Phys. **56**, 224 (1964).
[16] G. A. Baker, Jr., B. J. Hill, and R. J. McKee, Jr., Phys. Rev. **135**, A922 (1964).
[17] Reference 4, p. 770.
[18] B. D. Day, private communication.

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Eigenvalues and Eigenfunctions of the Spheroidal Wave Equation*

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A technique is presented for the calculation of the oblate and prolate spheroidal wave equation eigenvalues and eigenfunctions. The eigenvalue problem is cast in matrix form and a tridiagonal, symmetric matrix is obtained. This formulation permits the immediate calculation of the eigenvalues to the desired accuracy by means of the bisection method. The eigenfunction expansion coefficients are then obtained by a recursion method. This technique is quite simple to program, and the computation speed is rapid enough to allow its use as a function subroutine where values not previously tabulated or large numbers of values are required.

I. INTRODUCTION

The scalar wave equation

$$\nabla^2\psi + k^2\psi = 0 \tag{1}$$

is separable in both the oblate and prolate spheroidal coordinate systems. For this reason the formulation of physical problems in these coordinate systems has received much attention from a wide variety of disciplines. They offer an obvious generalization of physical processes described in spherical coordinate systems and, in addition, yield the extremely interesting limiting cases of the infinitely thin, finite "wire" and the infinitely thin, circular disk.

II. THE COORDINATE SYSTEMS

The notations and conventions of Flammer[1] will be used in the following. Due to the existence of thorough discussions of these coordinate systems and functions in the literature,[1,2] only that material necessary for a coherent presentation will be given here.

The prolate coordinate system (ξ, η, ϕ) may be defined in terms of a rectangular coordinate system by

$$x = \tfrac{1}{2}d[(1-\eta^2)(\xi^2-1)]^{\frac{1}{2}}\cos\phi, \tag{2}$$

$$y = \tfrac{1}{2}d[(1-\eta^2)(\xi^2-1)]^{\frac{1}{2}}\sin\phi, \tag{3}$$

$$z = \tfrac{1}{2}d\eta\xi, \tag{4}$$

where d is the interfocal distance. The oblate spheroidal coordinate system is obtained by replacing ξ with $i\xi$ and d with $-id$. In view of this simple transformation between the prolate and oblate coordinate systems, all expressions, although valid in both systems, will be written in terms of the prolate system. Both coordinate systems are shown in Fig. 1.

The scalar wave equation (1) now becomes

$$\frac{\partial}{\partial\eta}\left((1-\eta^2)\frac{\partial\psi}{\partial\eta}\right) + \frac{\partial}{\partial\xi}\left((\xi^2-1)\frac{\partial\psi}{\partial\xi}\right) + \frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2\psi}{\partial\phi^2} + c^2(\xi^2-\eta^2)\psi = 0, \tag{5}$$

[5] B. H. Brandow, Phys. Rev. **152**, 863 (1966).
[6] G. H. Hardy, *Divergent Series* (Oxford U.P., New York, 1956).
[7] V. V. Tolmachev, Dokl. Akad. Nauk. S.S.S.R. **141**, 582 (1961) [Sov. Phys. Dokl. **6**, 976 (1962)].
[8] G. A. Baker, Jr. and J. Kahane, J. Math. Phys. **10**, 1647 (1969).
[9] K. A. Brueckner, *The Many Body Problem*, C. de Witt, Ed. (Wiley, New York, 1959).
[10] G. A. Baker, Jr., Phys. Rev. **140**, B9 (1965).
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[13] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).
[14] K. A. Brueckner and K. S. Masterson, Phys. Rev. **128**, 2267 (1962).
[15] C. W. Wong, Nucl. Phys. **56**, 224 (1964).
[16] G. A. Baker, Jr., B. J. Hill, and R. J. McKee, Jr., Phys. Rev. **135**, A922 (1964).
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The scalar wave equation

$$\nabla^2\psi + k^2\psi = 0 \tag{1}$$

is separable in both the oblate and prolate spheroidal coordinate systems. For this reason the formulation of physical problems in these coordinate systems has received much attention from a wide variety of disciplines. They offer an obvious generalization of physical processes described in spherical coordinate systems and, in addition, yield the extremely interesting limiting cases of the infinitely thin, finite "wire" and the infinitely thin, circular disk.

II. THE COORDINATE SYSTEMS

The notations and conventions of Flammer[1] will be used in the following. Due to the existence of thorough discussions of these coordinate systems and functions in the literature,[1,2] only that material necessary for a coherent presentation will be given here.

The prolate coordinate system (ξ, η, ϕ) may be defined in terms of a rectangular coordinate system by

$$x = \tfrac{1}{2}d[(1-\eta^2)(\xi^2-1)]^{\frac{1}{2}}\cos\phi, \tag{2}$$

$$y = \tfrac{1}{2}d[(1-\eta^2)(\xi^2-1)]^{\frac{1}{2}}\sin\phi, \tag{3}$$

$$z = \tfrac{1}{2}d\eta\xi, \tag{4}$$

where d is the interfocal distance. The oblate spheroidal coordinate system is obtained by replacing ξ with $i\xi$ and d with $-id$. In view of this simple transformation between the prolate and oblate coordinate systems, all expressions, although valid in both systems, will be written in terms of the prolate system. Both coordinate systems are shown in Fig. 1.

The scalar wave equation (1) now becomes

$$\frac{\partial}{\partial\eta}\left((1-\eta^2)\frac{\partial\psi}{\partial\eta}\right) + \frac{\partial}{\partial\xi}\left((\xi^2-1)\frac{\partial\psi}{\partial\xi}\right) + \frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2\psi}{\partial\phi^2} + c^2(\xi^2-\eta^2)\psi = 0, \tag{5}$$

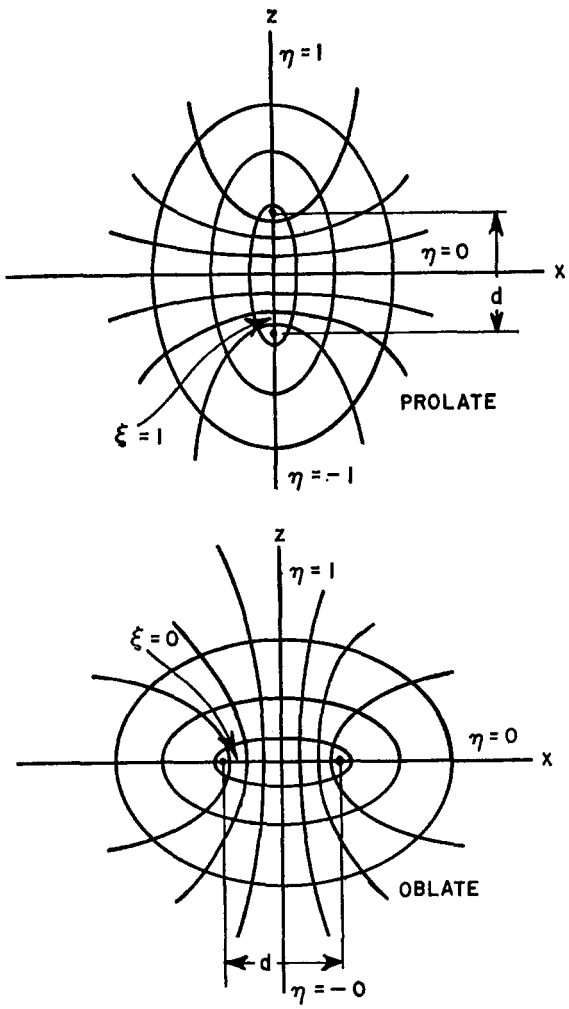

FIG. 1. Prolate and oblate coordinate systems.

where

$$c = \tfrac{1}{2}kd. \tag{6}$$

Solutions of the form

$$\psi_{mn} = S_{mn}(c, \eta)R_{mn}(c, \xi)\begin{matrix}\cos\\ \sin\end{matrix}(m\phi) \tag{7}$$

are assumed, and the separation of variables leads to the ordinary differential equations for the angular and radial functions, respectively,

$$\frac{d}{d\eta}\left((1-\eta^2)\frac{d}{d\eta}S_{mn}(c,\eta)\right) + \left(\lambda_{mn}(c) - c^2\eta^2 - \frac{m^2}{1-\eta^2}\right)S_{mn}(c,\eta) = 0, \tag{8}$$

$$\frac{d}{d\xi}\left((\xi^2-1)\frac{d}{d\xi}R_{mn}(c,\xi)\right) - \left(\lambda_{mn}(c) - c^2\xi^2 + \frac{m^2}{\xi^2-1}\right)R_{mn}(c,\xi) = 0. \tag{9}$$

The condition that ψ_{mn} be single valued requires that m take on only integer values and, without loss of generality, m may be assumed to be nonnegative. The eigenvalue $\lambda_{mn}(c)$ remains to be determined.

III. THE EIGENFUNCTIONS

When $c = 0$, Eq. (8) reduces to the defining equation for the associated Legendre polynomials; therefore, the following representation is chosen for the angular functions of the first kind:

$$S_{mn}(c, \eta) = \sum_{r=0,1}^{\infty}{}' d_r^{mn}(c)P_{m+r}^m(\eta). \tag{10}$$

The prime indicates that the summation is over only even values of r if $n - m$ is even and over odd values of r if $n - m$ is odd. The condition that

$$\lambda_{mn}(0) = n(n+1), \quad n \geq m, \tag{11}$$

is also obtained if $c = 0$. The angular functions of the second kind are necessary for a general solution of Eq. (8), but are seldom used and, therefore, will not be discussed here.

The radial functions of the first, second, third, and fourth kinds, $R_{mn}^{(1),(2),(3),(4)}(c, \xi)$, may be expanded in terms of the spherical Bessel, Neumann, and Hankel functions. Due to the similarity between the defining equation (9) for these functions and that [Eq. (8)] for the angular functions, the required radial function expansion coefficients are identical to the angular function expansion coefficients $d_r^{mn}(c)$. Thus, the determination of the coefficients $d_r^{mn}(c)$ suffices for the determination of all of the spheroidal functions. The necessary expansions are

$$R_{mn}^{(1),(2),(3),(4)}(c,\eta) = \frac{1}{\alpha}\left(\frac{\xi^2-1}{\xi^2}\right)^{\frac{1}{2}m}\sum_{r=0,1}^{\infty}{}' i^{r+m-n}d_r^{mn}(c)\frac{(2m+r)!}{r!} \times z_{m+r}^{(1),(2),(3),(4)}(c,\xi), \tag{12}$$

where

$$\alpha = \sum_{r=0,1}^{\infty}{}' d_r^{mn}(c)\frac{(2m+r)!}{r!} \tag{13}$$

and the $z_n^{(i)}$, $i = 1, 2, 3, 4$, are the spherical Bessel, Neumann, and Hankel functions of the first and second kind, respectively.

The substitution of Eq. (10) into Eq. (8) yields the following recursion relation for the angular-function-expansion coefficients:

$$A_r^m(c)d_{r+2}^{mn}(c) + [B_r^m(c) - \lambda_{mn}(c)]d_r^{mn}(c) + C_r^m(c)d_{r-2}^{mn}(c) = 0, \quad r \geq 0, \tag{14}$$

where

$$A_r^m(c) = \frac{(2m + r + 2)(2m + r + 1)}{(2m + 2r + 3)(2m + 2r + 5)} c^2, \quad (15)$$

$$B_r^m(c) = \frac{2(m + r)(m + r + 1) - 2m^2 - 1}{(2m + 2r - 1)(2m + 2r + 3)} c^2 + (m + r)(m + r + 1), \quad (16)$$

$$C_r^m(c) = \frac{r(r - 1)}{(2m + 2r - 3)(2m + 2r - 1)} c^2. \quad (17)$$

Note that the coefficients in this recursion relation do not depend upon n. The n dependence is introduced solely through the eigenvalue $\lambda_{mn}(c)$. This recursion relation provides a ready means of determining the expansion coefficients and, thus, the spheroidal functions. However, the use of this recursion relation hinges upon the determination of the eigenvalue $\lambda_{mn}(c)$.

IV. THE DETERMINATION OF THE EIGENVALUES

Previous calculations of the spheroidal eigenvalues have used the methods of Bouwkamp[3] or Stuckey and Layton.[4] In the Bouwkamp method, a power-series expansion of $\lambda_{mn}(c)$ in terms of c is obtained. The first six coefficients in this series have been determined[1]; however, a general expression for an arbitrary coefficient in this series has not been found. Thus, this series expansion provides only a means of obtaining an approximate value for $\lambda_{mn}(c)$. A variational procedure is then used to obtain successive improvements in the estimate of $\lambda_{mn}(c)$.

In the Stuckey and Layton method, the infinite-continued-fraction solutions of Eq. (14) are developed in terms of $\lambda_{mn}(c)$. The roots of these solutions then yield the eigenvalues. Although these methods have indeed been valuable in the absence of other approaches, they are both cumbersome and, at times, troublesome.

In the following, the eigenvalue problem is cast in matrix form, and a tridiagonal, symmetric matrix is obtained. Standard matrix procedures may then be used for determination of the eigenvalues. Because of the simplicity of the tridiagonal, symmetric form, these procedures are simple and even allow the computation time required for a particular desired accuracy to be estimated prior to the calculation. This procedure is a generalization of a technique orignially used by Weeks.[5] Let

$$D_q = C_{2q+s}, \quad (18)$$

$$E_q = B_{2q+s}, \quad (19)$$

$$F_q = A_{2q+s}, \quad (20)$$

and

$$a_q = d_{2q+s}, \quad (21)$$

where

$$s = 0, \quad \text{if } n - m \text{ is even},$$
$$= 1, \quad \text{if } n - m \text{ is odd}, \quad (22)$$

and the superscripts m and n and the argument c have been suppressed for simplicity. Then Eq. (14) becomes

$$D_q a_{q-1} + (E_q - \lambda)a_q + F_q a_{q+1} = 0, \quad q \geq 0. \quad (23)$$

This method of indexing allows the index q to range upward from zero in integer steps for all cases.

A change of variable

$$a_q = (D_1 D_2 D_3 \cdots D_q / F_0 F_1 F_2 \cdots F_{q-1})^{\frac{1}{2}} b_q \quad (24)$$

is made in Eq. (23), and the resulting expression is multiplied by $(F_0 F_1 F_2 \cdots F_{q-1}/D_1 D_2 D_3 \cdots D_q)^{\frac{1}{2}}$. The following form of the recursion relation is then obtained:

$$(D_q F_{q-1})^{\frac{1}{2}} b_{q-1} + (E_q - \lambda)b_q + (D_{q+1} F_q)^{\frac{1}{2}} b_{q+1} = 0, \quad q \geq 0. \quad (25)$$

The set of equations represented by Eq. (25) may be written in matrix form as

$$\begin{pmatrix} (E_0 - \lambda) & (D_1 F_0)^{\frac{1}{2}} & 0 & 0 & \cdots \\ (D_1 F_0)^{\frac{1}{2}} & (E_1 - \lambda) & (D_2 F_1)^{\frac{1}{2}} & 0 & \cdots \\ 0 & (D_2 F_1)^{\frac{1}{2}} & (E_2 - \lambda) & (D_3 F_2)^{\frac{1}{2}} & \cdots \\ 0 & 0 & (D_3 F_2)^{\frac{1}{2}} & (E_3 - \lambda) & \cdots \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}. \quad (26)$$

Thus, the spheroidal eigenvalue problem has been reduced to that of determining the eigenvalues of a real, tridiagonal, symmetric matrix. In practice, it is necessary to truncate this matrix to, say, an $N \times N$ matrix. The N eigenvalues then determined are denoted by $\lambda_{mn}(c)$, $n = m, m + 2, m + 4, \cdots, m + 2N - 2$ when arranged in order of increasing algebraic value.

The eigenvalues of the $N \times N$ tridiagonal, symmetric matrix are determined by the bisection method. It can be shown[6] that the eigenvalues lie in the range

$$|\lambda_{mn}(c)| \leq \max_q [|(D_q F_{q-1})^{\frac{1}{2}}| + |E_q| + |(D_{q+1} F_q)^{\frac{1}{2}}|]. \tag{27}$$

In successive steps of the bisection procedure, this range is halved, and the Sturm sequence property is used to determine in which resulting range the desired eigenvalue lies. Thus each successive application of the bisection procedure results in a reduction of the uncertainty of the eigenvalue by a factor of one-half. Typically, seven- or eight-digit accuracy can be obtained after about 30 bisections.

The bisection procedure also has the additional advantages of

(1) permitting the immediate calculation of any single desired eigenvalue without the calculation of other values and

(2) utilizing previously calculated values to reduce the uncertainty range and, thus, the computation time of subsequent values.

The bisection method is described in detail by Wilkinson[6] and will not be further treated here.

V. THE DETERMINATION OF THE EXPANSION COEFFICIENTS

Having obtained the eigenvalues, we may now use the recursion relation to determine the spheroidal-function-expansion coefficients $d_r^{mn}(c)$. For fixed m, n, and c, we note that $d_r^{mn}(c)$ assumes its largest values when

$$r \approx n - m. \tag{28}$$

This statement is an equality when c is zero as a consequence of the initial expansion in terms of the spherical eigenfunctions. In this particular case, $d_{n-m}^{mn}(0) = 1$ and all other coefficients $r \neq n - m$ are zero.

Since minimum error generally occurs when a recursive calculation proceeds toward larger values, the recursion is started at $r = s$. Assuming a value for the first coefficient, i.e.,

$$h_s^{mn}(c) = g d_s^{mn}(c) = 1, \tag{29}$$

where g is an unknown constant, we solve the recursion relation

$$h_{r+2}^{mn}(c) = -\frac{[B_r^m(c) - \lambda_{mn}(c)]h_r^{mn}(c) + C_r^m(c)h_{r-2}^{mn}(c)}{A_r^m(c)} \tag{30}$$

upward to obtain $h_{n-m}^{mn}(c)$. This is made possible by the fact that $C_s^m(c) = 0$. Now, for some large p where $p > n - m$, it is assumed that

$$h_{p+2}'^{mn}(c) = g' d_{p+2}^{mn}(c) \approx 0 \tag{31}$$

and

$$h_p'^{mn}(c) = g' d_p^{mn}(c) = t, \tag{32}$$

where g' is another unknown constant, t is an arbitrary small constant, and the prime indicates that the normalization is different than that used in Eq. (29). The recursion relation

$$h_{r-2}'^{mn}(c) = -\frac{A_r^m(c)h_{r+2}'^{mn}(c) + [B_r^m(c) - \lambda_{mn}(c)]h_r'^{mn}(c)}{C_r^m(c)} \tag{33}$$

is then solved downward to obtain $h_{n-m}'^{mn}(c)$.

The ratio of the two values obtained when $r = n - m$ can now be used to obtain a consistent set of coefficients having only one normalization constant; i.e.,

$$h_r^{mn}(c) = \frac{h_{n-m}^{mn}(c)}{h_{n-m}'^{mn}(c)} h_r'^{mn}(c), \tag{34}$$

for $r > n - m$.

Flammer's normalization[1] is used to determine the remaining constant g. This normalization is

$$\sum_{r=s}^{\infty}{}' F_r^m d_r^{mn}(c) = F_{n-m}^m, \tag{35}$$

where

$$F_r^m = \frac{(-1)^{r-s}(r + 2m + s)!}{2^r[\frac{1}{2}(r - s)]! \, [\frac{1}{2}(r + 2m + s)]!}. \tag{36}$$

Therefore,

$$g = \frac{1}{F_{n-m}^m} \sum_{r=s}^{\infty}{}' F_r^m h_r^{mn}(c) \tag{37}$$

and

$$d_r^{mn}(c) = g^{-1} h_r^{mn}(c). \tag{38}$$

Having obtained the expansion coefficients, we can readily generate the spheroidal functions from the expansions in terms of the spherical eigenfunctions.

This technique has been used for the calculation of both prolate and oblate functions over the ranges $n = 0, 1, \cdots, 22$, $m = 0, 2$, and $C = 0.2, 0.4, \cdots, 15.2$. These values have been compared with good agreement whenever possible with existing tabulated values.[1,4,7] Programs have been run on IBM 7094 and Com-Share SDS 940 time-sharing computers. No computational problems have been encountered. Listings of the programs used may be found in Ref. 8.

Sample computed values of the oblate spheroidal eigenvalues, expansion coefficients, and eigenfunctions are shown in Tables I, II, and III. An accuracy

TABLE I. Sample oblate spheroidal eigenvalue calculations. Matrix truncation size: $N = 5$; accuracy criteria: 7 digits.

	$\lambda_{on}(-i4.0)$			
n	Hodge	Flammer[1]	Stuckey and Layton[4]	Hanish[7]
0	−9.150793213E + 00	−9.15080E + 00	−9.1507933808E + 00	−9.150793381E + 00
2	2.214079039E − 01	2.2141 E − 01	2.2140790999E − 01	2.214079100E − 01
4	1.237214448E + 01	—	1.2372144801E + 01	1.237214480E + 01
6	3.415256711E + 01	—	3.4152567410E + 01	3.415256741E + 01
8	6.408657399E + 01	—	6.4086572621E + 01	6.408657262E + 01

TABLE II. Sample oblate spheroidal eigenfunction expansion coefficient calculations. Downward recursion started at $p = 26$.

	$d_r^{06}(-i4.0)$	
r	Hodge	Stuckey and Layton[4]
0	−6.531966221E − 04	−6.5319660505E − 04
2	+1.209002662E − 02	+1.2090026397E − 02
4	−1.426437444E − 01	−1.4264374300E − 01
6	9.260509647E − 01	9.2605096847E − 01
8	1.438420222E − 01	1.4384202427E − 01
10	9.474026638E − 03	9.4740268162E − 03
12	3.642271321E − 04	3.6422713995E − 04
14	9.365921365E − 06	9.3659215831E − 06
16	1.740994242E − 07	1.7409942846E − 07
18	2.461650191E − 09	2.4616502542E − 09
20	2.745315670E − 11	2.7453157421E − 11
22	2.481746195E − 13	2.4817462624E − 13
24	1.857856240E − 15	1.8578562941E − 15
26	1.171756940E − 17	1.1717939083E − 17

criterion of seven digits was set on the eigenvalue calculations. This criterion is simply determined by the number of bisections performed and, of course, subsequently limits the accuracy of the expansion coefficients and eigenfunctions. The other accuracy determining parameters are the truncation size of the eigenvalue matrix and the starting point of the expansion coefficient downward recursion. The choice of these parameters appears to present no problem. The parameters presented in Tables I and II are typical of the values used over the ranges of independent variables and orders investigated. Average computation times on the SDS 940 time-sharing system for the values shown were 0.4 sec per eigenvalue, 0.01 sec per expansion coefficient, and 0.018 sec per eigenfunction.

VI. SUMMARY

A new technique has been presented for the calculation of the eigenvalues and eigenfunctions of the scalar oblate and prolate spheroidal wave equations. This technique is based upon the reduction of the eigenvalue problem to that of finding the eigenvalues of a real, tridiagonal, symmetric matrix. This reduction permits well-known procedures which are both rapid and accurate to be used for the eigenvalue calculations. The spheroidal function expansion coefficients are determined, subsequently, by a recursive method.

TABLE III. Sample oblate spheroidal eigenfunction calculations.

Function	Hodge	Hanish[7]
$S_{06}(-i4.0, 0.0)$	−3.12500000E − 01	—
$S_{06}(-i4.0, 1.0)$	9.48533868E − 01	—
$R_{06}^{(1)}(-i4.0, i0.0)$	6.88638164E − 04	6.886381410E − 04
$R_{06}^{(2)}(-i4.0, i0.0)$	−6.18960815E + 01	−6.189608272E + 01

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[1] C. Flammer, *Spheroidal Wave Functions* (Stanford U.P., Stanford, Calif., 1957).
[2] J. A. Stratton, P. M. Morse, L. J. Chu, D. C. Little, and F. J. Corbato, *Spheroidal Wave Functions* (Wiley, New York, 1956).
[3] C. J. Bouwkamp, J. Math. & Phys. **26**, 79 (1947).
[4] M. M. Stuckey and L. L. Layton, David Taylor Model Basin, Washington, D.C., AML Report 164, 1964.
[5] W. L. Weeks, Electrical Engineering Research Laboratory, University of Illinois, Technical Report No. 38, 1959.
[6] J. H. Wilkinson, *Algebraic Eigenvalue Problem* (Clarendon, Oxford, 1965), p. 229.
[7] S. Hanish, Naval Research Laboratory, Washington, D.C. (private communication).
[8] D. B. Hodge, ElectroScience Laboratory, Department of Electrical Engineering, The Ohio State University, Columbus, Report 2415-4, 1969, prepared under Contract F19628-67-C-0239 for Air Force Cambridge Research Laboratories.

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New Theorems about Spherical Harmonic Expansions and $SU(2)$*

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Despite the heroic efforts of Laplace, Legendre, Maxwell, Hobson, and company, there are still new chapters to be written in the theory of spherical harmonics. This paper describes some of the special windfalls that result when one expands analytic functions. In technical language, we are concerned with Fourier series of analytic functions on $SU(2)$.

1. INTRODUCTION

Suppose we wish to consider a function f of a real variable x. In the course of our study, we may attempt to expand f in a Taylor series about a point x_0. As every student knows, or should know, the behavior of a Taylor series cannot be completely understood until one introduces the notion of a complex plane and considers f as a function of a complex variable. Indeed, the Taylor series for f converges within the largest circle (in the complex plane) about x_0 which does not contain any singularities of f.

Analogous results hold if we attempt to expand f in some other manner. For example, if we attempt to expand f in terms of a set of orthogonal polynomials on the interval $[a, b]$, we will find that the expansion converges within the largest ellipse (in the complex plane) which has a and b as foci and which does not contain singularities of f.[1] Similarly, if we attempt to expand f in terms of polynomials which are orthogonal on an infinite interval, such as Hermite or Laguerre polynomials, we will find that the expansion converges in certain other characteristic regions such as strips or parabolas.[1,2]

In this paper, we will study the expansion in spherical harmonics of functions f defined on the surface of a sphere. In analogy with the case of functions defined on the real line and just discussed in the previous paragraphs, we will find that the sphere should be regarded as the "real part" of a certain complex manifold and that we will need to examine the "analytic" behavior of f on this complex manifold. Thus, we will enlarge the domain of definition of f and consider what it means for f to be singular or free of singularities in this larger domain. We shall find that the spherical harmonic expansion for f,

$$f = \sum a_{lm} Y_l^m(\theta, \phi), \tag{1.1}$$

actually converges in a certain characteristic region in our "complexified" sphere and that the size of this region depends on the location of the singularities of f. We shall also find that the behavior of the coefficients a_{lm} for large l [i.e., the rate of convergence of the series (1.1)] is governed by the location of these singularities. Finally, we shall discover a new formula for the expansion coefficients a_{lm} which differs from the usual formula

$$a_{lm} = \int d\Omega f \bar{Y}_l^m \tag{1.2}$$

in that it involves contour integrals of the function f over the complexified sphere.

To be more precise, what we shall actually study in this paper is the expansion, in terms of the Wigner D^j functions, of various functions f defined on the group $SU(2)$. Formulas (1.1) and (1.2) are special cases of more general formulas holding for such expansions. In fact, we shall see that the results that we have just advertised for spherical-harmonic expansions are special cases of similar results for "Wigner" expansions. Section 2 presents a review of facts about the group $SU(2)$, its complexification $SL(2, C)$, and some of their representations. Section 3 defines what is meant by an analytic manifold and what it means for a function to be analytic on such a manifold. Section 4 is devoted to studying when, where, and how a Wigner expansion converges. Section 5 derives the relationship between the analytic properties of a function f and bounds on its expansion coefficients. A final section contains new formulas for these expansion coefficients, a curious version of Cauchy's theorem for functions defined on $SU(2)$, and similar results for spherical-harmonic expansions.

It is anticipated that our results [which in a mathematician's language are concerned with "Fourier series of analytic functions on $SU(2)$"] can be fairly easily extended to the general case of simply connected compact Lie groups.

2. FACTS ABOUT $SU(2)$ AND $SL(2, C)$

In this section we summarize various facts about $SU(2)$ and $SL(2, C)$ which will be needed in subsequent sections. Most results will be stated without proof but with references to appropriate literature.

A. The Group $SU(2)$

The group $SU(2)$ is the set of all 2×2 unitary matrices with determinant $+1$. If u is any element in $SU(2)$, it can be conveniently written in the form[3,4]

$$u = \exp(\tfrac{1}{2}i\boldsymbol{\beta}\cdot\boldsymbol{\sigma}), \tag{2.1}$$

where $\boldsymbol{\beta}$ is a real 3-vector,

$$\boldsymbol{\beta}\cdot\boldsymbol{\sigma} = \sum_{j=1}^{3}\beta_j\sigma_j, \tag{2.2}$$

and the σ_j are the Pauli matrices

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \tag{2.3a}$$

$$\sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \tag{2.3b}$$

$$\sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{2.3c}$$

We shall also need a matrix σ_4 defined by

$$\sigma_4 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{2.3d}$$

It is easily verified that

$$(\boldsymbol{\beta}\cdot\boldsymbol{\sigma})^2 = (\boldsymbol{\beta}\cdot\boldsymbol{\beta})\sigma_4 = \beta^2\sigma_4. \tag{2.4}$$

Thus, the Taylor series for (2.1) can be explicitly summed to give

$$u = \sigma_4\cos(\tfrac{1}{2}\beta) + i\boldsymbol{\beta}\cdot\boldsymbol{\sigma}\beta^{-1}\sin(\tfrac{1}{2}\beta). \tag{2.5}$$

The parametrization (2.1) is unique for $\beta < 2\pi$. In the case $u = -\sigma_4$, we may choose any $\boldsymbol{\beta}$ with $\beta = 2\pi$.

As is well known, the group $SU(2)$ is the covering group for the 3-dimensional rotation group $O(3)$. In fact, if $R(\theta, \hat{\mathbf{n}})$ is the 3×3 rotation matrix for a rotation by an angle θ about the axis in the direction of the unit vector $\hat{\mathbf{n}}$, we have the explicit relations

$$u^\dagger\sigma_j u = \sum_k R_{jk}\sigma_k, \quad 1 \le j, k \le 3, \tag{2.6a}$$

$$R_{jk}(\theta, \hat{\mathbf{n}}) = \tfrac{1}{2}\,\mathrm{Tr}\,(u^\dagger\sigma_j u\sigma_k), \tag{2.6b}$$

when u is given by the expression

$$u = \exp(\tfrac{1}{2}i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}). \tag{2.6c}$$

Formulas (2.1) and (2.5) show that the topology of $SU(2)$ is that of a ball of radius 2π with all points on the surface identified. The topology of $SU(2)$ is also that of S^3, the 3-dimensional surface of a sphere in 4-dimensional space. To see this, we need to examine the form of a unitary matrix. We write

$$u = \begin{pmatrix}a & b\\ c & d\end{pmatrix}. \tag{2.7}$$

The conditions $u^\dagger u = uu^\dagger = \sigma_4$ require that both the rows and columns of u are orthonormal unit vectors. It follows that $|a|^2 + |b|^2 = 1$ and $|b|^2 + |d|^2 = 1$, whence $|a| = |d|$. Similarly, $|b| = |c|$. Thus we can also write u in the form

$$u = \begin{pmatrix}a & b\\ -\xi\bar{b} & \eta\bar{a}\end{pmatrix}, \tag{2.8}$$

where ξ and η have modulus one. The condition that the rows be orthogonal gives $\xi = \eta$, and the requirement that $\det u = 1$ gives $\eta = 1$. Now write $a = x_4 + ix_3$ and $b = x_2 + ix_1$ with the x_i real. Then

$$u = \begin{pmatrix}x_4 + ix_3 & x_2 + ix_1\\ -x_2 + ix_1 & x_4 - ix_3\end{pmatrix} = i\mathbf{x}\cdot\boldsymbol{\sigma} + x_4\sigma_4 \tag{2.9}$$

and the condition $\det u = 1$ gives

$$\sum_{i=1}^{4}x_i^2 = 1. \tag{2.10}$$

If (2.10) is satisfied, u is also unitary.

The matrices $\frac{1}{2}\sigma_i$ (with $i = 1, 2, 3$) form a Lie algebra with the commutation rules

$$[\tfrac{1}{2}\sigma_a, \tfrac{1}{2}\sigma_b] = i\tfrac{1}{2}\sigma_c, \tag{2.11}$$

where a, b, c denotes a cyclic permutation of 1, 2, 3. Let J_a with $a = 1, 2, 3$ denote a set of matrices obeying the $SU(2)$ commutation rules:

$$[J_a, J_b] = iJ_c. \tag{2.12}$$

The finite-dimensional irreducible representations of (2.12) are well known.[3,5] Each irreducible representation, which can be chosen in such a manner that the J's are Hermitian, is labeled by an integer or half-integer j, and is of dimension $(2j + 1)$. Vectors within a representation are labeled by a number m which ranges between $-j$ and j in integer steps. The vectors, which we denote by $|jm\rangle$, obey the relations

$$J_3|jm\rangle = m|jm\rangle, \tag{2.13a}$$

$$\sum_{k=1}^{3}J_k^2|jm\rangle = j(j+1)|jm\rangle. \tag{2.13b}$$

The representations of the Lie algebra of $SU(2)$ can be exponentiated to give a representation of the group. To each element u of $SU(2)$ we assign a unitary matrix $U(u)$ by the rule

$$U(u) = \exp(i\boldsymbol{\beta}\cdot\mathbf{J}), \tag{2.14}$$

where u has the parametrization (2.1). That this produces a representation of $SU(2)$, i.e.,

$$U(u_1)U(u_2) = U(u_1u_2), \tag{2.15}$$

is a consequence of the Campbell–Baker–Hausdorff (CBH) theorem.[6,7] It states that, for any two $n \times n$

matrices A and B and for s and t sufficiently small, one has the relation

$$\exp(sA)\exp(tB) = \exp(C). \tag{2.16}$$

The matrix C can be expressed as a double-power series in s and t which is convergent for s and t sufficiently small. Further, and most importantly, the coefficients in this power series are all elements formed by taking multiple commutators of A and B. That is, the coefficients are all elements of the Lie algebra generated by A and B. Thus, if we have two sets of matrices which obey the same commutation rules, they will combine in the same manner under the operation (2.16).

B. The Group $SL(2, C)$

The group $SL(2, C)$ is the group of all 2×2 matrices, unitary or otherwise, with determinant $+1$. The symbol C denotes our willingness to work over the complex-number field. $SU(2)$ is evidently a subgroup of $SL(2, C)$. If g is an element in $SL(2, C)$ which is sufficiently near the identity σ_4, it can be written uniquely in the form

$$g = \exp(\tfrac{1}{2}\boldsymbol{\gamma}\cdot\boldsymbol{\sigma}), \tag{2.17}$$

where $\boldsymbol{\gamma}$ is in general some *complex* 3-vector.

It is not true that every element in $SL(2, C)$ can be written in the form (2.17). [The element $(-\sigma_4 - \frac{1}{2}\sigma_1 - \frac{1}{2}i\sigma_2)$ provides a counter example.] However, every element can be written in the form[4]

$$g = \exp(\tfrac{1}{2}\boldsymbol{\alpha}\cdot\boldsymbol{\sigma})\exp(\tfrac{1}{2}i\boldsymbol{\beta}\cdot\boldsymbol{\sigma}), \tag{2.18}$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are real 3-vectors. The first factor is Hermitian and positive definite. The second belongs to $SU(2)$. Both factors are uniquely defined. We record for future reference an explicit formula for α,

$$2\cosh\alpha = \mathrm{Tr}\,(gg^{\dagger}), \tag{2.19}$$

which follows from (2.18) and the complex forms of (2.1) and (2.5). Unlike $\boldsymbol{\beta}$, the domain of $\boldsymbol{\alpha}$ is completely unrestricted. Thus the topology of $SL(2, C)$ is $E^3 \times S^3$.

As with $SU(2)$, representations of $SL(2, C)$ can be obtained by exponentiating J matrices. If g is any element in $SL(2, C)$, we define a matrix $G(g)$ by the rule

$$G(g) = \exp(\boldsymbol{\alpha}\cdot\mathbf{J})\exp(i\boldsymbol{\beta}\cdot\mathbf{J}). \tag{2.20}$$

Here we have used the parametrization (2.18). If g is sufficiently near the identity, we may also write

$$G(g) = \exp(\boldsymbol{\gamma}\cdot\mathbf{J}), \tag{2.21}$$

in keeping with the parametrization (2.17). The CBH theorem guarantees that the definitions (2.20) and (2.21) agree and that the matrices $G(g)$ form a representation of $SL(2, C)$. [In fact, using one of the standard notations, the representations obtained in this way are $D(j, 0)$.][8]

C. Group Integration

The last tool we shall need is group integration over $SU(2)$. We assign to $SU(2)$ the unique left and right invariant measure du having the property

$$\int f(u)\,du = \int f(u_1 u u_2)\,du, \tag{2.22}$$

for any elements u_1 and u_2 in $SU(2)$ and any function f. If u is parametrized in terms of Euler angles,

$$u = \exp(-\tfrac{1}{2}i\phi\sigma_3)\exp(-\tfrac{1}{2}i\theta\sigma_2)\exp(-\tfrac{1}{2}i\psi\sigma_3), \tag{2.23}$$

the measure du is given by

$$du = (16\pi^2)^{-1}\sin\theta\,d\theta\,d\phi\,d\psi. \tag{2.24}$$

Carrying out the multiplications indicated in (2.23) and comparing the result with (2.9) give the relations

$$x_1 = +\sin\tfrac{1}{2}\theta\sin\tfrac{1}{2}(\phi - \psi), \tag{2.25a}$$

$$x_2 = -\sin\tfrac{1}{2}\theta\cos\tfrac{1}{2}(\phi - \psi), \tag{2.25b}$$

$$x_3 = -\cos\tfrac{1}{2}\theta\sin\tfrac{1}{2}(\phi + \psi), \tag{2.25c}$$

$$x_4 = +\cos\tfrac{1}{2}\theta\cos\tfrac{1}{2}(\phi + \psi). \tag{2.25d}$$

It is easily verified that S^3 is covered once, and only once, when the angular variables take on the values $\phi \in [0, 2\pi]$, $\theta \in [0, \pi]$, and $\psi \in [0, 4\pi]$.[9] With this region of integration and the measure (2.24), the integral of du over the whole group is unity. In calculations to be done later on, we shall sometimes find it useful to replace ϕ and ψ by sum and difference variables:

$$\sigma = \tfrac{1}{2}(\phi + \psi), \tag{2.26a}$$

$$\delta = \tfrac{1}{2}(\phi - \psi). \tag{2.26b}$$

In this case du is given by the expression

$$du = (8\pi^2)^{-1}\sin\theta\,d\theta\,d\delta\,d\sigma, \tag{2.27}$$

and the group is covered once when the variables take on the values $\delta, \sigma \in [0, 2\pi]$ and $\theta \in [0, \pi]$.

3. ANALYTIC MANIFOLDS AND FUNCTIONS THEREON

A. Analytic Manifolds

Loosely speaking, a manifold is a set which locally looks like a Euclidean space of some dimension. That is, there exists a 1-to-1 bicontinuous mapping (a homeomorphism) between a neighborhood of any point in the manifold and some Euclidean space. The groups $SU(2)$ and $SL(2, C)$ are manifolds. If u_0 is any element of $SU(2)$ and u is near u_0, then uu_0^{-1} is near the

identity so that we may write

$$u = \exp(\tfrac{1}{2}i\boldsymbol{\beta}\cdot\boldsymbol{\sigma})u_0\,, \tag{3.1}$$

with $\boldsymbol{\beta}$ being a "small" vector. Equation (3.1) gives an explicit map between points near the origin of E^3 and a small neighborhood of u_0. Similarly, if g_0 is any element of $SL(2, C)$ and g is near g_0, we may write

$$g = \exp(\tfrac{1}{2}\boldsymbol{\gamma}\cdot\boldsymbol{\sigma})g_0\,, \tag{3.2}$$

where $\boldsymbol{\gamma}$ is a "small" complex 3-vector. By treating the real and imaginary parts of $\boldsymbol{\gamma}$ separately, we see that (3.2) is a map between points near the origin of E^6 and a neighborhood of g_0. In keeping with the standard terminology, we shall call the images of Euclidean space under the mappings (3.1) and (3.2) *coordinate patches* for the groups $SU(2)$ and $SL(2,C)$, respectively. The real components of $\boldsymbol{\beta}$ and the real and imaginary components of $\boldsymbol{\gamma}$ will be called local coordinates.

We are now in a position to say what it means for a manifold to be analytic. Suppose two coordinate patches overlap. Then a group element in the overlap region has two sets of local coordinates, and it is possible in this region to express one set of coordinates in terms of the other. We thus get a mapping of E^n into E^n where, in our cases, $n = 3$ or 6. A manifold is said to be *real analytic* if one set of coordinates has a convergent Taylor-series expansion in terms of the other. Note that all terms in the Taylor series are real, for the coordinates are real by definition.

Evidently, as defined, the property of being real analytic is a joint property of both the manifold and the choice of coordinates. However, each choice of coordinates can be uniquely extended to a maximal family of coordinate systems by considering all those coordinate systems which are related in a (real) analytic way to the initial coordinate system. Since many choices of coordinate systems lead to the same maximal family, we can, in this manner, remove much of the arbitrariness pertaining to a particular choice of coordinates.[10]

The groups $SU(2)$ and $SL(2, C)$ are both real analytic manifolds: Suppose u_0 and u_0' are two nearby elements in $SU(2)$ and $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ are the coordinates for the corresponding coordinate patches. In the region of overlap, we have, using (3.1), the relation

$$\exp(\tfrac{1}{2}i\boldsymbol{\beta}'\cdot\boldsymbol{\sigma}) = \exp(\tfrac{1}{2}i\boldsymbol{\beta}\cdot\boldsymbol{\sigma})u_0(u_0')^{-1}. \tag{3.3}$$

Since u_0 and u_0' are nearby, the element $u_0(u_0')^{-1}$ can be written in exponential form with a small exponent. Applying the CBH theorem, we conclude that the components of $\boldsymbol{\beta}'$ can be expressed as convergent power series in the components of $\boldsymbol{\beta}$. A similar argument may be made for $SL(2, C)$. In this case, we find that the six components of Re $\boldsymbol{\gamma}'$ and Im $\boldsymbol{\gamma}'$ are related to the six components of Re $\boldsymbol{\gamma}$ and Im $\boldsymbol{\gamma}$ by six Taylor series in the six components of Re $\boldsymbol{\gamma}$ and Im $\boldsymbol{\gamma}$. The knowledgeable reader will observe that what we have been saying is a consequence of the fact that $SU(2)$ and $SL(2, C)$ are Lie groups. It is, in fact, part of the definition of what it means for a group to be a Lie group.[10]

The group $SL(2, C)$ is also a *complex* analytic manifold. We observe that the expression (3.2) may also be viewed as a mapping between a neighborhood of $SL(2, C)$ and C^3, the space of three complex variables. That is, we may treat each component of $\boldsymbol{\gamma}$ as a complex variable. Looking at the analog of (3.3) for $SL(2, C)$ and the CBH theorem, we see that, in fact, the three components of $\boldsymbol{\gamma}'$, when viewed as complex numbers, are analytic functions of the three complex components of $\boldsymbol{\gamma}$. That is, the three components of $\boldsymbol{\gamma}'$ each have a convergent Taylor expansion (a triple-power series) in the three components of $\boldsymbol{\gamma}$.

Evidently, every complex analytic manifold of complex dimension n is also a real analytic manifold of dimension $2n$. However, the reader is warned that not every real analytic manifold of dimension $2n$ is a complex analytic manifold of complex dimension n. S^4 provides a counterexample.[11] Finally, we remark that $SL(2, C)$ may be viewed as the complexification of $SU(2)$, and hence $SU(2)$ may be regarded as the real part of $SL(2, C)$.[12,13]

B. Analytic Functions

The last topic to be discussed in this section is what it means for a function to be real or complex analytic. A function f on a manifold is a rule which assigns a number, in general complex, to each point in the manifold. At each point in the manifold, we may introduce a local coordinate patch with real coordinate variables. Our function f then becomes (locally) a function of the real coordinate variables. The function f is said to be *real analytic* on the manifold if, *at each point*, it has a convergent multiple Taylor expansion in the local real coordinate variables. (Note that the function itself need not take on only real values.) Evidently, our definition as it stands appears to depend on the choice of coordinate system. However, since "an analytic function of an analytic function is again analytic," our definition is, in fact, coordinate free.

To get the feel of what it means to be real analytic, consider functions defined on S^2, the surface of a sphere in 3-dimensional space. It is easily verified that S^2 becomes a real analytic manifold, if we take as a

family of coordinate systems spherical polar coordinates with various polar axes. Each polar-coordinate system provides a good set of coordinates, i.e., a homeomorphic mapping between S^2 and E^2, everywhere except at its poles. Where two coordinate systems overlap and are both good, they are analytically related.

Let us choose the z axis as polar axis, and let the polar angles θ, ϕ be defined by the standard relations

$$x = \sin\theta\cos\phi, \tag{3.4a}$$

$$y = \sin\theta\sin\phi, \tag{3.4b}$$

$$z = \cos\theta. \tag{3.4c}$$

We claim that the function $\cos\theta$ is real analytic on S^2, but $\sin\theta$ is not. Evidently, both are entire functions of θ and are therefore real analytic functions wherever θ, ϕ form a good coordinate system. To examine their behavior at the poles $\theta = 0, \pi$ (where ϕ is undefined), we need a different coordinate system. A suitable choice is the coordinate pair x, y. It produces two coordinate patches, one covering the northern hemisphere and the other the southern. It is easily verified that these patches are analytically related to those provided by spherical coordinates wherever they overlap. At the north pole, we have

$$\cos\theta = +(1 - x^2 - y^2)^{\frac{1}{2}}, \tag{3.5a}$$

$$\sin\theta = +(x^2 + y^2)^{\frac{1}{2}}. \tag{3.5b}$$

We see that $\cos\theta$ has a double Taylor-series expansion in x and y, but $\sin\theta$ does not. A similar result holds at the south pole. Thus, $\cos\theta$ is real analytic on S^2, but $\sin\theta$ is not.

We shall next demonstrate that all the spherical harmonics $Y_l^m(\theta, \phi)$ are real analytic on S^2. Firstly, we already know that Y_1^0 is real analytic, since it is proportional to $\cos\theta$. Let us examine Y_1^1. We have the relation

$$Y_1^1 \propto \sin\theta e^{i\phi}, \tag{3.6}$$

which shows that Y_1^1 is real analytic wherever θ, ϕ are good coordinates. At the north pole we have

$$Y_1^1 \propto x + iy, \tag{3.7}$$

which is manifestly a convergent Taylor expansion. A similar result holds at the south pole. Thus Y_1^1 is real analytic. The same arguments succeed for Y_1^{-1}. Finally, since all the Y_l^m can be built up by taking finite sums of finite products of the Y_1^m, we conclude that all the Y_l^m are real analytic.

We now return to $SU(2)$. Consider the functions $D^j_{\mu\lambda}(u)$ defined on $SU(2)$ by the formula

$$D^j_{\mu\lambda}(u) = \langle j\mu|\, U(u)\,|j\lambda\rangle, \tag{3.8}$$

where we have used the notation of (2.13) and (2.14). If u is parametrized by the Euler angles, Eq. (2.23), $D^j_{\mu\lambda}(u)$ is just the Wigner rotation function $D^j_{\mu\lambda}(\phi\theta\psi)$. We claim that the functions $D^j_{\mu\lambda}$ are real analytic on $SU(2)$. At least two proofs of this statement are possible. One proceeds in a similar fashion to that given for the Y_l^m on S^2. We shall present another.

Suppose u is near u_0. We introduce local coordinates as in (3.1) to obtain the relation

$$D^j_{\mu\lambda}(u) = \langle j\mu|\, U(\boldsymbol{\beta})U(u_0)\,|j\lambda\rangle \tag{3.9a}$$

$$= \sum_\nu \langle j\mu|\, U(\boldsymbol{\beta})\,|j\nu\rangle\, D^j_{\nu\lambda}(u_0), \tag{3.9b}$$

where

$$U(\boldsymbol{\beta}) = \exp(i\boldsymbol{\beta}\cdot\mathbf{J}). \tag{3.9c}$$

Here, we have used the representation property (2.15). Note that the sum on ν in (3.9b) is over a finite range. Thus, if we can show that the terms $D^j_{\mu\nu}(\boldsymbol{\beta}) = \langle j\mu|\, U(\boldsymbol{\beta})\,|j\nu\rangle$ have a convergent Taylor expansion in the components of $\boldsymbol{\beta}$, we will have shown that $D^j_{\mu\lambda}$ is real analytic on $SU(2)$. By definition, we have

$$U(\boldsymbol{\beta}) = \sum_{n=0}^{\infty} (n!)^{-1}(i\boldsymbol{\beta}\cdot\mathbf{J})^n. \tag{3.10}$$

Therefore, $D^j_{\mu\nu}(\boldsymbol{\beta})$ is an infinite sum of polynomials in the components of $\boldsymbol{\beta}$. We shall show that this sum is absolutely and uniformly convergent on any compact set and hence analytic in the components of $\boldsymbol{\beta}$. Define the matrix A by the rule

$$A = i\boldsymbol{\beta}\cdot\mathbf{J} \tag{3.11}$$

and the number $\|A\|$ by the rule

$$\|A\| = \max_{\mu,\nu} |\langle j\mu|\, A\,|j\nu\rangle|. \tag{3.12}$$

It is easily verified that

$$\|A^n\| \leq (2j+1)^n \|A\|^n, \tag{3.13}$$

since the matrices $\mathbf{J}$ are of dimension $(2j+1) \times (2j+1)$.[14] Lastly, the series

$$\sum_{n=0}^{\infty} (n!)^{-1}(2j+1)^n \|A\|^n \tag{3.14}$$

is convergent for all $\|A\|$. This completes the proof.

So far, we have defined what it means for a function to be real analytic and have discussed some important examples. We next define what it means for a function f to be *complex analytic*. First of all, it must be defined on a complex analytic manifold. Secondly, we require that f depend on the local coordinates in a complex analytic manner. That is, suppose p is some point in the manifold and $z_1, z_2, \cdots, z_n$ are local coordinates which map the neighborhood of p into C^n, with p

having the coordinates $z_i = 0$. We say that f is complex analytic at p, if it has a convergent multiple Taylor expansion in the variables z_i. Observe that, for f to be real analytic on a complex analytic manifold, it need only have a convergent Taylor expansion in the variables z_i and $\bar{z}_i$. Thus, complex analytic functions are a special subclass of real analytic functions. The importance of complex analytic functions will become apparent in Sec. 5. We note that, if a function f is complex analytic on a set in $SL(2, C)$ which contains $SU(2)$, then f is automatically real analytic on $SU(2)$.

Consider the functions $D^j_{\mu\lambda}(g)$ defined on $SL(2, C)$ by the rule

$$D^j_{\mu\lambda}(g) \stackrel{\text{def}}{=} \langle j\mu|\, G(g)\,|j\lambda\rangle, \tag{3.15}$$

where we have used the notation of (2.20) and (2.21). We assert that the functions $D^j_{\mu\lambda}(g)$ are *complex analytic everywhere* on $SL(2, C)$. The proof is straightforward. If g is any element of $SL(2, C)$ in the neighborhood of g_0, we introduce complex local coordinates γ as in (3.2). We then follow steps analogous to those in Eqs. (3.9)–(3.14), to discover that $D^j_{\mu\lambda}(g)$ has a convergent expansion in the components of γ as required.

4. INFINITE SERIES

We have seen that the functions $D^j_{\mu\lambda}(g)$ are complex analytic everywhere on $SL(2, C)$. They, in fact, play somewhat the same role as do polynomials on C^3. In this section, we will consider sums of the form

$$S(g) = \sum_{j=0}^{\infty} \sum_{\mu=-j}^{j} \sum_{\lambda=-j}^{j} (2j+1) a^j_{\mu\lambda} D^j_{\mu\lambda}(g). \tag{4.1}$$

The sum S will be a complex analytic function in any region of $SL(2, C)$, in which it converges uniformly. For computational convenience, the term $(2j + 1)$ has been explicitly separated out. The reader is reminded of the relation for integer j and m[3],

$$D^j_{m,0}(\phi, \theta, \psi) = [4\pi/(2j+1)]^{\frac{1}{2}}(-1)^m Y^{-m}_j(\theta, \phi), \tag{4.2}$$

which shows that the sum (1.1) is a special case of (4.1).

We begin by finding a bound for the functions $D^j_{\mu\lambda}(g)$.

Theorem 1: If g is parametrized as in (2.18), then

$$|D^j_{\mu\lambda}(g)| \leq \Delta^j(\alpha), \tag{4.3}$$

where

$$\Delta^j(\alpha) = [\sinh(j + \tfrac{1}{2})\alpha][\sinh \tfrac{1}{2}\alpha]^{-1}. \tag{4.4}$$

Proof: Note that the second factor in (2.18) belongs to $SU(2)$, so that we may write

$$g = \exp(\tfrac{1}{2}\boldsymbol{\alpha} \cdot \boldsymbol{\sigma})u. \tag{4.5}$$

We next use (2.6) to infer the existence of an element $u_1 \in SU(2)$ such that

$$\exp(\tfrac{1}{2}\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}) = u_1(\exp \tfrac{1}{2}\alpha\sigma_3)u_1^{-1}. \tag{4.6}$$

Combining (4.5) and (4.6), we find that g has the form

$$g = u_1(\exp \tfrac{1}{2}\alpha\sigma_3)u_2 \tag{4.7}$$

and

$$D^j_{\mu\lambda}(g) = \sum_{\nu,\tau} D^j_{\mu\nu}(u_1) D^j_{\nu\tau}(\exp \tfrac{1}{2}\alpha\sigma_3) D^j_{\tau\lambda}(u_2). \tag{4.8}$$

Since $U(u)$ is unitary, we have

$$|D^j_{ab}(u)| \leq 1. \tag{4.9}$$

Also, from (2.13a) and (2.21),

$$D^j_{\nu\tau}(\exp \tfrac{1}{2}\alpha\sigma_3) = \delta_{\nu\tau} e^{\alpha\tau}. \tag{4.10}$$

Consequently,

$$|D^j_{\mu\lambda}(g)| \leq \sum_{\tau=-j}^{j} \exp \alpha\tau = \Delta^j(\alpha). \tag{4.11}$$

We remark that $\Delta^j(\alpha)$ increases monotonically with increasing α. From (4.11), we have the estimate

$$e^{j\alpha} \leq \Delta^j(\alpha) \leq (2j+1)e^{j\alpha}. \tag{4.12}$$

A region in which (4.1) converges can now be determined by techniques similar to those for Taylor series. Consider the sequence of numbers $b^j_{\mu\lambda}(\alpha)$ generated by the formula

$$b^j_{\mu\lambda}(\alpha) = (2j+1)\,|a^j_{\mu\lambda}|\,\Delta^j(\alpha), \tag{4.13}$$

as j, μ, and λ range over the values indicated in the sum (4.1). We define α_0 to be the least upper bound of those α's for which the sequence $\{b^j_{\mu\lambda}(\alpha)\}$ is bounded.

This definition leads to an explicit formula for α_0.

Theorem 2: We have the formula

$$\alpha_0 = -\log[\limsup |a^j_{\mu\lambda}|^{1/j}], \tag{4.14}$$

where the limit superior is taken over all j, μ, and λ indicated in (4.1).

Proof: Suppose $\alpha < \alpha_0$. Then, by the definition of α_0, there exists an M such that

$$b^j_{\mu\lambda}(\alpha) \leq M. \tag{4.15}$$

From (4.12) and (4.15), it follows that

$$|a^j_{\mu\lambda}| \leq Me^{-j\alpha}, \tag{4.16}$$

whence

$$\log[\limsup |a^j_{\mu\lambda}|^{1/j}] \leq -\alpha_0. \tag{4.17}$$

Now suppose $\alpha > \alpha_0$. Then for any M we have

$$b^j_{\mu\lambda}(\alpha) \geq M, \tag{4.18}$$

for infinitely many triplets j, μ, λ. Therefore, we have

$$|a^j_{\mu\lambda}| \geq M(2j+1)^{-2}e^{-j\alpha} \tag{4.19}$$

for infinitely many j, μ, and λ, whence

$$\log[\limsup |a^j_{\mu\lambda}|^{1/j}] \geq -\alpha_0. \tag{4.20}$$

Comparison of (4.17) and (4.20) verifies (4.14).

We assert that the quantity α_0 defines a region of $SL(2, C)$ in which the series (4.1) converges.

Theorem 3: Suppose g is such that its α [given explicitly by (2.19)] satisfies $\alpha < \alpha_1 < \alpha_0$. Then $S(g)$ converges absolutely.

Proof: We obtain from (4.3) the inequality

$$|(2j+1)a^j_{\mu\lambda}D^j_{\mu\lambda}(g)| \leq b^j_{\mu\lambda}(\alpha). \tag{4.21}$$

From the definition of α_0 there exists an M such that

$$b^j_{\mu\lambda}(\alpha_1) \leq M, \tag{4.22}$$

whence

$$b^j_{\mu\lambda}(\alpha) \leq M[b^j_{\mu\lambda}(\alpha)/b^j_{\mu\lambda}(\alpha_1)]. \tag{4.23}$$

From (4.12) we observe that

$$[b^j_{\mu\lambda}(\alpha)/b^j_{\mu\lambda}(\alpha_1)] \leq (2j+1)e^{j(\alpha-\alpha_1)}. \tag{4.24}$$

But the comparison series

$$\sum_{j\mu\lambda} M(2j+1)e^{j(\alpha-\alpha_1)} = M\sum_{j=0}^{\infty}(2j+1)^3 e^{j(\alpha-\alpha_1)} \tag{4.25}$$

converges for $\alpha < \alpha_1$. Hence, S converges absolutely as advertised.

Several comments are in order. The first concerns the region of convergence found in Theorem 3. We saw in Sec. 2 that the topology of $SL(2, C)$ is $E^3 \times S^3$. The condition on $\boldsymbol{\alpha}$, in Theorem 3, is that its length be less than α_0. This condition characterizes the interior of a ball in E^3 of radius α_0 which we denote by $B^3(\alpha_0)$. Under the hypotheses of Theorem 3, the convergence of $S(g)$ is independent of the "$SU(2)$ part" of g. Thus, the domain of absolute convergence is $B^3(\alpha_0) \times S^3$. We shall call this region a *superball* of radius α_0 and denote it by $B^6(\alpha_0)$.

A second comment is that Theorem 3 can easily be extended to show that the convergence of $S(g)$ is uniform in any superball of radius less than α_0. *Therefore $S(g)$ converges to a complex analytic function within $B^6(\alpha_0)$.*

A third comment is that Theorem 3 contains within it the celebrated result that the region of convergence of a Legendre series (more generally a series of Jacobi polynomials) is the interior of an ellipse with foci ± 1. It is easily checked that a general element in $SL(2, C)$ can be written in the form (2.9), provided the numbers x_1 to x_4 are allowed to become complex but still subject to the condition (2.10). Reference to (2.25) then shows that a general element in $SL(2, C)$ can also be parametrized by complex Euler angles. We find, using (2.9), (2.19), (2.25), and (2.26), that the α for a general g is related to its Euler angles by the expression

$$2\cosh\alpha = |1+\cos\theta|\cosh(2\,\mathrm{Im}\,\sigma) + |1-\cos\theta|\cosh(2\,\mathrm{Im}\,\delta). \tag{4.26}$$

We next remind the reader of the relation

$$D^j_{00}(\phi\theta\psi) = P_j(\cos\theta). \tag{4.27}$$

Hence, a Legendre sum is a special case of (4.1), in which $a^j_{\mu\lambda}$ vanishes unless $\mu = \lambda = 0$. In this case, $S(g)$ depends only on $\cos\theta$ and is independent of δ and σ. According to Theorem 3, the Legendre sum converges absolutely when $\alpha < \alpha_0$. Looking at (4.26), we see that $\cos\theta$ reaches the edge of its domain when $\sigma = \delta = 0$ [which condition does not change the value of $S(g)$]. Hence, the series converges when

$$2\cosh\alpha_0 > |1+\cos\theta| + |1-\cos\theta|. \tag{4.28}$$

The condition (4.28) describes the interior of an ellipse in the complex $\cos\theta$ plane with foci ± 1 and semi-major axis $\cosh\alpha_0$. A similar argument can be given for sums of Jacobi polynomials.

The last item to be discussed in this section is something about the region in which the series $S(g)$ diverges. In the case of a Taylor series in a single variable, we know that the series converges everywhere inside its circle of convergence, diverges everywhere outside, and may or may not converge at points on the circle itself depending upon the detailed nature of its coefficients. The behavior of the Wigner series $S(g)$ is more complicated, as will be seen from a well chosen example.

Let us write a general element $g \in SL(2, C)$ in the form

$$g = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{4.29}$$

We may view a, b, and c as independent complex parameters, and compute d from the constraint

$$\det g = 1 \tag{4.30a}$$

or

$$d = a^{-1}(1+bc). \tag{4.30b}$$

Consider the function f defined by

$$f(g) = (1-\tau a)^{-1} = \sum_0^{\infty} \tau^n a^n, \tag{4.31}$$

where τ is some number satisfying $|\tau| < 1$. We note the two relations

$$D^{\frac{1}{2}}_{\frac{1}{2}\frac{1}{2}}(g) = a, \tag{4.32}$$

$$[D^{\frac{1}{2}}_{\frac{1}{2}\frac{1}{2}}]^n = D^{\frac{1}{2}n}_{\frac{1}{2}n\frac{1}{2}n}. \tag{4.33}$$

Thus, f has the Wigner expansion

$$f(g) = \sum_{j=0}^{\infty} \tau^{2j} D^j_{jj}(g). \tag{4.34}$$

It is easily verified that f is complex analytic except at $a = \tau^{-1}$. Indeed, f as a function of a has only a pole, and, by (4.32) and Sec. 3, a is an entire function of g.

Let us compute α, when g is parametrized by (4.29). We find, using (2.19) and (4.30b), that

$$2 \cosh \alpha = |a|^2 + |b|^2 + |c|^2 + |a|^{-2} |1 + bc|^2. \tag{4.35}$$

Let us also compute α_0 using (4.14). We obtain

$$\alpha_0 = -\log [\limsup |(2j + 1)^{-1} \tau^{2j}|^{1/j}] = -2 \log |\tau|. \tag{4.36}$$

It is evident from (4.31) that the expansion (4.34) converges absolutely provided $|a| < |\tau|^{-1}$. Comparing (4.35) and (4.36), we see that there are many points outside of $B^6(\alpha_0)$, where this condition is satisfied since $|b|$ and $|c|$ can be arbitrarily large. We conclude that a Wigner series may also converge at points, and indeed within whole regions, outside its superball of convergence.

What is the largest superball in which the function f of our example is complex analytic? Put another way, what is the smallest superball in which f is singular? To answer this question, we set $a = \tau^{-1}$ and vary b and c to minimize (4.35). A short calculation shows that the minimum occurs when $b = c = 0$, and we obtain

$$2 \cosh \alpha_{\min} = |\tau|^2 + |\tau|^{-2} \tag{4.37}$$

or

$$\alpha_{\min} = -2 \log |\tau|. \tag{4.38}$$

Thus, in our example, the maximal superball of analyticity coincides with the superball of convergence for the Wigner series! We shall see in Sec. 5 that this is always true.

Suppose we anticipate this result. We can then show that there are cases in which a Wigner series has no meaning outside its superball of convergence. What we shall show is that there are functions which are complex analytic within a given superball, but are not analytic anywhere outside the superball and hence may not even be defined anywhere else. In the technical language of the theory of many complex variables, a superball is an envelope of holomorphy.[15]

To show that a given superball is an envelope of holomorphy, it is sufficient to show that given any point p on the boundary of the superball, there exists a function which is complex analytic inside any smaller superball, but singular at p.[16] Let $f_0(g)$ denote the function defined by (4.31) using a real value of τ with $\tau = \tau_0$, $0 < \tau_0 < 1$. The function f_0 is complex analytic within $B^6(\alpha_0)$, where

$$\alpha_0 = -2 \log \tau_0, \tag{4.39}$$

and is singular at the boundary point

$$g_0 = \begin{pmatrix} \tau_0^{-1} & 0 \\ 0 & \tau_0 \end{pmatrix} = \exp(\tfrac{1}{2}\alpha_0 \sigma_3). \tag{4.40}$$

Now consider the function f_{12} defined by

$$f_{12}(g) = f_0(u_1^{-1} g u_2^{-1}), \tag{4.41}$$

where u_1 and u_2 are any elements in $SU(2)$. It is easily verified that the arguments of f_{12} and f_0 have the same α. Further, any matrix element of the argument of f_0 is an entire function of g. It follows that f_{12} is also complex analytic within $B^6(\alpha_0)$. Finally, f_{12} is singular when $g = g_s$, where

$$u_1^{-1} g_s u_2^{-1} = g_0 \tag{4.42}$$

or

$$g_s = u_1 g_0 u_2. \tag{4.43}$$

Employing (4.7), we see that, with a proper choice of u_1 and u_2, g_s can be made to coincide with an arbitrary point on the boundary of $B^6(\alpha_0)$.

5. EXPANSION OF ANALYTIC FUNCTIONS

Suppose f is a function defined on $SU(2)$. Then, under certain conditions, f has an expansion of the form (4.1). For the most part, we shall be concerned with the expansion of functions which are real analytic on $SU(2)$ or complex analytic within some superball of $SL(2, C)$. (In fact, we shall see that these two conditions are equivalent.) However, some discussion is given to the case where f possesses a finite number of derivatives or is only continuous.

Consider the set of functions defined on $SU(2)$. This set is evidently a vector space under the operations of pointwise addition and multiplication by complex numbers. If f and g are any two such functions, we define a scalar product by the rule

$$(f, g) = \int du \bar{f}(u) g(u). \tag{5.1}$$

It is easily verified that this scalar product is real and positive definite.

Consider the functions $D^j_{\mu\lambda}(u)$. The reader is reminded, using the notation of (2.24) and (5.1), that they obey the relation[3,5]

$$(D^j_{\mu\lambda}, D^{j'}_{\mu'\lambda'}) = (2j+1)^{-1}\delta_{jj'}\delta_{\mu\mu'}\delta_{\lambda\lambda'}. \quad (5.2)$$

Therefore, if f has an expansion of the form (4.1), the coefficients are given by the relation

$$a^j_{\mu\lambda} = (D^j_{\mu\lambda}, f). \quad (5.3)$$

Using (5.3), we get an immediate estimate for the coefficients $a^j_{\mu\lambda}$ by the Schwarz inequality,

$$|a^j_{\mu\lambda}| \leq (2j+1)^{-\frac{1}{2}}(f,f)^{\frac{1}{2}}. \quad (5.4)$$

There still remains the question of whether the Wigner functions form a complete set. The answer is yes.

Theorem 4: Suppose f is continuous on $SU(2)$; then the Wigner series (4.1) for f is Abel summable, in the sense that

$$\lim_{t\to 1}\sum_{j\mu\lambda}(2j+1)t^{2j}a^j_{\mu\lambda}D^j_{\mu\lambda}(u) = f(u). \quad (5.5)$$

Proof: From (4.9) and (5.4), it is evident that (5.5) is absolutely convergent for $0 \leq t < 1$, and hence there is something to take the limit of. We shall proceed in a somewhat circuitous manner. We first define a "δ function" $\delta(u)$ on $SU(2)$ by the rule

$$\int du\delta(u)f(u) = f(\sigma_4) \quad (5.6)$$

for any continuous function f. Since the measure du is left and right invariant, we have the result

$$\int du\delta(uu'^{-1})f(u) = f(u'). \quad (5.7)$$

Thus, proving (5.5) is equivalent to demonstrating that

$$\lim_{t\to 1}\delta(t,u) = \delta(u), \quad (5.8)$$

where

$$\delta(t,u) = \sum(2j+1)t^{2j}\delta_{\mu\lambda}D^j_{\mu\lambda}(u). \quad (5.9)$$

Note that

$$(D^j_{\mu\lambda}, \delta) = \bar{D}^j_{\mu\lambda}(\sigma_4) = \delta_{\mu\lambda}. \quad (5.10)$$

We first calculate the sum

$$\sum_{\mu,\lambda}\delta_{\mu\lambda}D^j_{\mu\lambda}(u) = \mathrm{Tr}\, D^j(u). \quad (5.11)$$

If u is parametrized as in (2.1), there exists by (2.6) an element u_1 such that

$$u = u_1^{-1}\exp(\tfrac{1}{2}i\beta\sigma_3)u_1.$$

Consequently,

$$\mathrm{Tr}\, D^j(u) = \sum_\lambda \langle j\lambda|\, U^{-1}(u_1)\exp i\beta J_3 U(u_1)\,|j\lambda\rangle$$
$$= \sum_\lambda \langle j\lambda|\exp i\beta J_3\,|j\lambda\rangle = \sum_\lambda e^{i\beta\lambda} = \Delta^j(i\beta). \quad (5.12)$$

The sum (5.9) can now be easily evaluated. We obtain

$$\delta(t,u) = \sum_0^\infty (2j+1)t^{2j}\Delta^j(i\beta)$$
$$= (1-t^2)(1-2t\cos\beta/2+t^2)^{-2}. \quad (5.13)$$

Evidently,

$$\lim_{t\to 1}\delta(t,u) = 0, \quad \text{if} \quad \beta \neq 0, \quad 4\pi \quad \text{or} \quad u \neq \sigma_4,$$
$$= \infty, \quad \text{if} \quad \beta = 0, \quad 4\pi \quad \text{or} \quad u = \sigma_4. \quad (5.14)$$

Thus, $\delta(t,u)$ becomes strongly peaked about $u = \sigma_4$ as $t \to 1$. Finally, it is easily checked from (5.9) that

$$\int du\delta(t,u) = (D^0_{00}, \delta[t,u]) = 1 \quad (5.15)$$

since, by (5.2), only the first term in the sum contributes. Thus, (5.8) is correct. Because δ is manifestly real, we may also write

$$\delta(uu'^{-1}) = \sum_{j\mu\lambda}(2j+1)\delta_{\mu\lambda}\bar{D}^j_{\mu\lambda}(uu'^{-1}). \quad (5.16)$$

Insertion of (5.16) into (5.7) and use of the group property for the $D^j_{\mu\lambda}$ produces the desired Wigner expansion for f.

It might be imagined that the convergence of a Wigner expansion for a function f depends on how "nice" f is. This is indeed the case. We shall see that the estimate (5.4) can be improved if f is differentiable, and greatly improved if it is analytic. By way of definition, a function f on an analytic manifold is said to be differentiable at a point p if it is a differentiable function of the local coordinates at p. If f is differentiable at all points of a manifold, we simply say that it is differentiable.

Suppose f is defined on $SU(2)$ and is differentiable at u_0. We define three Lie differential operators $\mathfrak{d}_k$ by the rule

$$i\mathfrak{d}_k f(u_0) = \frac{d}{d\lambda}\{f[(\exp -\tfrac{1}{2}i\lambda\sigma_k)u_0]\}|_{\lambda=0}. \quad (5.17)$$

Let us apply this definition to the Wigner functions. We have

$$D^j_{\mu\lambda}[(\exp -\tfrac{1}{2}i\lambda\sigma_k)u_0] = \langle j\mu|\,(\exp -i\lambda J_k)U(u_0)\,|j\lambda\rangle, \quad (5.18)$$

from which it follows from (2.13) and (5.17) that

$$\mathfrak{J}_3 D^j_{\mu\lambda} = -\mu D^j_{\mu\lambda} \tag{5.19}$$

and

$$\left(\sum_k \mathfrak{J}_k^2\right) D^j_{\mu\lambda} = j(j+1) D^j_{\mu\lambda}. \tag{5.20}$$

We assert that the operators $\mathfrak{J}_k$ are Hermitian. That is, if f and g are two differentiable functions, then

$$(\mathfrak{J}_k f, g) = (f, \mathfrak{J}_k g). \tag{5.21}$$

Theorem 5: The operators $\mathfrak{J}_k$ are Hermitian.

Proof: We first show that

$$(1, \mathfrak{J}_k f) = 0, \tag{5.22}$$

where 1 denotes the function which is one on $SU(2)$ and f is uniformly differentiable. By definition, we have the relation

$$f\{[\exp(-\tfrac{1}{2}i\lambda\sigma_k)]u\} - f(u) = \lambda i \mathfrak{J}_k f(u) + O(\lambda^2). \tag{5.23}$$

Take the scalar product of both sides of (5.23) with 1. The left-hand side gives a vanishing scalar product because of (2.22). Division of the right-hand side by λ and setting $\lambda = 0$ give (5.22). Next observe that $\mathfrak{J}_k$ is a differential operator, so that

$$\mathfrak{J}_k[\bar{f}g] = [\mathfrak{J}_k \bar{f}]g + \bar{f}[\mathfrak{J}_k g]. \tag{5.24}$$

It is also "pure imaginary,"

$$\mathfrak{J}_k \bar{f} = -\overline{[\mathfrak{J}_k f]}. \tag{5.25}$$

Taking the scalar product of both sides of (5.24) with 1 and using (5.22) and (5.25) give (5.21).

We are now prepared to state a theorem concerning differentiable functions.

Theorem 6: Suppose f has $2n$ derivatives. Then the coefficients $a^j_{\mu\lambda}$ obey the inequality

$$|a^j_{\mu\lambda}| \leq [j(j+1)]^{-n}(2j+1)^{-\frac{1}{2}}(\mathfrak{J}^{2n}f, \mathfrak{J}^{2n}f)^{\frac{1}{2}}, \tag{5.26}$$

where

$$\mathfrak{J}^{2n} = \left(\sum_k \mathfrak{J}_k^2\right)^n. \tag{5.27}$$

Proof: A simple calculation gives

$$\begin{aligned}(D^j_{\mu\lambda}, \mathfrak{J}^{2n}f) &= (\mathfrak{J}^{2n}D^j_{\mu\lambda}, f) \\ &= [j(j+1)]^n (D^j_{\mu\lambda}, f) = [j(j+1)]^n a^j_{\mu\lambda}.\end{aligned} \tag{5.28}$$

Now apply Schwarz's inequality to obtain (5.26).[17]

We turn now to the case of real analytic functions on $SU(2)$. The first tools we shall need are three theorems concerning multiple Taylor series. For our needs, a discussion of triple Taylor series will suffice.

Theorem 7: Consider the Taylor series

$$T(x_1x_2x_3) = \sum_{\alpha,\beta,\gamma} a_{\alpha\beta\gamma}(x_1 - x_1')^\alpha (x_2 - x_2')^\beta (x_3 - x_3')^\gamma. \tag{5.29}$$

Define a number R by the expression

$$R^{-1} = \limsup |a_{\alpha\beta\gamma}|^{(\alpha+\beta+\gamma)^{-1}}. \tag{5.30}$$

Then T converges absolutely and is analytic in the polydisk

$$|x_j - x_j'| < R, \quad j = 1, 2, 3, \tag{5.31}$$

and diverges when

$$|x_j - x_j'| > R, \quad j = 1, 2, 3. \tag{5.32}$$

Proof: The proof proceeds along lines similar to that for a single complex variable.[18]

Theorem 8: Suppose $f(x_1x_2x_3)$ is analytic in the polydisk $|x_i - x_i'| < r$. Then f has a convergent expansion of the form (5.29) and $R \geq r$.

Proof: Apply Cauchy's theorem three times and expand the denominators in a geometric series.[18]

Theorem 9: The radius of convergence R is a continuous function of the expansion point x_1', x_2', x_3'.

Proof: Let $x_1'x_2'x_3'$ be a fixed point and $x_1x_2x_3$ denote a variable point. Consider the polydisk of convergence about $x_1'x_2'x_3'$ with its radius denoted by $R(x_1'x_2'x_3')$. Choose the variable point sufficiently near the fixed point, so that

$$\sum_{i=1}^{3} |x_i - x_i'| < R(x_1'x_2'x_3'), \tag{5.33}$$

whence

$$|x_i - x_i'| < R(x_1'x_2'x_3'), \quad i = 1, 2, 3. \tag{5.34}$$

We can now place a polydisk about $x_1x_2x_3$ which fits inside the polydisk about $x_1'x_2'x_3'$. It follows from Theorems 7 and 8 that

$$R(x_1x_2x_3) \geq \min_i [R(x_1'x_2'x_3') - |x_i - x_i'|], \tag{5.35}$$

whence

$$R(x_1x_2x_3) \geq R(x_1'x_2'x_3') - \sum_i |x_i - x_i'|. \tag{5.36}$$

However, the polydisk of convergence about $x_1x_2x_3$ cannot be too large, for otherwise it would contain the polydisk about $x_1'x_2'x_3'$ which would again violate

Theorems 7 and 8. Therefore, we must have

$$R(x_1x_2x_3) \leq \max_i [R(x_1'x_2'x_3') + |x_i - x_i'|], \quad (5.37)$$

whence

$$R(x_1x_2x_3) \leq R(x_1'x_2'x_3') + \sum_i |x_i - x_i'|. \quad (5.38)$$

(See Figs. 1 and 2.) Combining (5.36) and (5.38) gives

$$|R(x_1x_2x_3) - R(x_1'x_2'x_3')| \leq \sum_i |x_i - x_i'|, \quad (5.39)$$

which completes the proof.

We are now prepared to proceed. Suppose that f is a real analytic function on $SU(2)$. At each point u_0 we introduce local coordinates $\boldsymbol{\beta}$ using (3.1). Then, since f is real analytic, we have

$$f[(\exp \tfrac{1}{2}i\boldsymbol{\beta}\cdot\boldsymbol{\sigma})u_0] = \sum_{jkl} c_{jkl}\beta_1^j\beta_2^k\beta_3^l. \quad (5.40)$$

Compute the radius R of convergence for this series using (5.30). By hypothesis, we have $R > 0$. Therefore, by Theorem 7, the series (5.40) also converges for small complex $\boldsymbol{\beta}$. But elements of the form

$$(\exp \tfrac{1}{2}i\boldsymbol{\beta}\cdot\boldsymbol{\sigma})u_0$$

with $\boldsymbol{\beta}$ complex are elements in $SL(2, C)$. We draw the important conclusion that a function on $SU(2)$ which is real analytic at u_0 can be locally extended to a complex analytic function on $SL(2, C)$.

Can these local extensions be pieced together to make a global extension? The answer is yes. We first show that a certain minimal local extension is possible at each point in $SU(2)$.

Theorem 10: Suppose, given a function f real analytic on $SU(2)$, that we make an expansion of the form (5.40) at each point u in $SU(2)$. At each u, we compute the radius of convergence using (5.30), and denote its value by $R(u)$. Then, there exists a number $r > 0$ such that

$$R(u) \geq r$$

for all elements $u \in SU(2)$.

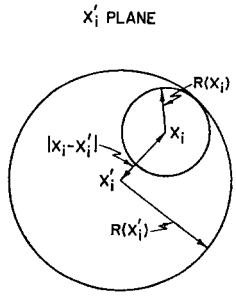

FIG. 1. The inequality (5.35).

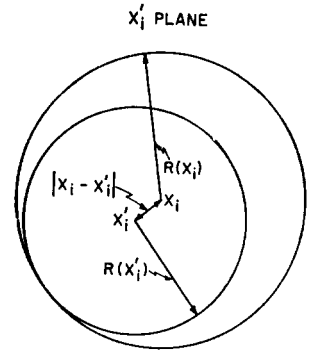

FIG. 2. The inequality (5.37).

Proof: Since $SL(2, C)$ is locally homeomorphic to C^3 and (5.40) is a Taylor series in C^3, we know by Theorem 9 that $R(u)$ is continuous. Further, by hypothesis, $R(u) > 0$ at each point in $SU(2)$, since f is real analytic. Finally, the group $SU(2)$ is compact. This completes the proof, for a continuous positive function on a compact manifold must be bounded away from zero.

Theorem 10 states that f is complex analytic at each point u in a neighborhood satisfying $|\beta_i| < r$. Take the union of all these neighborhoods as u ranges over $SU(2)$. It is geometrically evident that this union contains *within* it a superball $B^6(r')$ with $r > r' > 0$. We now show that the local expansions within $B^6(r')$ can be pieced together to produce a function which is globally complex analytic in $B^6(r')$. We need two more results from the theory of complex variables.

Theorem 11: Suppose a function f is known to be complex analytic at some point p in a complex analytic manifold. Then its values in any small neighborhood of p determine its values at any other point p', which can be reached by analytic continuation along some path.

Proof: This is the uniqueness theorem for analytic continuation.[18]

Theorem 12: If a function can be analytically continued along any path in a simply connected region D, then the value obtained at any point is independent of the path of continuation.

Proof: This is the monodromy theorem.[18]

We assert that the conditions of Theorems 11 and 12 are satisfied in our case. First, we already know that f is complex analytic at each "$SU(2)$" point in $SL(2, C)$. Secondly, since $B^6(r')$ is covered by polydisks of radius r, it is possible to analytically continue

f along any path in $B^6(r')$. Finally, $B^6(r')$ is simply connected since it is the topological product of S^3 and a ball in E^3, both of which are simply connected. We conclude that f can be analytically continued into $B^6(r')$ and that its values there are completely determined by its values on $SU(2)$.

Still more can be said. Applying Theorem 11, we may attempt to continue f into a larger superball. If we are able to continue into a larger superball, we can try continuing along all possible paths within it. If we cannot get into a larger superball, we may conclude that the original superball has singularities of f everywhere dense on its boundary. (This is a possibility, since we saw in Sec. 4 that a superball is an envelope of holomorphy.) In either case, we are able to completely determine the singularity structure of f in $SL(2, C)$. In particular, there exists for each function f a certain maximal superball (which may have infinite radius) inside of which f is free of singularities. We conclude that, if f is real analytic on $SU(2)$, it must also be complex analytic on $SL(2, C)$ within a certain maximal superball.

We now have sufficient tools to state and prove results about Wigner expansions of analytic functions. A key result is the following.

Theorem 13: Suppose f is complex analytic within a superball of radius r_0. Then, for any $r_1 < r_0$, the coefficients $a^j_{\mu\lambda}$ satisfy the bound

$$|a^j_{\mu\lambda}| \leq M(r_1)(2j+1)^{\frac{1}{2}}[\Delta^j(r_1)]^{-1}. \tag{5.41}$$

Proof: Let u be an arbitrary element in $SU(2)$. Consider the element $g(t)$ defined by

$$g(t) = (\exp \tfrac{1}{2}t\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})u, \tag{5.42}$$

where $\hat{\mathbf{n}}$ is a real unit vector and t is a real or complex number. It is evident that g is contained in a superball whose radius α is given by

$$\alpha = |\mathrm{Re}\, t|. \tag{5.43}$$

Thus, g will be contained within $B^6(r_0)$, if

$$|t| \leq r_1. \tag{5.44}$$

By hypothesis, f is complex analytic in $B^6(r_0)$. Hence, it can be continued analytically along any path given by (5.42) as t varies over a path in the complex t plane, starting at $t = 0$, provided (5.44) is obeyed. Therefore, we may write

$$f[g(t)] = \sum_0^\infty c_m t^m \tag{5.45}$$

with the assurance that (5.45) is absolutely convergent in the disk (5.44). Using (5.17), we may also write (5.45) in the symbolic form

$$f(g) = O(t, \hat{\mathbf{n}})f(u), \tag{5.46}$$

where $O(t, \hat{\mathbf{n}})$ denotes the operator

$$O(t, \hat{\mathbf{n}}) = \exp(-t\hat{\mathbf{n}} \cdot \mathfrak{z}). \tag{5.47}$$

We say that $f(u)$ "admits" the operator $O(t, \hat{\mathbf{n}})$ for t in the disk (5.44), when the series (5.45) converges. Note that $O(t, \hat{\mathbf{n}})$ is Hermitian, when t is real. Now define an operator $O(t)$ by the rule

$$O(t) = (4\pi)^{-1}\int d\Omega_{\hat{\mathbf{n}}} O(t, \hat{\mathbf{n}}), \tag{5.48}$$

where $d\Omega_{\hat{\mathbf{n}}}$ indicates an integration over the surface of the unit sphere in "$\hat{\mathbf{n}}$" space. Evidently, $O(t)$ is Hermitian for real t and is admissible on $f(u)$ for t satisfying (5.44), provided f is complex analytic in $B^6(r_0)$. Let us apply $O(t)$ to $D^j_{\mu\lambda}(u)$. We have the relation

$$O(t)D^j_{\mu\lambda}(u) = (4\pi)^{-1}\int d\Omega_{\hat{\mathbf{n}}} D^j_{\mu\lambda}[(\exp \tfrac{1}{2}t\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})u]. \tag{5.49}$$

But, by the group property,

$$D^j_{\mu\lambda}[(\exp \tfrac{1}{2}t\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})u] = \sum_\nu D^j_{\mu\nu}(\exp \tfrac{1}{2}t\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})D^j_{\nu\lambda}(u). \tag{5.50}$$

Also, using (4.6), (2.24), and the unitarity relation $U(u_1^{-1}) = U^\dagger(u_1)$, we have

$$\begin{aligned}(4\pi)^{-1}&\int d\Omega_{\hat{\mathbf{n}}} D^j_{\mu\nu}(\exp \tfrac{1}{2}t\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \\ &= \int du_1 D^j_{\mu\nu}[u_1(\exp \tfrac{1}{2}t\sigma_3)u_1^{-1}] \\ &= \sum_{c,d}\int du_1 D^j_{\mu c}(u_1)D^j_{cd}(\exp \tfrac{1}{2}t\sigma_3)D^j_{d\nu}(u_1^{-1}) \\ &= \sum_{c,d}\delta_{c,d}\exp(td)(D^j_{\nu d}, D^j_{\mu c}) \\ &= \delta_{\mu\nu}(2j+1)^{-1}\Delta^j(t).\end{aligned} \tag{5.51}$$

Thus, we obtain the remarkable result

$$O(t)D^j_{\mu\lambda}(u) = (2j+1)^{-1}\Delta^j(t)D^j_{\mu\lambda}(u). \tag{5.52}$$

The verification of (5.41) is now straightforward. We have

$$\begin{aligned}(D^j_{\mu\lambda}, O[r_1]f) &= (O[r_1]D^j_{\mu\lambda}, f) \\ &= (2j+1)^{-1}\Delta^j(r_1)(D^j_{\mu\lambda}, f) \\ &= (2j+1)^{-1}\Delta^j(r_1)a^j_{\mu\lambda}.\end{aligned} \tag{5.53}$$

Application of the Schwarz inequality gives

$$M(r_1) = (O[r_1]f, O[r_1]f)^{\frac{1}{2}}. \tag{5.54}$$

Theorem 13 has several immediate consequences.

Theorem 14: If f has $B^6(r_0)$ as its maximal superball of analyticity, then its Wigner series converges and is complex analytic within $B^6(r_0)$. Further, the Wigner series converges to the function f. Conversely, if the Wigner series for a function f on $SU(2)$ has $B^6(\alpha_0)$ as its superball of convergence, then f can be analytically continued into $B^6(\alpha_0)$, its continuation is complex analytic within $B^6(\alpha_0)$, and its continuation agrees with its Wigner series.

Proof: Apply the results of Sec. 4 to (5.41) to see that the Wigner series converges and is complex analytic. Then use Theorem 4 to conclude that f agrees with its Wigner series on $SU(2)$. Finally, use Theorem 11 and the discussion following it to show that, since f agrees with its Wigner series on $SU(2)$, it must agree with its Wigner series in $B^6(r_0)$.

6. NEW FORMULAS

A. Functions on $SU(2)$

In Sec. 5 we saw that the coefficients $a^j_{\mu\lambda}$ in a Wigner expansion of a function f can be computed from (5.3). Formula (5.3) involves an integration of f over $SU(2)$ using the measure du. In part A of this section, we will see that, if f is real analytic on $SU(2)$ and hence complex analytic in some superball in $SL(2, C)$, then the coefficients $a^j_{\mu\lambda}$ can also be computed in terms of contour integrals of f over $SL(2, C)$. When available, formulas involving contour integrals are often to be preferred because contours may be deformed to exploit various analytic properties of the integrand. Part B will be devoted to analogous results for functions on S^2.

The functions $D^j_{\mu\lambda}$ can be explicitly expressed in terms of Jacobi functions.[5] We use the Euler parametrization (2.23) and introduce a variable w by the expression

$$w = \cos\theta. \tag{6.1}$$

One finds, using a standard notation,[1] the relation

$$D^j_{\mu\lambda}(\phi\theta\psi) = C(j\mu\lambda)e^{-\mu i(\phi+\lambda\psi)} \times (1-w)^{\frac{1}{2}|\mu-\lambda|}(1+w)^{\frac{1}{2}|\mu+\lambda|} \times P^{(|\mu-\lambda|,|\mu+\lambda|)}_{j-m}(w), \tag{6.2a}$$

where

$$m = \max\{|\mu|, |\lambda|\} \tag{6.2b}$$

and $C(j\mu\lambda)$ is a constant whose magnitude can be determined from (5.2) and the normalization of Jacobi polynomials.

Let us substitute (6.2) into (5.3). We find, using (2.24) and (5.1),

$$a^j_{\mu\lambda} = (16\pi^2)^{-1}\bar{C}(j\mu\lambda)\int_{-1}^{1} dw(1-w)^{|\mu-\lambda|}(1+w)^{|\mu+\lambda|} \times P^{(|\mu-\lambda|,|\mu+\lambda|)}_{j-m}(w)g(w), \tag{6.3a}$$

where $g(w)$ is given by

$$g(w) = (1-w)^{-\frac{1}{2}|\mu-\lambda|}(1+w)^{-\frac{1}{2}|\mu+\lambda|} \times \int_0^{2\pi} d\phi \int_0^{4\pi} d\psi e^{i(\mu\phi+\lambda\psi)} f. \tag{6.3b}$$

The apportioning of factors of $(1-w)$ and $(1+w)$ in (6.3) may appear a bit strange. It has been done in the way indicated because of the following result.

Theorem 15: Suppose $g(w)$ is analytic in a region R of the w plane which includes the interval $[-1, 1]$. Then the integral (6.3a) can be rewritten as a contour integral in the form

$$a^j_{\mu\lambda} = (16\pi^2)^{-1}\bar{C}(j\mu\lambda)(\pi i)^{-1} \times \oint_C dw(w-1)^{|\mu-\lambda|}(w+1)^{|\mu+\lambda|} \times Q^{(|\mu-\lambda|,|\mu+\lambda|)}_{j-m}(w)g(w), \tag{6.4}$$

where C is any contour in R which encloses the interval $[-1, 1]$ in a counterclockwise direction and Q is a Jacobi function of the second kind.

Proof: The Jacobi function $Q^{(|\lambda-\mu|,|\lambda+\mu|)}_{j-m}(w)$ is analytic in the w plane when it is cut along the interval $[-1, 1]$. Along the interval $[-1, 1]$ it obeys the relation

$$[(w-1)^a(w+1)^b Q^{(a,b)}_c(w)]\Big|^{w+i\epsilon}_{w-i\epsilon} = -\pi i(1-w)^a(1+w)^b P^{(a,b)}_c(w), \tag{6.5}$$

when a, b, and c are integers. [Note that the quantities $|\lambda \pm \mu|, j-m$ are always integers.] Indeed, $Q^{(a,b)}_c$ has the integral representation[19]

$$2(w-1)^a(w+1)^b Q^{(a,b)}_c(w) = \int_{-1}^{1}(w-t)^{-1}(1-t)^a(1+t)^b P^{(a,b)}_c(t)\,dt. \tag{6.6}$$

This information is sufficient to verify (6.4). For further details, see Szegö.[1]

We will have achieved our announced goal if we can show that $g(w)$, as given by (6.3b), is analytic in a neighborhood of $[-1, 1]$. This is indeed the case if f is real analytic on $SU(2)$.

Theorem 16: Suppose f is real analytic on $SU(2)$. Then $g(w)$ as defined by (6.1) and (6.3b) is analytic in a neighborhood of $[-1, 1]$.

Proof: From (2.25) we see that ϕ, θ, and ψ provide a good coordinate system on $SU(2)$ except at $\theta = 0$ and π. Hence, f must be an analytic function of θ on

the open interval $(0, \pi)$. The inverse of (6.1),

$$\theta(w) = \cos^{-1}(w) = -i \log [w + i(1 - w^2)^{\frac{1}{2}}], \quad (6.7)$$

shows that θ in turn is an analytic function of w on the open interval $(-1, 1)$. Therefore, f must be an analytic function of w on the open interval $(-1, 1)$. At the end points, $w = \pm 1$, $\theta(w)$ has branch points. However, at these branch points $\theta = 0$ or π, which is precisely where the Euler angle coordinates fail. Next observe that $g(w)$ involves a ϕ, ψ integration over f and multiplication by powers of $(1 - w)$ and $(1 + w)$. The latter factors are also analytic in w on the interval $(-1, 1)$. We conclude that $g(w)$ is analytic on $(-1, 1)$, but that the status of the points $w = \pm 1$ is still unclear.

We will now show that g is also analytic at $w = \pm 1$. For brevity, we shall only treat the point $w = +1$. The argument for $w = -1$ is similar. Let us rewrite (2.25) using (2.26) and (6.1). We find

$$x_1 = [(1 - w)/2]^{\frac{1}{2}} \sin \delta, \quad (6.8a)$$

$$x_2 = -[(1 - w)/2]^{\frac{1}{2}} \cos \delta, \quad (6.8b)$$

$$x_3 = -[(1 + w)/2]^{\frac{1}{2}} \sin \sigma, \quad (6.8c)$$

$$x_4 = [(1 + w)/2]^{\frac{1}{2}} \cos \sigma. \quad (6.8d)$$

Thus, near $w = 1$, x_1 and $x_2 \approx 0$, and x_3 and x_4 are nearly on the unit circle. A good coordinate system at these points is given by the variables x_1, x_2, and σ. Since f is real analytic at these points, we may make the convergent expansion

$$f(u) = \sum_{j,k=0}^{\infty} a_{jk}(\sigma) s_+^j s_-^k, \quad (6.9a)$$

where

$$s_\pm = -x_2 \pm i x_1 \quad (6.9b)$$

and the coefficients a_{jk} depend on σ. Inserting (6.8a) and (6.8b) into (6.9), we find

$$f = \sum_{j,k} a_{jk}(\sigma)[(1 - w)/2]^{(j+k)/2} e^{-i\delta(k-j)}. \quad (6.10)$$

Next observe that we may write

$$e^{i(\mu\phi + \lambda\psi)} = e^{i\sigma(\mu+\lambda)} e^{i\delta(\mu-\lambda)}. \quad (6.11)$$

Employing (6.10) and (6.11) and using δ and σ as new variables of integration [see (2.27)], we find

$$g(w) = 2(1 - w)^{-\frac{1}{2}|\mu-\lambda|}(1 + w)^{-\frac{1}{2}|\mu+\lambda|} \times \sum_{j,k} [(1 - w)/2]^{(j+k)/2} \int_0^{2\pi} d\sigma a_{jk}(\sigma) e^{i\sigma(\mu+\lambda)} \times \int_0^{2\pi} d\delta e^{-i\delta(k-j)} e^{i\delta(\mu-\lambda)}. \quad (6.12)$$

A simple integration gives

$$\int_0^{2\pi} d\delta e^{-i\delta(k-j)} e^{i\delta(\mu-\lambda)} = 2\pi \delta_{\mu-\lambda, k-j}. \quad (6.13)$$

Thus we need to consider the sum

$$S(\sigma, w) = \sum_{j,k} a_{jk}[(1 - w)/2]^{(j+k)/2} \delta_{\mu-\lambda, k-j}. \quad (6.14)$$

Three cases need to be distinguished:

$$\mu - \lambda < 0, \quad \text{for which} \quad j = k + |\mu - \lambda|, \quad (6.15a)$$

$$\mu - \lambda = 0, \quad \text{for which} \quad j = k, \quad (6.15b)$$

$$\mu - \lambda > 0, \quad \text{for which} \quad k = j + |\mu - \lambda|. \quad (6.15c)$$

For these cases S becomes

$$S = \sum_{k=0}^{\infty} a_{j,k}[(1 - w)/2]^{\frac{1}{2}|\mu-\lambda|}[(1 - w)/2]^k, \quad (6.16a, b)$$

or

$$S = \sum_{j=0}^{\infty} a_{j,k}[(1 - w)/2]^{\frac{1}{2}|\mu-\lambda|}[(1 - w)/2]^j. \quad (6.16b, c)$$

Note that in all cases the sum is over only one index since the remaining index is constrained by (6.15). Examination of (6.16) shows that $(1 - w)^{-\frac{1}{2}|\mu-\lambda|} \times S$ is always analytic at $w = 1$. This completes the proof that $g(w)$ is analytic at $w = 1$.

In summary, we may rewrite the contents of Theorems 15 and 16 to obtain the new formula

$$a^j_{\mu\lambda} = (16\pi^2)^{-1} \bar{C}(j\mu\lambda)(\pi i)^{-1} \times \oint_C dw (w - 1)^{|\mu-\lambda|}(w + 1)^{|\mu+\lambda|} \times Q_{j-m}^{(|\mu-\lambda|, |\mu+\lambda|)}(w) g(w), \quad (6.17a)$$

where

$$g(w) = 2(1 - w)^{-\frac{1}{2}|\mu-\lambda|}(1 + w)^{-\frac{1}{2}|\mu+\lambda|} \times \int_0^{2\pi} d\delta \int_0^{2\pi} d\sigma e^{i\delta(\mu-\lambda)} e^{i\sigma(\mu+\lambda)} f. \quad (6.17b)$$

Initially, the contour C is near $[-1, 1]$. However, since $Q_c^{(a,b)}(w)$ and the terms involving $(1 \pm w)$ are analytic off the interval $[-1, 1]$, the contour C may be deformed at will provided one does not encounter singularities of f. By suitably deforming contours and using the behavior of $Q_c^{(a,b)}(w)$ for large w, it should be possible to obtain and perhaps even sharpen the bound (5.41). We shall not pursue this intriguing question any further here. Instead we shall explore another implication of (6.17).

Suppose we insert (6.2) and (6.17) into the sum (4.1). We obtain the relation

$$f(u) = \int dw' \, d\delta' \, d\sigma' f(u') K(u, u'), \quad (6.18)$$

where

$$K(u,u') = (8\pi^3 i)^{-1}\sum_{j,\mu\lambda}(2j+1)\,|C(j\mu\lambda)|^2 \times (1-w)^{\frac{1}{2}|\mu-\lambda|}(1-w')^{-\frac{1}{2}|\mu-\lambda|} \times (1+w)^{\frac{1}{2}|\mu+\lambda|}(1+w')^{-\frac{1}{2}|\mu+\lambda|} \times (w'-1)^{|\mu-\lambda|}(w'+1)^{|\mu+\lambda|} \times Q_{j-m}^{(|\mu-\lambda|,|\mu+\lambda|)}(w')P_{j-m}^{(|\mu-\lambda|,|\mu+\lambda|)}(w) \times e^{i(\mu-\lambda)(\delta'-\delta)}e^{i(\mu+\lambda)(\sigma'-\sigma)}. \tag{6.19}$$

Thus, $K(u,u')$ is a reproducing kernel which relates values of f on $SU(2)$ to its values on $SL(2,C)$, and (6.18) may be regarded as an integral representation for f.

The sum (6.19) is absolutely convergent for u sufficiently near σ_4, and can be explicitly evaluated by first summing over j and then over μ, λ. The sum over j can be evaluated from the relation[1]

$$2\sum_{n=0}^{\infty}h^{-1}(n,a,b)Q_n^{(a,b)}(w')P_n^{(a,b)}(w) = (w'-1)^{-a}(w'+1)^{-b}(w'-w)^{-1}, \tag{6.20}$$

where h^{-1} is proportional to $(2j+1)\,|C(j\mu\lambda)|^2$. The remaining sums over μ, λ are geometric series and thus trivial. Sparing the reader algebraic details, we find the simple result

$$K(u,u') = -(32\pi^3 i)^{-1}(w-w') \times [(s_+ - s'_+)(s_- - s'_-)(t_+ - t'_+)(t_- - t'_-)]^{-1}, \tag{6.21}$$

where $s\pm$ are given by (6.9b) and

$$t_\pm = x_4 \pm ix_3. \tag{6.22}$$

Putting everything together, we obtain a version of Cauchy's theorem for $SL(2,C)$:

$$f(u) = -(32\pi^3 i)^{-1}\oint dw'\int_0^{2\pi}d\delta'\int_0^{2\pi}d\sigma' f(u')(w-w') \times [(s_+ - s'_+)(s_- - s'_-)(t_+ - t'_+)(t_- - t'_-)]^{-1}. \tag{6.23}$$

B. Functions on S^2

We shall end our discussion with a special consideration of spherical-harmonic expansions using the functions $Y_l^m(\theta,\phi)$. Many of the results obtained so far for Wigner expansions can be applied to Y_l^m expansions simply by setting $\lambda = 0$ and using (4.2). For example, given the expansion (1.1), we may compute a number α_0' from the formula

$$\alpha_0' = -\log\,[\limsup |a_{lm}|^{1/l}], \tag{6.24}$$

and then use the discussion leading to (4.26), bearing in mind that f is now independent of ψ, to conclude that (1.1) converges absolutely in the domain

$$2\cosh\alpha_0' > \cosh(\mathrm{Im}\,\phi)[|1+\cos\theta| + |1-\cos\theta|]. \tag{6.25}$$

The manifold S^2 may be viewed as a coset space of $SU(2)$. To see this, note that (2.6b) can also be written in the form

$$R_{jk} = \tfrac{1}{2}\,\mathrm{Tr}\,(\sigma_j u\sigma_k u^{-1}). \tag{6.26}$$

Now set $k=3$ and define quantities x_1, x_2, and x_3 [not to be confused with the x_i of (2.9) and (2.25)] by the rule

$$x_j(u) = R_{j3}. \tag{6.27}$$

It is evident that the x_j are the components of a vector obtained by applying a rotation to a unit vector in the 3 direction and hence must satisfy

$$x_1^2 + x_2^2 + x_3^2 = 1. \tag{6.28}$$

Further, if we replace u by the element $u\exp(\frac{1}{2}i\psi\sigma_3)$, we see from (6.26) and (6.27) that the values of the x_j are unchanged. Elements of the form $\exp(\frac{1}{2}i\psi\sigma_3)$ form a $U(1)$ subgroup of $SU(2)$. Thus, the quantities x_j depend only on the cosets of $SU(2)$ with respect to a particular $U(1)$ subgroup. We denote this coset space by $SU(2)/U(1)$. Finally, using the Euler-angle parametrization (2.23), we obtain the explicit relations

$$x_1 = \sin\theta\cos\phi, \quad x_2 = \sin\theta\sin\phi, \quad x_3 = \cos\theta. \tag{6.29}$$

Equation (6.29) shows that the relation between the cosets of $SU(2)$ and points on S^2 is 1-to-1 and bicontinuous. We summarize these conclusions by writing

$$SU(2)/U(1) \approx S^2, \tag{6.30}$$

where the symbol "$\approx$" denotes topological equivalence.

Suppose that f is a real analytic function on S^2. We may extend f to $SU(2)$ by giving it the same value on all elements belonging to a given coset and assigning to each coset the value of f at the corresponding point in S^2 given by (6.26), (6.27), and (6.29). We claim that the f obtained in this fashion is real analytic on $SU(2)$. The proof is straightforward. We identify the triplet $(x_1x_2x_3)$ with (xyz) and note that, at any point p on S^2, a good local coordinate patch can be obtained by dropping perpendiculars from the sphere to the tangent plane through p. Thus, at any point p, there are two appropriate linear combinations of x, y, and z which can serve as good local coordinates, and f, since it is real analytic on S^2, must have a convergent Taylor expansion in these two linear combinations. Also, we

know from (4.2) and relations like (3.7) that any linear combination of x, y, and z is a linear combination of the functions $D^1_{m,0}(u)$ [with $m = 0, \pm 1$] and hence our local coordinates are in turn real analytic functions on $SU(2)$. Therefore, by the chain rule, f is also real analytic on $SU(2)$.

With the conclusion of the previous paragraph in mind, we may apply the methods of Sec. 5 to conclude that the coefficients a_{lm} must obey a bound similar to (5.41). The only difference arises from the lack of a $(2j + 1)$ factor in (1.1) and its presence in (4.2).

A little reflection shows that what we have in essence been doing is taking the real analytic manifold S^2 defined by (6.28), and letting the quantities x_j become complex but still subject to the constraint (6.28). The resulting manifold, which we denote by S^{2C}, is easily shown to be complex analytic. The function f, which was originally real analytic on S^2, becomes complex analytic on S^{2C} in the neighborhood of S^2. Finally, the behavior of the series (1.1) is governed by the "singularity structure" of f on S^{2C}.

The last topic we shall consider is the analog of (6.23) for functions on S^2. Theorem 15 can immediately be specialized to the S^2 case simply by setting $\lambda = 0$ and making appropriate changes in factors of $(2j + 1)$. The resulting integral expression for the coefficients a_{lm} can then be inserted into (1.1) and, as before, the sum can be explicitly evaluated. We find the integral representation

$$f(\theta, \phi) = -(4\pi^2 i)^{-1} \oint dz' \int_0^{2\pi} d\phi' f(\theta', \phi')(z + z') \times [(x_+ - x'_+)(x_- - x'_-)]^{-1}, \tag{6.31}$$

where

$$x_\pm = x \pm iy \tag{6.32}$$

and the integration contour encloses $[-1, 1]$. Equation (6.31) may be viewed as a Cauchy formula which relates values of f on S^2 to values on S^{2C}.

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[1] G. Szegö, *Orthogonal Polynomials* (American Mathematical Society, New York, 1959), Vol. XXIII.

[2] R. P. Boas Jr. and R. C. Buck, *Polynomial Expansions of Analytic Functions* (Academic, New York, 1964).

[3] M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957).

[4] N. Jacobson, *Lectures in Abstract Algebra* (Van Nostrand, Princeton, N.J., 1953), Vol. II.

[5] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, N.J., 1957).

[6] N. Jacobson, *Lie Algebras* (Interscience, New York, 1962).

[7] W. Magnus, Commun. Pure Appl. Math. **7**, 649 (1954).

[8] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and All That* (Benjamin, New York, 1964).

[9] Note that this range of integration differs from that of Rose and Edmonds who only integrate over half the group. In their case, no harm is done since, in keeping with a superselection rule of quantum mechanics, they never mix integral and half-integral j.

[10] For a more precise and detailed discussion of analytic manifolds, see P. M. Cohn, *Lie Groups* (Cambridge U.P., Cambridge, England, 1961).

[11] S. S. Chern, *Complex Manifolds Without Potential Theory* (Van Nostrand, Princeton, N.J., 1967).

[12] S. Helgason, *Differential Geometry and Symmetric Spaces* (Academic, New York, 1962).

[13] G. P. Hochschild, *The Structure of Lie Groups* (Holden-Day, San Francisco, 1965).

[14] C. Chevalley, *Theory of Lie Groups* (Princeton U.P., Princeton, N.J., 1946).

[15] A. S. Wightman, "Analytic Functions of Several Complex Variables," in *Dispersion Relations and Elementary Particles*, C. DeWitt and R. Omnes, Eds. (Wiley, New York, 1960).

[16] L. Bers, *Introduction to Several Complex Variables*, Notes on lectures delivered at the Courant Institute of Mathematical Sciences at New York University, 1962–1963 (unpublished).

[17] Note that the estimate (5.26) is adequate to assure the absolute convergence of a Wigner series if $n \geq 2$. For further details concerning the convergence of Wigner series for continuous and piecewise differentiable functions, the reader is referred to the work of R. A. Mayer, Duke Math. J. **34**, 549 (1967a); Amer. J. Math. **89**, 661 (1967b); Trans. Am. Math. Soc. **130**, 414 (1968a); Ill. J. Math. **12**, 325 (1968b).

[18] B. A. Fuks, *Theory of Analytic Functions of Several Complex Variables* (American Mathematical Society, Providence, R.I., 1963).

[19] *Higher Transcendental Functions*, Arthur Erdélyi, Ed. (McGraw-Hill, New York, 1953), Vol. II.

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Theory of Particles with Variable Mass. I. Formalism

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The equivalence principle (through the mechanism of the gravitational red shift) allows one to set up a classical formalism with the proper time as an extra degree of freedom, independent of the coordinate time, and with an immediate physical interpretation. Then proper time and mass occur as conjugate variables in a canonical formalism, leading to a gravitational theory of particles with variable mass. The nonrelativistic theory and a relativistic vector theory of gravity are described as models. The theory is capable of providing a dynamical framework for cosmological models with the creation of matter. Some simple examples are discussed, including the steady-state universe with continuous creation, where the correct relation between the density of matter and the Hubble constant appears automatically, with no free parameters.

INTRODUCTION

Conservation of mass is deeply imbedded into the formalism of nonrelativistic classical physics. The so-called "changing mass" problems one encounters, such as rocket or falling chain problems, actually involve a redistribution of mass, not a creation or destruction of it. Even classical relativity theory, which can handle the kinematics of a particle decaying into several others, has no natural means for providing a mechanism for such decay.

Yet the phenomenon of creation and destruction of mass does arise in practice, in the most widely divergent scale of events possible. On the one hand, elementary particles freely change into each other, and all the standard techniques such as field theory, S-matrix theory, bootstraps, etc., have absolutely no classical analogs to appeal to.[1] And on the other hand, the possibility of continuous creation exists in cosmology.[2] Even if the "perfect comological principle"[3] is untrue[4] the possibility of such creation is still open, but the only known way to provide for such a theory is to corrupt Einstein's field equations in a clever but ad hoc manner.[5] Again there is no classical guide, even within general relativity.

The purpose of this paper is to point out that the principle of equivalence actually provides a rather natural take-off point, not only for general relativity, but also for a classical gravitational theory which includes the possibility of particles changing their masses. The theory is "natural" in the sense that, while new phenomena enter, no new ad hoc parameters are needed in the classical theory. In this paper we shall treat the theory as a mathematical exercise, as none of its physical implications have yet been tested. However such a theory, if true, has some important conceptual consequences, which are experimentally verifiable, and in the following paper[6] we will point out some of them.

First we discuss the rationale for the theory, namely that the equivalence principle allows one to introduce the proper time of a particle as an independent degree of freedom, independent of coordinate time. This is not a purely formal procedure, but has a direct observational significance. The proper time enters the canonical formalism as any other coordinate would, and mass plays the role of its canonically conjugate variable. The theory is then developed for the nonrelativistic case and for a relativistic field and particle. The equivalence principle enters the formalism in a very specific manner. Next some simple examples are solved, including the case of an expanding steady-state universe with continuous creation, and it is shown that the model leads to the correct relation between the rate of expansion and the density of matter, with no free parameters.

The important point here is not the numerical agreement, which arises automatically, but the fact that the theory provides a dynamics which can be incorporated into models with mass creation. The usual steady-state theory is not actually a theory at all, but only the boundary condition on a theory, so its results may be worked out without a specific model, if one accepts the perfect cosmological principle. However,if the perfect cosmological principle is not valid, which is probably the case, then one cannot alter the steady-state theory to produce a theory of, say, partly continuous creation and partly "big bang," or any other variation of this type, unless one has a specific dynamics. The usual steady-state theory provides no guide along these lines, while the present theory offers a complete dynamics.

We also make some preliminary remarks concerning the 2-body problem within the theory.

1. RATIONALE

The main idea of the present theory is the elevation of the proper time, as read by a clock located on a

particle, to the role of a new independent internal coordinate, or degree of freedom, and it is the principle of equivalence that makes this possible. (There are other theories in five dimensions[7] making formal use of proper time, however we will impart to it an immediate physical reality and observability.)

First, we must say a few words about the question of what determines the number of degrees of freedom in a problem. The question has strong philosophical and psychological overtones, but, for a physicist, the answer to the question of whether a particular variable is an independent degree of freedom depends on the mathematical role it plays in the formalism being used.

For example, we could treat the problem of a point mass confined to motion in a plane, by either of the following mathematical expedients: First, we could set up a Hamiltonian with two independent variables, and never acknowledge the existence of a dimension outside the plane; and second, we could imbed the problem in 3-space, with a constraint imposed on the motion. In the latter case, the reward for the extra complexity involved is that one can solve for the constraining forces. However, if there were no possibility of ever observing motion in the third dimension, the distinction would be an arbitrary mathematical one, and the idea of constraining forces merely a useful fiction. The "reality" of the third dimension rests on our ability to relax the constraint.

In our formalism the variable conjugate to the proper time is the mass (rest energy) of the particle, and by relaxing the constraint connecting proper time to coordinate time, the extra "forces" one observes can change the rest mass of the particle. However, even if one is not particularly interested in treating particles of changing mass, the very possibility has important implications in quantum mechanical discussions of the localization and rigidity of inertial frames, and we shall touch upon these in Paper II.[6]

But there is a further role that an independent degree of freedom plays in the setting up of a mechanics problem, and this to some degree determines the physical significance of the concept. Since the laws of motion are second-order differential equations, we have the freedom to set up two independent experimental parameters for each degree of freedom, the initial position r_0 and velocity v_0. Then the future behavior of the system is uniquely determined from its initial state (r_0, v_0) at time t_0, and all its previous history is irrevelant. This ability to mathematically prescribe arbitrary initial conditions acquires physical significance from the circumstance that we are in fact physically free to interfere with the system (at least in principle) and to alter these initial conditions,[8] and it is of course crucial that the future behavior of a spring, once we have released it, does not depend on the physiological machinations required to set it up initially, prior to t_0.

In classical nonrelativistic physics, the proper time as registered by a clock on a particle at rest is the same as that on a clock in the laboratory. Special relativity partly transcends this restriction. For, even if a particle's proper time is set to coincide with that of the laboratory, once it has been accelerated it will disagree with the laboratory clock, even after it has again come to rest in the laboratory. The proper time cannot be eliminated by writing $\tau = \tau(\mathbf{r}, t)$, a single-valued function of the coordinates, since it depends on the trajectory (i.e., the past history) of the particle. But once the particle returns to rest in the laboratory, its subsequent behavior will be independent of how its clock came to differ with that in the laboratory. In this sense we can say that we have reset the clock, as we could an independent coordinate. However $d\tau/dt = (1 - v^2/c^2)^{\frac{1}{2}}$ *is* a single-valued function of the coordinates, since the velocity is, and thus the clock rate is uniquely determined at every instant, which is why τ is not an independent degree of freedom.

In general relativity the situation is different. Imagine two small laboratories, as in Fig. 1. One is located inside a hollow spherical mass shell at P_1 and the other at infinity, i.e., at $P_2(r)$, where $r \gg R$. Both of them are in a force-free region of space, and both of them can determine that they are inertial frames, even over a finite spatial extent. And in fact they can determine by local measurements that all their local laws of physics are identical. However, when they communicate, point P_2 will notice a red shift in the signal from P_1, due to their different gravitational potentials. Thus, although they observe identical local physics, their clocks run at different rates. We see, then, that local physical laws do not depend on what rate local proper time runs, relative to some prescribed coordinate time. (Because of the arbitrary nature of coordinates in general relativity, we should perhaps be more

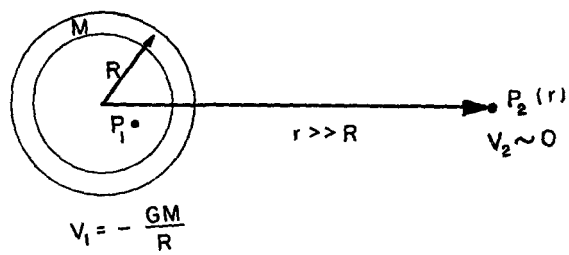

FIG. 1. Setting Proper Time. Two laboratories, P_1 inside a spherical mass shell and P_2, very far away at $r \gg R$, are both in essentially force-free regions, yet at different potentials. Their rest clocks run at different rates.

specific. In our example, because of the static nature of the field, clocks can be synchronized everywhere,[9] thus setting up a universal coordinate time t, say by using radiation from a standard atom located at P_2. Then the observer at P_1 will see that the same atom at rest in his laboratory runs at a different rate τ, i.e., it has $d\tau/dt \neq 1$. Alternatively, this can be converted to a description wherein every observer uses local atoms to set his clocks, in which case it would be coordinate time that changes.) The rate $d\tau/dt$ is merely a measure of the distribution of masses in the universe and can be taken as an arbitrary initial parameter, a different initial value corresponding to a different mass distribution. But one need not know the details of how this mass distribution was set up—their effect is summed up in the value of $d\tau/dt$.

Thus, in principle, one can affect the value of both τ and $d\tau/dt$ relative to local coordinate time, and, after choosing initial values, the subsequent motion of the system will be independent of the past history[10] prior to t_0. It only remains to be said that τ can be fitted into a canonical formalism, in the same manner as the coordinate $\mathbf{r}$, and we will assume that it is a universal, internal degree of freedom, to be associated with any mass point. (In fact, one parameter may not be enough, but we are not going to develop the theory in its most general form.)

2. NONRELATIVISTIC THEORY

The theory we shall develop is both a theory of gravity and of mass creation. Actually, one can develop an entire hierarchy of theories along these lines, and we will ultimately be concerned with a tensor theory, which will be a generalization of general-relativity. However, in this paper we will develop only the nonrelativistic theory, and a relativistic generalization to a vector theory, as this is easier than the tensor theory and introduces the principle ideas and complications, including nonlinearity.

In the nonrelativistic limit, we consider a single particle with coordinates q_i, proper time τ, velocities $\dot{q}_i$, $\dot{\tau}$ (where the overhead dot, as usual, indicates the derivative with respect to t), situated in an external potential $\varphi(q_i, \tau)$, and having a Lagrangian

$$L = L(q_i, \dot{q}_i, \tau, \dot{\tau}, t). \tag{2.1}$$

We shall assume that the coordinate τ enters the canonical formalism in the same way as any other degree of freedom, and that the momentum conjugate to τ will be the mass of the particle, which physical interpretation will be confirmed by its role in the theory. The canonical momenta are defined by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \quad mc^2 = \frac{\partial L}{\partial \dot{\tau}}. \tag{2.2}$$

(Note that what we have called "mass" actually has the units of energy—c being a constant conversion factor.)

In choosing the coordinates and momenta for the canonical formalism the following convention will be assumed: all the coordinates are independent of the mass; and the momenta are linearly dependent on it, i.e., of the form $mf(q_i, \dot{q}_i)$. There will exist a Hamiltonian

$$H(q_i, p_i, \tau, m, t) = p_i\dot{q}_i + c^2 m\dot{\tau} - L, \tag{2.3}$$

and Hamilton's equations will be satisfied:

$$\frac{\partial H}{\partial p_i} = \dot{q}_i, \quad \frac{\partial H}{\partial q_i} = -\dot{p}_i,$$
$$c^2\frac{\partial H}{\partial m} = \dot{\tau}, \quad \frac{\partial H}{\partial \tau} = -\dot{m}c^2. \tag{2.4}$$

We can already prove at this stage an important theorem characterizing the role of the principle of weak equivalence[11] in this theory. According to this principle any two particles released in an external gravitational field with the same set of initial coordinates and velocities will follow identical trajectories, i.e., the trajectory will be independent of the masses of the particles. It follows from this that the total energy will depend linearly on the mass [since the kinetic, potential, and rest energies are all of the form $mf(x, v)$].

Then, since H depends on m only through the momenta p_i and m itself, we have, from Euler's theorem for a linear homogeneous function,

$$H = p_i\frac{\partial H}{\partial p_i} + m\frac{\partial H}{\partial m}. \tag{2.5}$$

But, from Eqs. (2.4), this gives

$$H = p_i\dot{q}_i + c^2 m\dot{\tau}, \tag{2.6}$$

which implies from Eq. (2.3) that

$$L = 0. \tag{2.7}$$

Thus, in our theory of a single particle in an external field, the principle of equivalence is guaranteed by the condition $L = 0$ (which follows from the equations of motion and is not an identity). The condition $L = 0$ also guarantees that the theory obeys scale invariance[12] though we will not exploit this fact in this paper.

However, we will use the fact that $L = 0$ to help construct a Lagrangian for the theory. In general relativity we note that the Lagrangian L_0 is proportional to the proper time,

$$\int L_0\,dt = -m_0c^2\int d\tau = -m_0c^2\int (g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu)^{\frac{1}{2}}\,dt. \tag{2.8}$$

The only components of $g_{\mu\nu}$ that contribute in the nonrelativistic limit are

$$g_{00} \approx 1 + 2\varphi/c^2, \tag{2.9}$$

where φ is the gravitational potential, and the other diagonal components,

$$g_{ii} \approx -1/c^2, \quad i = 1, 2, 3. \tag{2.10}$$

Then

$$\int L_0\, dt \approx -m_0c^2 \int \left(1 + \frac{2\varphi}{c^2} - \frac{v^2}{c^2}\right)^{\frac{1}{2}} dt$$

$$\approx \int (-m_0c^2 + \tfrac{1}{2}m_0v^2 - m_0\varphi)\, dt. \tag{2.11}$$

Since $L = 0$ in our theory, we will take

$$L = c^2\alpha(\dot\tau + L_0/m_0c^2) = c^2\alpha[\dot\tau - (g_{\mu\nu}\dot x^\mu \dot x^\nu)^{\frac{1}{2}}]$$
$$\approx c^2\alpha(\dot\tau - 1 + v^2/2c^2 - \varphi/c^2), \tag{2.12}$$

where α is some function of the coordinates, and possibly velocities,

$$\alpha = \alpha(x_i, \tau, v_i, \dot\tau), \tag{2.13}$$

which we need not specify in detail. It will be determined by the equations of motion. Thus,

$$L = c^2\alpha X, \quad X = (\dot\tau - 1 - \varphi/c^2 + v^2/2c^2), \tag{2.14}$$

and, in taking derivatives, we will anticipate the fact that by virtue of the equations of motion,

$$X = 0. \tag{2.15}$$

For the momenta we have

$$p_i = \frac{\partial L}{\partial v_i} = \alpha v_i + X\frac{\partial \alpha}{\partial v_i} = \alpha v_i,$$

$$mc^2 = \frac{\partial L}{\partial \dot\tau} = \alpha c^2 + Xc^2\frac{\partial \alpha}{\partial \dot\tau} = \alpha c^2, \tag{2.16}$$

so that $m = \alpha$, and is not necessarily a constant. If we assume that φ is some given function $\varphi(x, \tau, t)$, then the equations of motion are

$$\dot p_i = \frac{\partial L}{\partial x_i} = -\alpha\frac{\partial \varphi}{\partial x_i} = -m\frac{\partial \varphi}{\partial x_i},$$

$$c^2\dot m = \frac{\partial L}{\partial \tau} = -\alpha\frac{\partial \varphi}{\partial \tau} = -m\frac{\partial \varphi}{\partial \tau}. \tag{2.17}$$

Thus it is explicitly the τ dependence of φ that gives rise to a varying mass for the particle.

We can then introduce the Hamiltonian

$$H = p_iv_i + c^2m\dot\tau - L$$
$$= mv_i^2 + c^2m\dot\tau - (mc^2\dot\tau - mc^2 - m\varphi + \tfrac{1}{2}mv_i^2)$$
$$= mc^2 + \tfrac{1}{2}mv_i^2 + m\varphi$$
$$= mc^2 + p_i^2/2m + m\varphi. \tag{2.18}$$

The Hamiltonian equations of motion are

$$v_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m},$$

$$\dot p_i = -\frac{\partial H}{\partial x_i} = -m\frac{\partial \varphi}{\partial x_i},$$

$$\dot\tau = \frac{1}{c^2}\frac{\partial H}{\partial m} = 1 - \tfrac{1}{2}p_i^2/mc^2 + \frac{\varphi}{c^2} = 1 + \frac{\varphi}{c^2} - \frac{v_i^2}{2c^2},$$

$$c^2\dot m = -\frac{\partial H}{\partial \tau} = -m\frac{\partial \varphi}{\partial \tau}. \tag{2.19}$$

We see from this that $X = 0$. Also, the equation for the p_i can be expressed in terms of the v_i,

$$\dot p_i = m\dot v_i + v_i\dot m = -m\frac{\partial \varphi}{\partial x_i},$$

$$\dot v_i = -\frac{\partial \varphi}{\partial x_i} + \frac{v}{c^2}\frac{\partial \varphi}{\partial \tau}, \tag{2.20}$$

and we see that the trajectory is independent of the mass of the particle. The fact that in mechanics $L = T - V$, while $H = T + V$, is reflected here by the fact that m appears explicitly in the numerator in L and in the denominator in H.

The last term in Eq. (2.20) is the correction to the motion due to the changing particle mass. It is a $1/c^2$ correction to the equation of motion. To this same order there are kinematical corrections from special relativity, and also corrections from general relativity, which are not included. We have written a Newtonian theory, with nonconstant mass.

The potential $\varphi(x, \tau)$ is not purely arbitrary, but must be restricted by a gauge condition (5.1). We will also note in passing that the form of the terms in the Lagrangian

$$L \sim \int \alpha\dot\tau\, dt = \int \alpha\, d\tau \tag{2.21}$$

is very suggestive of the conformal line element[13] and we believe that this theory should be helpful in providing a guide to the interpretation of conformal theories.

3. RELATIVISTIC THEORY-FIELDS

In a full relativistic theory of gravity, the external field φ of the previous section would presumably be related to the component g_{00} of the metric tensor. However, in this paper we are going to construct a vector theory, as it is much easier to work with, has an analog in electrodynamics, and yet contains all the essential complications of the full theory.

We are seeking a vector potential $B_\mu(x_\nu, \tau)$ to be coupled to a matter field $\Psi(x_\nu, \tau)$. We can construct the theory by noting that it contains a type of gauge

invariance, insofar as the forces do not depend on the actual value of τ at any point. Thus we can change τ independently at every point in space

$$\tau \to \tau' = \tau - g\sigma(x), \tag{3.1}$$

where g is a coupling constant,[14] and cancel this effect by introducing a gauge transformation in the field B_μ. This is quite similar to the problem of making a gauge change in electrodynamics (EM case), a main difference being that in EM theory we have a 1-parameter transformation, the phase of the wave-function, while for this case we have a continuous parameter τ, on which the potential may depend, and which may be changed independently at every point. The technique is due to Yang and Mills.[15] It was elaborated by Utiyama[16] for an arbitrary Lie group, and the continuous parameter case was treated by Greenberger,[12] from which paper the following theory is taken.

The second main difference between this and the EM case is that in the EM case the transformation is a pure gauge transformation, at a particular point in space–time, while here the transformation (3.1) induces a combination coordinate and gauge transformation. Under the transformation (3.1) the matter field Ψ transforms as

$$\Psi(x, \tau) \to \Psi'(x, \tau') = \Psi(x, \tau). \tag{3.2}$$

The field $B_\mu(x, \tau)$ acquires a gradient under this transformation,

$$B_\mu(x, \tau) \to B'_\mu(x, \tau') = B_\mu(x, \tau) - \partial_\mu\sigma. \tag{3.3}$$

The "minimal" gauge-invariant coupling is produced by the recipe

$$\partial_\mu \to \left(\partial_\mu - gB_\mu \frac{\partial}{\partial\tau}\right) \equiv D_\mu. \tag{3.4}$$

Then, since

$$\partial_\mu\Psi'(x, \tau') = (\partial_\mu)_{\tau'}\Psi'(x, \tau') - g(\partial_\mu\sigma)\frac{\partial\Psi'(x, \tau')}{\partial\tau'} \tag{3.5}$$

and

$$\frac{\partial\Psi'(\tau')}{\partial\tau'} = \frac{\partial\Psi(\tau)}{\partial\tau}, \tag{3.6}$$

it follows that

$$\begin{aligned}\left(\partial_\mu - gB'_\mu(\tau')\frac{\partial}{\partial\tau'}\right)\Psi'(\tau') &= \left\{\partial_\mu - g[B_\mu(\tau) - \partial_\mu\sigma]\frac{\partial}{\partial\tau'}\right\}\Psi'(\tau') \\ &= \left(\partial_\mu - gB_\mu(\tau)\frac{\partial}{\partial\tau}\right)\Psi(\tau).\end{aligned} \tag{3.7}$$

These formulas are analogous to those used to introduce the EM field, in which case

$$\begin{aligned}&\Psi \to \Psi e^{-ie\sigma(x)}, \\ &A_\mu \to A_\mu - \partial_\mu\sigma, \\ &\partial_\mu \to \partial_\mu - ieA_\mu.\end{aligned} \tag{3.8}$$

In the EM case there is no coordinate transformation induced in Ψ, whereas in our case the point (x, τ) becomes (x, τ').

In the EM case the field A_μ is restricted by the gauge condition

$$\partial_\mu A_\mu = 0, \tag{3.9}$$

while the phase function σ must be a solution of the equation

$$\Box\sigma = 0. \tag{3.10}$$

The gauge-invariant field tensor is

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{3.11}$$

Analogous formulas hold in our case. If we choose the gauge condition

$$\partial_\mu B_\mu - gB_\mu \frac{\partial B_\mu}{\partial\tau} = D_\mu B_\mu = 0, \tag{3.12}$$

then σ can be consistently restricted to be a function of x alone, i.e., $\sigma \neq \sigma(\tau)$, and will then also be restricted to solutions of Eq. (3.10).

The invariant field tensor in this case is

$$\begin{aligned}F_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu - g\left(B_\mu \frac{\partial B_\nu}{\partial\tau} - B_\nu \frac{\partial B_\mu}{\partial\tau}\right) \\ &= D_\mu B_\nu - D_\nu B_\mu.\end{aligned} \tag{3.13}$$

The quantities Ψ, $D_\mu B_\mu$, and $F_{\mu\nu}$ all transform as

$$f(x, \tau) \to f'(x, \tau') = f(x, \tau), \tag{3.14}$$

while B_μ itself is not invariant but transforms according to Eq. (3.3). However, when B_μ is properly coupled, via the recipe of Eq. (3.4), then the Lagrangian density $\mathfrak{L}(x, \tau)$ also transforms as

$$\mathfrak{L}'(x, \tau') = \mathfrak{L}(x, \tau). \tag{3.15}$$

The action A, given by

$$A = \int d^4x \int d\tau \mathfrak{L}(x, \tau), \tag{3.16}$$

is invariant under the transformation, and leads to the field equations

$$\partial_\mu\left[\frac{\partial\mathfrak{L}}{\partial(\partial_\mu u)}\right] + \frac{\partial}{\partial\tau}\left[\frac{\partial\mathfrak{L}}{\partial(\partial u/\partial\tau)}\right] - \frac{\partial\mathfrak{L}}{\partial u} = 0, \qquad u = \Psi, B_\nu. \tag{3.17}$$

We should point out two important distinctions between our equations and those of EM theory.

First, in EM theory, (3.8) give

$$(\partial_\mu - ieA'_\mu)\Psi' = e^{-ie\sigma}(\partial_\mu - ieA_\mu)\Psi, \quad (3.18)$$

and in order to make the action an invariant, the phase factor must be killed. So Ψ must be a complex field to carry charge, and must be coupled quadratically, such as through terms $\Psi^*\Psi$, in order to insure charge conservation. In our case the action is invariant automatically, so that even a 1-component field will couple to gravity. Second, the EM field couples through the universal constant e. Our field has a derivative coupling to τ, and this derivative plays the role of the mass operator, so that our coupling is proportional to the mass of the matter field. For the simple τ dependence

$$\Psi = \Psi_0(x)e^{im\tau}, \quad (3.19)$$

we have

$$D_x\Psi = e^{im\tau}(\partial_\mu - igmB_\mu)\Psi_0 \quad (3.20)$$

and the field appears similar to a Maxwell field, but with the coupling proportional to the mass of the particle.

If we choose for the free-field Lagrangian corresponding to B_μ, the expression

$$\mathfrak{L}_0 = -\tfrac{1}{4}F_{\mu\nu}F_{\mu\nu}, \quad (3.21)$$

then the free-field equation generated by Eq. (3.17) is

$$D_\mu F_{\mu\nu} - 2g\left(\frac{\partial B_\mu}{\partial\tau}\right)F_{\mu\nu} = 0. \quad (3.22)$$

The example of B_μ interacting with a Dirac field is treated in Ref. 12. In the presence of a matter field Eq. (3.22) is altered to the form

$$D_\mu F_{\mu\nu} - 2g\left(\frac{\partial B_\mu}{\partial\tau}\right)F_{\mu\nu} = -4\pi g\mathfrak{J}_\nu. \quad (3.23)$$

We can write these equations out in an explicit metric. We will use the following conventions: Latin letters run from 1–3, Greek from 1–4, and

$$g_{ii} = 1, \quad g_{44} = -1. \quad (3.24)$$

Keeping track of covariant vs contravariant indices, we define

$$\begin{aligned} F_{ij} &\equiv \epsilon_{ijk}H^k \quad (= F^{ij}), \\ F^{4i} &\equiv E^i \qquad (= -F_{4i}), \end{aligned} \quad (3.25)$$

and introduce the potentials

$$B^i \equiv \mathbf{A}, \quad B^4 \equiv \varphi. \quad (3.26)$$

Then from Eq. (3.13) we have

$$\begin{aligned} \mathbf{H} &= \nabla \times \mathbf{A} - g\mathbf{A} \times \mathbf{A}', \\ E &= -\nabla\varphi - \dot{\mathbf{A}} + g\mathbf{A}\varphi' - g\varphi\mathbf{A}', \end{aligned} \quad (3.27)$$

where the superscript primes denotes the (partial) derivative with respect to τ, the overhead dot denotes the partial derivative with respect to t, and $c = 1$.

The gauge condition (3.12) becomes

$$\nabla \cdot \mathbf{A} + \dot{\varphi} - g\mathbf{A} \cdot \mathbf{A}' + g\varphi\varphi' = 0. \quad (3.28)$$

The inhomogeneous equations of motion (3.23) become

$$\begin{aligned} \nabla \times \mathbf{H} - g\mathbf{A} \times \mathbf{H}' - 2g\mathbf{A}' \times \mathbf{H} - \dot{\mathbf{E}} - g\varphi\mathbf{E}' \\ - 2g\varphi'\mathbf{E} = 4\pi g\mathbf{J}, \\ \nabla \cdot \mathbf{E} - g\mathbf{A} \cdot \mathbf{E}' - 2g\mathbf{A}' \cdot \mathbf{E} = 4\pi g\rho. \end{aligned} \quad (3.29)$$

The homogeneous field equations

$$\tfrac{1}{2}\epsilon_{\lambda\mu\nu\kappa}\partial^\mu F^{\nu\kappa} = 0 \quad (3.30)$$

are identical to Maxwell's

$$\begin{aligned} \nabla \times \mathbf{E} &= -\dot{\mathbf{H}}, \\ \nabla \times \mathbf{H} &= 0. \end{aligned} \quad (3.31)$$

One important caution must be made concerning this model, namely that we do not know whether the forces between particles are attractive or repulsive. In analogy with Maxwell's equations we can write the equations of motion to make like particles either attract or repel. The reason why like particles must repel in EM theory is because the requirement of a positive-definite energy demands it. In our nonlinear theory we have not worked out the details of the energy tensor because we do not intend to take the specific model seriously. If our example of continuous creation in Sec. 6 actually predicts a contracting universe, with repulsion, then the tensor form of the theory will correct it. The important point of our continuous-creation calculation will be to show that the mechanism exists and automatically predicts the correct order of magnitude.

One more point should also be noted. It appears that one solution to our equations is for there to be no τ dependence at all, in which case the equations reduce to Maxwell's equations. This is only true if there are no gravitating fields around. In the presence of a $\mathfrak{J}_\mu$, τ becomes a complicated path-dependent nonintegrable function of x_μ. If one could write $\tau = \tau(x_\mu)$, then one could eliminate the τ dependence and it would have no physical effect. This is similar to the statement that in EM, if one could integrate $\int \mathbf{A} \cdot \mathbf{dl}$, one could eliminate the vector potential. The physics is present *because* of its nonintegrability. Although we have only considered an external potential B_μ, the presence of gravitating bodies also produces the τ dependence of B_μ, and therefore mass nonconservation. The question of current conservation is treated in Ref. 12.

4. RELATIVISTIC THEORY—CLASSICAL PARTICLE

If instead of a classical matter field Ψ, we have a classical particle whose coordinates are (x_μ, τ), we can easily determine the coupling equivalent to Eq. (3.4). If we define the Poisson bracket of two functions $F(x, p, \tau, m)$ and $G(x, p, \tau, m)$ as[17]

$$\{F, G\} = \left(\frac{\partial F}{\partial x_i}\frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial x_i}\right) + \frac{1}{c^2}\left(\frac{\partial F}{\partial \tau}\frac{\partial G}{\partial m} - \frac{\partial F}{\partial m}\frac{\partial G}{\partial \tau}\right), \quad (4.1)$$

so that

$$\{p_i, F\} = -\frac{\partial F}{\partial x_i},$$
$$\{m, F\} = -\frac{1}{c^2}\frac{\partial F}{\partial \tau}, \quad (4.2)$$

which is to be compared to the commutator

$$[\partial_i, F] = \frac{\partial F}{\partial x_i}. \quad (4.3)$$

So we see that the Poisson bracket for a function $F(x, \tau)$,

$$\{p_\mu - gmc^2 B_\mu, F\} = -\left(\partial_\mu F - gB_\mu \frac{\partial F}{\partial \tau}\right) = -D_\mu F, \quad (4.4)$$

is the analog of the commutator

$$[D_\mu, F] = D_\mu F. \quad (4.5)$$

Thus for a classical particle, the recipe analogous to Eq. (3.4) is

$$p_\mu \to p_\mu - gmc^2 B_\mu, \quad (4.6)$$

which is linear in the mass, as required by equivalence.

We can construct a particle Lagrangian as in the nonrelativistic case, by noting that our theorem $L = 0$ is still valid. By analogy with special relativity,[18] we choose

$$A = c^2 \int \alpha\left(d\tau - d\lambda + \frac{g}{c^2} B_\mu \, dx^\mu\right), \quad (4.7)$$

where $d\lambda$ is the time element which would be an invariant in special relativity, i.e.,

$$d\lambda = \left(1 - \frac{v^2}{c^2}\right)^{\frac{1}{2}} dt. \quad (4.8)$$

In our theory it is still an invariant with respect to homogeneous Lorentz transformations, but not inhomogeneous ones.

In noncovariant form,

$$A = c^2 \int \alpha\left(\dot\tau - \left(1 - \frac{v^2}{c^2}\right)^{\frac{1}{2}} + \frac{g}{c^2}\frac{1}{c}\mathbf{v}\cdot\mathbf{A} - \frac{g}{c^2}\varphi\right) dt. \quad (4.9)$$

As before, we have

$$c^2 m = \frac{\partial L}{\partial \dot\tau} = c^2\alpha = mc^2, \quad m = \alpha,$$
$$p_i = \frac{\partial L}{\partial v_i} = mv_i\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}} + \frac{1}{c} gmA_i. \quad (4.10)$$

We can invert the last equation to get

$$\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}} = \frac{1}{mc}\left[\left(\mathbf{p} - \frac{gm}{c}\mathbf{A}\right)^2 + (mc)^2\right]^{\frac{1}{2}}. \quad (4.11)$$

The Hamiltonian then takes the form

$$\begin{aligned} H &= \mathbf{p}\cdot\mathbf{v} + mc^2\dot\tau - L \\ &= \frac{mv^2}{(1 - v^2/c^2)^{\frac{1}{2}}} + \frac{gm}{c}\mathbf{v}\cdot\mathbf{A} + mc^2\dot\tau \\ &\quad - \left[mc^2\dot\tau + \frac{gm}{c}\mathbf{v}\cdot\mathbf{A} - mg\varphi - mc^2\left(1 - \frac{v^2}{c^2}\right)^{\frac{1}{2}}\right] \\ &= \frac{mc^2}{(1 - v^2/c^2)^{\frac{1}{2}}} + mg\varphi \\ &= c\left[\left(\mathbf{p} - \frac{gm}{c}\mathbf{A}\right)^2 + (mc)^2\right]^{\frac{1}{2}} + mg\varphi. \end{aligned} \quad (4.12)$$

Hamilton's equations become

$$\frac{v_i}{c} = \left(\frac{1}{c}\right)\frac{\partial H}{\partial p_i} = \frac{[p - (gm/c)A]_i}{\{[p - (gm/c)A]^2 + (mc)^2\}^{\frac{1}{2}}}, \quad (4.13)$$

which is equivalent to Eq. (4.10), and

$$\begin{aligned} \dot\tau &= \frac{1}{c^2}\frac{\partial H}{\partial m} \\ &= \frac{1}{c^2}\frac{c\{mc^2 - (g/c)\mathbf{A}\cdot[\mathbf{p} - (gm/c)\mathbf{A}]\}}{\{[\mathbf{p} - (gm/c)\mathbf{A}]^2 + (mc)^2\}^{\frac{1}{2}}} + \frac{g\varphi}{c^2} \\ &= \left(1 - \frac{v^2}{c^2}\right)^{\frac{1}{2}} - \left(\frac{g}{c^3}\right)\mathbf{v}\cdot\mathbf{A} + \frac{g\varphi}{c^2}, \end{aligned} \quad (4.14)$$

$$\begin{aligned} \dot m &= -\frac{1}{c^2}\frac{\partial H}{\partial \tau} \\ &\equiv -\frac{1}{c^2}H' = \frac{gm\mathbf{A}'\cdot[\mathbf{p} - (gm/c)\mathbf{A}]}{\{[\mathbf{p} - (gm/c)\mathbf{A}]^2 + (mc)^2\}^{\frac{1}{2}}} - \frac{gm}{c^2}\varphi' \\ &= \left(\frac{gm}{c}\right)\mathbf{A}'\cdot\mathbf{v} - \left(\frac{gm}{c^2}\right)\varphi', \end{aligned} \quad (4.15)$$

$$\begin{aligned} \dot p_i &= -\frac{\partial H}{\partial x_i} = \frac{gm(\partial_i A^j)[p - (gm/c)A]_j}{\{[\mathbf{p} - (gm/c)\mathbf{A}]^2 + (mc)^2\}^{\frac{1}{2}}} - mg\partial_i\varphi \\ &= \left(\frac{gm}{c}\right)v_j\partial_i A_j - gm\partial_i\varphi. \end{aligned} \quad (4.16)$$

If we introduce the parameter λ from Eq. (4.8), then we can write the previous equations "covariantly."

We define

$$\frac{dt}{d\lambda} \equiv \gamma = \left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}, \tag{4.17}$$

$$u^i = \frac{dx^i}{d\lambda} = v^i\gamma, \quad u^4 = c\gamma. \tag{4.18}$$

Then, from Eq. (4.10),

$$p^i - (gm/c)A^i = mu^i, \tag{4.19}$$

and, from Eq. (4.12),

$$H - gm\varphi = c[p^4 - (gm/c)B^4] = mc\gamma = mcu^4, \tag{4.20}$$

so that

$$mu^\mu = p^\mu - (gm/c)B^\mu. \tag{4.21}$$

Thus

$$\frac{d\tau}{d\lambda} = 1 - \frac{g}{c^3}u_\mu B^\mu, \tag{4.22}$$

$$\frac{dm}{d\lambda} = \frac{gm}{c^3}u_\mu B^\mu, \tag{4.23}$$

$$\frac{dp^i}{d\lambda} = \frac{gm}{c}u_\mu \partial^i B^\mu. \tag{4.24}$$

To complete the last equation, we note that

$$\frac{dH}{dt} = \left(\frac{\partial H}{\partial x^i}\right)v^i + \left(\frac{\partial H}{\partial p_i}\right)\dot{p}^i + \left(\frac{\partial H}{\partial \tau}\right)\dot{\tau} + \left(\frac{\partial H}{\partial m}\right)\dot{m} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}, \tag{4.25}$$

from the equations of motion, and since the only explicit time dependence can be in B_μ,

$$\begin{aligned}\frac{dH}{dt} &= \frac{-gm(\partial \mathbf{A}/\partial t)\cdot[\mathbf{p} - (gm/c)\mathbf{A}]}{\{[\mathbf{p} - (gm/c)\mathbf{A}]^2 + (mc)^2\}^{\frac{1}{2}}} + gm\frac{\partial \varphi}{\partial t} \\ &= \frac{gm}{c}\frac{\partial \mathbf{A}}{\partial t}\cdot\mathbf{v} + gm\frac{\partial \varphi}{\partial t} = -\frac{gm}{\gamma}u_\mu \partial_4 B^\mu \\ &= \frac{gm}{\gamma}u_\mu \partial^4 B^\mu, \\ \frac{dp^4}{d\lambda} &= \frac{gm}{c}u_\mu \partial^4 B^\mu\end{aligned} \tag{4.26}$$

and, therefore,

$$\frac{dp^\nu}{d\lambda} = \frac{gm}{c}u_\mu \partial^\nu B^\mu. \tag{4.27}$$

The above equation can be converted into an equation for the acceleration by noting that, for any function $f(x, \tau)$,

$$\begin{aligned}\frac{df}{d\lambda} &= \frac{\partial f}{\partial x^\mu}\frac{dx^\mu}{d\lambda} + \frac{\partial f}{\partial \tau}\frac{d\tau}{d\lambda} \\ &= \frac{\partial f}{\partial x^\mu}u^\mu + \frac{\partial f}{\partial \tau}\left(1 - \frac{g}{c^3}u^\mu B_\mu\right) \\ &= u^\mu\left(\partial_\mu - \frac{g}{c^3}B_\mu\frac{\partial}{\partial \tau}\right)f + \frac{\partial f}{\partial \tau} \\ &= u^\mu D_\mu f + f'.\end{aligned} \tag{4.28}$$

Thus

$$\begin{aligned}\frac{d(mu^\nu)}{d\lambda} &= \frac{gm}{c}u_\mu \partial^\nu B^\mu - \frac{g}{c}\frac{d(mB^\nu)}{d\lambda} \\ &= \frac{gm}{c}u_\mu \partial^\nu B^\mu - \frac{g}{c}\frac{dm}{d\lambda}B^\nu \\ &\quad - \frac{gm}{c}\left(u_\mu D^\mu B^\nu + \frac{\partial B^\nu}{\partial \tau}\right) \\ &= \frac{gm}{c}u_\mu\left(\partial^\nu B^\mu - \frac{g}{c^3}B^{\mu'}B^\nu - D^\mu B^\nu\right) - \frac{gm}{c}\frac{\partial B^\nu}{\partial \tau} \\ &= -\frac{gm}{c}u_\mu F^{\mu\nu} - \frac{gm}{c}B^{\nu'}\end{aligned} \tag{4.29}$$

or

$$\frac{du^\nu}{d\lambda} = -\frac{g}{c}u_\mu F^{\mu\nu} - \frac{g}{c}B^{\nu'} - \frac{g}{c^3}u^\nu u_\mu B^{\mu'}. \tag{4.30}$$

Once again the mass has dropped out of the equation of motion, as it should.

Again it should be noted that it is the explicit τ dependence of B^μ that causes the mass to change. However, this explicit dependence, because of our gauge condition (3.12) and (3.28), generally means that B^μ also has an explicit t dependence, which implies that H will not be a constant.

In the nonrelativistic limit, Eq. (4.30) becomes

$$\mathbf{a} = -g\nabla\varphi + g\mathbf{v}\frac{\varphi'}{c^2} - \left(g\frac{v^2}{2c^2}\nabla\varphi + \frac{v^2}{c^2}\mathbf{a} + \frac{\mathbf{v}}{c^2}(\mathbf{v}\cdot\mathbf{a})\right). \tag{4.31}$$

On the right-hand side of this equation, the first term is the lowest-order force term, the second term is the correction due to changing mass and is of higher order. The terms in the final parentheses are special relativistic kinematical corrections of the same order, and which are not present in the nonrelativistic case (2.20).

5. A SIMPLE EXAMPLE

As an illustration of the theory we will work out two simple examples: first, the case of a decaying particle at rest, and second, the case of an expanding

steady-state universe with continuous creation of matter.

Before we begin, we must be able to solve our nonlinear gauge condition. For our examples, both taken in the nonrelativistic limit, we will be able to assume that $A = 0$. The gauge condition (3.28), for φ alone, becomes

$$\frac{\partial\varphi}{\partial t} + \frac{g}{c^2}\varphi\frac{\partial\varphi}{\partial\tau} = 0, \tag{5.1}$$

keeping powers of c^2. If we introduce the notation

$$\psi = (g/c^2)\varphi, \tag{5.2}$$

this condition becomes

$$\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi}{\partial\tau} = 0, \tag{5.3}$$

and we seek a potential of the form

$$\psi = \psi(\mathbf{r}, t, \tau). \tag{5.4}$$

While the condition (5.3) is nonlinear in ψ, it may be inverted to read

$$-\left(\frac{\partial\psi}{\partial t}\right)_\tau \Big/ \left(\frac{\partial\psi}{\partial\tau}\right)_t = +\left(\frac{\partial\tau}{\partial t}\right)_\psi = \psi. \tag{5.5}$$

Thus the gauge condition *is* linear if interpreted as defining

$$\tau = \tau(\mathbf{r}, t, \psi), \tag{5.6}$$

and the general solution is

$$\tau = t\psi + f(\mathbf{r}, \psi). \tag{5.7}$$

This is the most general solution under the assumption that $\partial\psi/\partial\tau \neq 0$; otherwise we have the simple solution

$$\psi = \psi(\mathbf{r}), \tag{5.8}$$

which gives no mass creation.

Now we will consider the problem of a particle at rest at the origin, but decaying under the influence of an external potential $\psi = \psi(t, \tau)$. In this case, the Eqs. (2.19) and (5.7) reduce to

$$\tau = t\psi + f(\psi), \tag{5.9}$$

$$\dot{\tau} = 1 + \psi, \tag{5.10}$$

$$\dot{m}/m = -\psi'. \tag{5.11}$$

Here the dot means the total time derivative.

Taking the derivatives d/dt and $\partial/\partial\tau$ of Eq. (5.9) gives

$$\psi' = \left(t + \frac{\partial f}{\partial\psi}\right)^{-1}, \tag{5.12}$$

$$\dot{\psi} = (\dot{\tau} - \psi)\left(t + \frac{\partial f}{\partial\psi}\right)^{-1} = (\dot{\tau} - \psi)\psi'. \tag{5.13}$$

From Eqs. (5.10) and (5.11), this gives

$$\dot{\psi} = \psi' = -\dot{m}/m \tag{5.14}$$

and, therefore,

$$m = m_0 e^{-\psi(t,\tau(t))}. \tag{5.15}$$

If we assume that $m = m(t)$ is known and we seek a potential $\psi(t, \tau)$ which can produce such a decay, then from Eqs. (5.14) and (5.15) we see that $\psi(t)$ and $\psi'(t)$ are known, and we can determine $f(\psi)$ by inverting Eq. (5.12).

As a particular case, assume exponential decay

$$m = m_0 e^{-\alpha t}. \tag{5.16}$$

Then

$$\dot{\psi}(t) = \psi'(t) = +\alpha \tag{5.17}$$

and

$$\psi(t) = \alpha t. \tag{5.18}$$

From Eq. (5.12), we have

$$\frac{\partial f}{\partial\psi} = \frac{1}{\psi'} - t = \frac{1}{\alpha} - \frac{\psi}{\alpha}, \tag{5.19}$$

and, therefore,

$$f(\psi) = \psi/\alpha - \psi^2/2\alpha. \tag{5.20}$$

This determines $\psi(t, \tau)$ from Eq. (5.9):

$$\begin{aligned} \tau &= \psi t + \psi/\alpha - \psi^2/2\alpha, \\ \psi(t, \tau) &= 1 + \alpha t - [(1 + \alpha t)^2 - 2\alpha\tau]^{\frac{1}{2}}. \end{aligned} \tag{5.21}$$

The negative root must be chosen to be consistent with the equation for $\tau(t)$. From Eq. (5.10),

$$\begin{aligned} \dot{\tau} &= 1 + \alpha t, \\ \tau &= t + \tfrac{1}{2}\alpha t^2, \end{aligned} \tag{5.22}$$

and this is consistent with Eq. (5.21), which then gives

$$\begin{aligned} [(1 + \alpha t)^2 - 2\alpha\tau]^{\frac{1}{2}} &\equiv \xi = 1, \\ \psi(t, \tau(t)) &= \alpha t, \\ \psi' &= \alpha/\xi = \alpha. \end{aligned} \tag{5.23}$$

Thus Eq. (5.21) represents the potential $\psi(t, \tau)$ which causes the exponential decay of Eq. (5.16).

In this example, we have worked out the mathematical details for a particle decaying into the void. Of course this violates energy conservation, and, in any other coordinate system moving with constant velocity, it would also violate momentum conservation. However this is not an objection to the theory since the external field, which in mechanics must absorb the momentum change of the particle, must here also absorb the energy change. In a more realistic example, the particle should be coupled to other particles, so that over-all energy and momentum can be conserved.

We will not consider the question of interacting particles here within the vector formalism; however, we will point out some characteristics of an interacting theory. If two nonrelativistic particles are coupled through a potential that depends on $(\tau_2 - \tau_1)$, then, if we write the potential energy as

$$V_{12} = m_1 m_2 \varphi(\tau_1 - \tau_2), \tag{5.24}$$

we see that

$$\frac{\dot{m}_1}{m_1} = -m_2 \frac{\partial \varphi}{\partial \tau_1},$$
$$\frac{\dot{m}_2}{m_2} = -m_1 \frac{\partial \varphi}{\partial \tau_2} = m_1 \frac{\partial \varphi}{\partial \tau_1}. \tag{5.25}$$

This in turn implies that

$$\dot{m}_1 + \dot{m}_2 = 0, \quad m_1 + m_2 = \text{const}, \tag{5.26}$$

and the total mass will be conserved. This result will be true for any number of interacting particles if the potential is of the form

$$V_{ij} = m_i m_j \varphi(\tau_i - \tau_j). \tag{5.27}$$

In that case we would obtain

$$\sum m_i = \text{const}. \tag{5.28}$$

Without giving a detailed treatment of the 2-body problem, we will point out, however, that the problem must be reparametrized differently from the usual formulation. Normally there are two sets of canonical variables, one for each particle, with Poisson brackets

$$\{x_{1i}, p_{1j}\} = \{x_{2i}, p_{2j}\} = \delta_{ij}, \quad \text{etc.} \tag{5.29}$$

In our case the Poisson brackets are defined as in Eq. (4.1), except that the sums run over the variables of both particles. We can then introduce, as in the usual case, center of mass and relative coordinates:

$$\mathbf{R} = (m_1/M)\mathbf{r}_1 + (m_2/M)\mathbf{r}_2, \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2,$$
$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{p} = (m_2/M)\mathbf{p}_1 - (m_1/M)\mathbf{p}_2, \tag{5.30}$$
$$M = m_1 + m_2,$$

which obey the rules

$$\{R_i, P_j\} = \{r_i, p_j\} = \delta_{ij}, \quad \text{etc.} \tag{5.31}$$

However in our case there are two other sets of variables τ_1, m_1 and τ_2, m_2 which obey the rules

$$\{\tau_1, m_1\} = \{\tau_2, m_2\} = 1, \quad \text{etc.} \tag{5.32}$$

and it is easy to see that these variables do not commute with the center of mass and relative coordinates because of the masses in their definition. For example,

$$\{\tau_1, \mathbf{R}\} = \{\tau_1, [m_1/(m_1 + m_2)]\mathbf{r}_1 + [m_2/(m_1 + m_2)]\mathbf{r}_2\}$$
$$= (m_2/M^2)\mathbf{r},$$
$$\{\tau_1, \mathbf{p}\} = \{\tau_1, [m_2/(m_1 + m_2)]\mathbf{p}_1 - [m_1/(m_1 + m_2)]p_2\}$$
$$= -(m_2/M^2)\mathbf{P}. \tag{5.33}$$

Nonetheless, we can introduce a set of canonical variables for the problem, which then obey all the usual commutation rules:

$$M = m_1 + m_2, \quad T = (m_1/M)\tau_1 + (m_2/M)\tau_2,$$
$$\Delta = (m_1 - m_2)/2M, \quad \delta = M(\tau_1 - \tau_2) + P \cdot r, \tag{5.34}$$

$$\{T, M\} = \{\delta, \Delta\} = 1, \quad \{T, R\} = \{T, p\} = 0, \quad \text{etc.} \tag{5.35}$$

Then if the Hamiltonian is a function of δ (which depends on $\tau_1 - \tau_2$), but not of T, then the total mass M will be conserved.

6. CONTINUOUS CREATION

As a further example of the theory we will calculate in the nonrelativistic limit the case of an expanding steady-state universe, with continuous creation. Since the vector theory will be inaccurate when the velocity of expansion v approaches that of light anyway, we will lose little by the nonrelativistic restriction, and gain simplicity. The main point is to show that the theory provides a reasonable model for the phenomenon, and yields a relation between the rate of expansion and the average mass density of the universe, which is in order of magnitude agreement with observation, with *no* free parameters. A tensor calculation would yield the same order of magnitude agreement, so that the theory is capable of providing a theoretical basis to steady-state cosmologies. It is of course also compatible with a big-bang theory—though then not necessary—or with any combination of the two.

In accord with the perfect cosmological principle, we assume that the expansion is everywhere uniform, both in space and time. This implies that if we choose an arbitrary origin, then the expansion will be radial, with

$$\mathbf{v} = \alpha \mathbf{r}, \tag{6.1}$$

where α is related to Hubble's constant T, the "age of the universe," by $\alpha = 1/T$. Thus,

$$\mathbf{r} = \mathbf{r}_0 e^{\alpha t}, \tag{6.2}$$

for any small aggregation of matter moving along with the general expansion.

The density ρ must satisfy

$$\rho = \text{const}, \tag{6.3}$$

because of the steady-state condition. Then, if we follow the surface of a sphere growing with the general expansion, the amount of matter contained inside is

$$m = \rho V = m_0 e^{3\alpha t}. \tag{6.4}$$

Since the problem is purely radial, if there were a vector potential it would be radial and would give rise to no field and could therefore be "gauged away." Therefore, we seek a solution

$$B^i = 0, \quad B^4 = \varphi. \tag{6.5}$$

Then our solution must satisfy Eqs. (2.19), (2.20), (5.1), and (5.7), which take the form (with $g = c = 1$)

$$\frac{\partial \varphi}{\partial t} + \varphi\varphi' = 0, \tag{6.6a}$$

$$\tau = t\varphi + f(r, \varphi), \tag{6.6b}$$

$$\dot{\tau} = 1 + \varphi - \tfrac{1}{2}v^2, \tag{6.6c}$$

$$\dot{v} = -\frac{\partial \varphi}{\partial r} + v\varphi', \tag{6.6d}$$

$$\dot{m}/m = -\varphi' = 3\alpha. \tag{6.6e}$$

The second equation above is the solution to the first, the gauge condition. The total time derivatives refer to motion comoving with the expanding distribution.

Since in this problem the potential is generated by the mass distribution itself, we must also have, from Eqs. (3.27) and (3.29),

$$\nabla^2\varphi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \varphi}{\partial r}\right) = -4\pi\rho,$$

$$\varphi'\nabla\varphi = \dot{\varphi}'\frac{\partial \varphi}{\partial r'} = 4\pi\rho v. \tag{6.7}$$

We seek functions $\varphi(r, t, \tau)$, $\tau(r, t)$, and $r(t)$. In analogy with the electrostatic case we assume that $\varphi(r, t, \tau(r, t)) \equiv \varphi(r, t)$ will be of the form

$$\varphi(r, t) = -3\alpha t + 3\alpha b r^2, \tag{6.8}$$

where the first term must be independent of r, and has been chosen so that τ will turn out to be equal to t plus corrections. In line with this we shall also rewrite Eq. (6.6b) more explicitly, as

$$\tau = t\varphi + g(r, \varphi) - \gamma r^2, \tag{6.9}$$

with $\gamma = \text{const}$. In Eqs. (6.8) and (6.9), the constants b and γ are assumed to be of the same order as α and in all our calculations we will work to the lowest order of α necessary.

From Eq. (6.9), we get

$$1 = \left(t + \frac{\partial g}{\partial \varphi}\right)\varphi', \tag{6.10a}$$

$$\dot{\tau} - \varphi = \frac{\dot{\varphi}}{\varphi'} + \left(\frac{\partial g}{\partial r} - 2\gamma r\right)v, \tag{6.10b}$$

$$\frac{\partial \varphi}{\partial r} = -\varphi'\left(\frac{\partial g}{\partial r} - 2\gamma r\right), \tag{6.10c}$$

and from Eqs. (6.8) and (6.6e) we get

$$\dot{\varphi} = -3\alpha + 6\alpha b r v = \varphi'(1 - 2brv). \tag{6.11}$$

Equation (6.10a) can be integrated to give

$$\frac{\partial g}{\partial \varphi} = -\frac{1}{3\alpha}(1 + 3\alpha t) = -\frac{1}{3\alpha}(1 + 3\alpha b r^2 - \varphi), \tag{6.12}$$

$$g(r, \varphi) = -\frac{\varphi}{3\alpha} - br^2\varphi + \frac{\varphi^2}{6\alpha}$$

and

$$\frac{\partial g}{\partial r} = -2br\varphi. \tag{6.13}$$

This then determines $\varphi(r, t, \tau)$ from Eq. (6.9). Equation (6.9) then gives

$$\dot{\tau} - \varphi = 1 + \left(-2br - 2\gamma r + \frac{\partial g}{\partial r}\right)v = 1 - \tfrac{1}{2}v^2. \tag{6.14}$$

The term in $\partial g/\partial r$ here is of higher order (α^2) and may be omitted. Then

$$-\tfrac{1}{2}v = (-2b - 2\gamma)\Gamma = -\tfrac{1}{2}\alpha r,$$

$$b + \gamma = \tfrac{1}{4}\alpha. \tag{6.15}$$

The equation of motion, Eq. (6.6d) gives

$$\dot{v} = \varphi'\left(\frac{\partial g}{\partial r} - 2\gamma r + v\right). \tag{6.16}$$

Again the term $\partial g/\partial r$ may be omitted and we have

$$\alpha^2 r = -3\alpha(-2\gamma + \alpha)r,$$

$$\gamma = \tfrac{2}{3}\alpha, \quad b = -\tfrac{5}{12}\alpha. \tag{6.17}$$

Thus Eq. (6.9) reads

$$\tau = t\varphi - (\varphi/3\alpha) - br^2\varphi + (\varphi^2/6\alpha) - \gamma r^2,$$

which can be inverted to give

$$\varphi(r, t, \tau) = -3\alpha t + 3\alpha b r^2 + 1 - \xi,$$

$$\xi = [(-3\alpha t + 3br^2 + 1)^2 + 6\alpha(\tau + \gamma r^2)]^{\frac{1}{2}}, \tag{6.18}$$

with γ and b given by Eq. (6.17). This equation is consistent if the square root equals unity,

$$\xi = 1, \tag{6.19}$$

which is equivalent to

$$\tau = -\varphi^2(r, t)/6\alpha - \varphi(r, t)/3\alpha - \gamma r^2, \tag{6.20}$$

which is true and may be checked for consistency with Eqs. (6.10b) and (6.14).

To lowest order, Eq. (6.19) becomes

$$\tau = t - \tfrac{3}{2}\alpha t^2 + 3br^2 t - \tfrac{1}{4}\alpha r^2. \tag{6.21}$$

Finally, using Eqs. (6.19) and (6.18) we may calculate ρ and j from Eqs. (6.7) and we find, to lowest order, that

$$\rho = 18\alpha\gamma/4\pi,$$
$$\rho v/c = 18\alpha\gamma^2 r. \tag{6.22}$$

Experimentally, the relation between ρ and Hubble's constant $T = 1/\alpha$ is given by one of Eddington's "magic relations," [3]

$$G\rho T^2 \sim 1, \quad \text{between } 10^{-2} \text{ and } 1, \tag{6.23}$$

while Eq. (6.22) gives (putting back a $g^2 = G$)

$$G\rho T^2 = 3/\pi. \tag{6.24}$$

We note that this result is obtained with no free parameters to fix. From Eqs. (6.6e) and (6.7) we see that the current caused by the expansion produces a τ dependence in φ just sufficient to generate the correct mass production. (However one should note the cautionary statement at the end of Sec. 3.)

The most significant aspect of this calculation is not the numerical agreement, but the fact that the theory provides a dynamical basis for performing such calculations.

It should be pointed out that the amount of continuous creation needed in the steady-state theory is exceedingly small, so that the classical theory exhibits no gross effects on a less than cosmological scale, except perhaps in the interior of stars. However, the very possibility of variable mass leads to some important qualitative results in the quantum domain, which will be discussed in the Paper II.

[1] This circumstance has even led practitioners to wonder exactly what the connection is between bootstraps and more conventional physics. See G. F. Chew, Science **161**, 762 (1968).

[2] H. Bondi and T. Gold, Monthly Notices Roy. Astron. Soc. **108**, 252 (1948).

[3] H. Bondi, *Cosmology* (Cambridge U.P., London, 1961).

[4] Apparently, the existence of black-body radiation from the primordial "fireball" may be irreconcilable with a steady-state universe. See P. Thaddeus, Bull. Am. Phys. Soc. **12**, 1031 (1968).

[5] The best known attempt is F. Hoyle, Monthly Notices Roy. Astron. Soc. **108**, 372 (1948); **109**, 365 (1949).

[6] D. M. Greenberger, J. Math. Phys. **11**, 2341 (1970), hereafter referred to as Paper II.

[7] One such approach was started by E. C. G. Stuckelberg, Helv. Phys. Acta **14**, 322 (1941); **15**, 23 (1942). Some more recent references to this work can be found in J. H. Cooke, Phys. Rev. **166**, 1293 (1968). A different theory, using coordinate time as a dynamical variable, has been recently proposed by P. Pearle, Phys. Rev. **168**, 1429 (1968).

[8] This assumes that one's equations do not describe every object in the universe, or else one can open a philosophical Pandora's Box.

[9] L. Landau and E. Lifshitz, *The Classical Theory of Fields* (Addison-Wesley, Reading, Mass., 1951), Chap. 10.

[10] This whole argument depends on the gravitational red shift, which in turn depends on the principle of equivalence, and not on the details of general relativity.

[11] "Weak" equivalence refers only to the fact that acceleration in an external gravitational field is mass independent. "Strong" equivalence is a generalization to cover the form of all the laws of physics. See R. Dicke, *The Theoretical Significance of Experimental Relativity* (Gordon and Breach, New York, 1964).

[12] D. M. Greenberger, Ann. Phys. (N.Y.) **25**, 290 (1963).

[13] Some important references, with lists of further references on conformal theories are T. Fulton, F. Rohrlich, and L. Witten, Rev. Mod. Phys. **34**, 442 (1962); H. A. Kastrup, Phys. Rev. **150**, 1183 (1966); Ann. Physik (Leipzig) **9**, 388 (1962); J. A. Schouten, Rev. Mod. Phys. **21**, 421 (1949). A recent work on the physical significance of such theories is J. Rosen, Ann. Phys. (N.Y.) **47**, 468 (1968). The classic attempt at a theory along these lines is that of Weyl, H. Weyl, *Space-Time-Matter* (Methuen, London, 1922).

[14] If G is the gravitational constant, then $g = G^{\frac{1}{2}}$, so that the appearance of G will generally be kept explicit in the relativistic theory.

[15] C. N. Yang and R. Mills, Phys. Rev. **96**, 191 (1954).

[16] R. Utiyama, Phys. Rev. **101**, 1597 (1956).

[17] In this section, $c \neq 1$.

[18] See, for example, Ref. 9.

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Theory of Particles with Variable Mass. II. Some Physical Consequences

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The formalism of the previous paper, in which mass and proper time are treated as independent dynamical variables in a canonical formalism, is shown to imply certain physical consequences. There will exist a mass vs proper time uncertainty relation; trajectories and proper time will be exactly determinable in an external gravitational field, while mass will be determinable in an external electromagnetic field; and conventional quantum mechanics will imply that equivalence is invalid for low-lying quantum states. This leads to a second possible way to quantize a system in a gravitational field, which introduces a fundamental length. It is shown that it is possible to test for quantum interference effects of gravitational systems with present technology and conventional techniques, using the earth's gravitational field.

INTRODUCTION

In the preceding paper,[1] we have shown that the principle of equivalence can be used to justify a formalism where the proper time of a particle, and its mass, enter as two additional independent variables. In the present paper, we show that, if one accepts this postulate of an additional degree of freedom in physical problems, then there are certain physical consequences that follow, and these provide a definite insight into the underlying quantum significance of the principle of equivalence. Our discussion is free of the details of the specific mathematical model of the Paper I, and as a prerequisite requires only a knowledge of the general idea of the theory, as presented there in Secs. 1 and 2.

In Sec. 1, we point out that if proper time and mass are independent variables, they must satisfy an uncertainty relation, and we give several examples, emphasizing how this uncertainty relation differs from that between energy and coordinate time. However, it is possible to proceed further, and we show that, because of the equivalence principle, one can actually measure the trajectory of a particle in an external gravitational field, and thus determine the proper time along the particle path exactly, while one learns nothing of the mass of the particle. In an external electromagnetic (EM) field, the exact opposite is true—one can measure the mass of a particle exactly, without learning its trajectory or proper time.

One then sees that the two classical situations, an external pure gravitational field (where $\Delta m = \infty$), and a pure electromagnetic field ($\Delta m = 0$), are represented by the two extreme poles of the mass-proper time uncertainty relation in much the same way as the classical wave-particle division is represented by the extremes of the Δx, Δp relation. Thus, the idea of mass and proper time as dynamical variables leads to the idea of a duality between gravity and electricity as two classical extremes of a unified quantum mechanical entity.

In Sec. 2, we show that for low-lying states quantum mechanics is incompatible with the equivalence principle, or more precisely, is irrelevant to it, and then, in Sec. 3, we point out that there exists a second method of quantizing a system in an external gravitational field which is consistent with equivalence. We also show that the quantum interference effects of the earth's gravitational field are large enough to be measured in the laboratory, and describe an experiment wherein this may be done.

1. THE MASS–PROPER TIME UNCERTAINTY RELATION

Since mass enters our theory as an operator conjugate to proper time, we might expect that there will be an uncertainty principle satisfied between rest energy and proper time, i.e.,

$$\Delta E_{\text{rest}} \cdot \Delta\tau = c^2 \Delta m \cdot \Delta\tau > \hbar, \tag{1.1}$$

and, in fact, the existence of the uncertainty principle between other pairs of conjugate variables forces this conclusion on us. We examine some simple cases in order to show how this comes about, and also to illustrate the difference between Eq. (1.1) and the similar appearing equation[2]

$$\Delta E \cdot \Delta t > \hbar, \tag{1.2}$$

which one usually sees in quantum mechanics.

The most significant difference between the two equations above is that Δt in Eq. (1.2) represents a time interval, as measured in a particular coordinate system, while $\Delta\tau$ expresses an uncertainty in one coordinate system of the reading of a clock at rest in another system, even though an observer in the rest system might read it exactly. This uncertainty can arise from an uncertain gravitational potential, or from an uncertain velocity in the kinematical factor $(1 - v^2/c^2)^{\frac{1}{2}}$

of special relativity. The energy uncertainty in Eq. (1.2) is generally due to the kinetic or potential energy of the body, rather than its rest energy.

As an illustration of Eq. (1.1), imagine an attempt to determine the mass M of a heavy body by gravitationally scattering off of it a light body of known mass m with $m \ll M$, and known velocity v (see Fig. 1). If the initial velocity of the light body is known accurately, then

$$\theta \sim p_x/p \sim \int F\,dt/mv, \tag{1.3}$$

where F is the gravitational force exerted by M,

$$F \sim \frac{GMm}{x^2}, \quad \int F\,dt \sim \frac{GMm}{xv}. \tag{1.4}$$

Thus,

$$\theta \sim GM/xv^2, \quad M \sim xv^2\theta/G \sim xvp_x/mG. \tag{1.5}$$

If the momentum transfer p_x is measured to within Δp_x, so that

$$\Delta m \sim xv\Delta p_x/mG, \tag{1.6}$$

then the distance of closest approach x cannot be known to within the amount

$$\Delta x \cdot \Delta p \sim \hbar. \tag{1.7}$$

However, while passing M, the particle m also exerts a gravitational force upon it, the potential of which is uncertain, at M, to the extent

$$\Delta\varphi \sim (Gm/x^2)\Delta x. \tag{1.8}$$

Over the period of closest approach $T \sim x/v$, we have

$$T\Delta\varphi \sim (Gm/xv)\Delta x \tag{1.9}$$

and the reading τ of a clock on M will be uncertain to an observer in the laboratory by an amount

$$\Delta\tau \sim T\Delta\varphi/c^2 \sim (Gm/xv)\Delta x, \tag{1.10}$$

even if the clocks reading t and τ were synchronized in the laboratory before the experiment, and even if an observer on M were continuously monitoring his own clock. Thus,

$$\Delta\tau \cdot c^2\Delta M = (xv\Delta p_x/mG)(Gm/xv)\Delta x > \hbar. \tag{1.11}$$

This result follows from the existence of the uncertainty relation (1.7), and needs no further assumptions—an accurate mass measurement depends on an accurate momentum determination, which precludes an accurate proper-time knowledge, and vice versa.

Similar to this experiment, except that the clock on the observed particle is actually read during the experiment, is the famous example discussed by Bohr and Einstein.[3] In that experiment, a box contains a gas of photons which is weighed accurately (in the earth's gravitational field) before the experiment see (Fig. 2). Inside, a clock is programmed to open a trap door at a specific time, for a specific interval, and a train of light is emitted. Afterward, the box is weighed again and the energy emitted, E, is determined. Ignoring gravity, these independent, accurate measurements of E and t would violate the uncertainty principle.

Bohr argued that to measure M accurately, the scale must be at rest. If the reading takes time T, then the uncertain momentum impulse imparted by the reading process must be less than $g\Delta mT$, where g is the earth's field, to yield an accuracy Δm. Then

$$\Delta x > \hbar/\Delta p > \hbar/(g\Delta mT). \tag{1.12}$$

But the gravitational potential is then uncertain, and

$$\Delta T/T \sim \Delta\varphi/c^2 = g\Delta x/c^2, \tag{1.13}$$

from which Eq. (1.1) follows.

This uncertainty results from the inability of the laboratory observer to know the rate at which the clock in the box is running. The experiment can be converted into one for which Eq. (1.2) holds by predicting in advance when the emitted photon train will

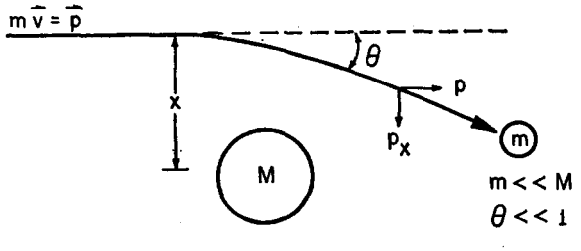

FIG. 1. Gravitational scattering experiment. A light particle m, of known mass and velocity, is gravitationally scattered off a heavy particle, to determine its mass M.

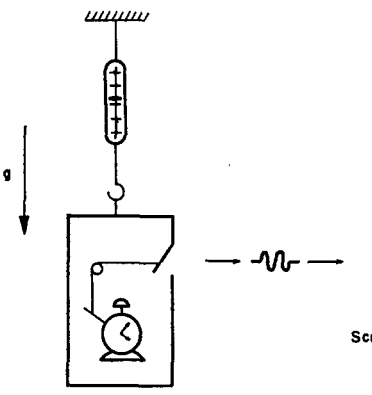

FIG. 2. The Einstein–Bohr experiment. A box of photons is weighed (m_1) in the earth's gravitational field. Then a trap door is opened at a preset time, releasing a photon packet. Next, the box is reweighted (m_2) so that both the photon energy $c^2(m_1 - m_2)$ and proper time of the box are determined. This can be transformed into a laboratory time by predicting when the photon will strike a screen at rest in the laboratory.

strike a screen, at rest in the laboratory, a known distance away. Then Δt represents an interval in the laboratory where the observer, after the weighing, cannot know exactly when the trap door will open.[4]

As an example where the time scale uncertainty is due to kinematical effects of special relativity, we consider the determination of the mass of a particle by use of the Aston mass spectrometer (Fig. 3). In this device, an ion beam is sent along the z axis through parallel static electric and magnetic fields, directed along the y axis. Then the deflections are given by

$$y = eEL^2/2mv^2, \quad x = eHL^2/mcv, \tag{1.14}$$

where $T = L/v$ is the time of flight. The velocity spread of the beam will cause the trace on the screen to be parabolic, where

$$y = \frac{c}{2L^2}\left(\frac{m}{e}\right)\frac{E}{H^2}x^2. \tag{1.15}$$

The slope of the parabola then gives m.

If we choose to determine m by an accurate measure of y and x, then, since $m \sim y/x^2$, we have[5]

$$\left|\frac{\Delta m}{m}\right| = \left|\frac{\Delta y}{y}\right| + 2\left|\frac{\Delta x}{x}\right| > \left|\frac{\Delta y}{y}\right| + \left|\frac{\Delta x}{x}\right|. \tag{1.16}$$

From the measurements, m and v can be fairly accurately determined. However, there will be a resulting inaccuracy in the transverse momenta,

$$\Delta x \cdot m\Delta v_x > \hbar,$$
$$\Delta y \cdot m\Delta v_y > \hbar, \tag{1.17}$$

and since

$$v_x \sim x/T, \quad v_y \sim y/T, \tag{1.18}$$

then

$$(\Delta x/x)mTv_x\Delta v_x > \hbar,$$
$$(\Delta y/y)mTv_y\Delta v_y > \hbar. \tag{1.19}$$

Therefore,

$$(\Delta m/m)mT(v_x\Delta v_x + v_y\Delta v_y) > \hbar. \tag{1.20}$$

But

$$\Delta v^2 \sim v_x\Delta v_x + v_y\Delta v_y, \tag{1.21}$$

so that

$$(\Delta m)c^2T(\Delta v^2)/c^2 > \hbar, \tag{1.22}$$

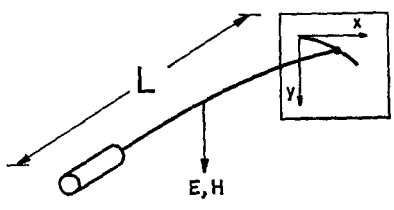

FIG. 3. The Aston mass spectrometer. Parallel E and H fields cause a 2-dimensional deflection pattern, the accuracy of which is controlled by the uncertainty principle Eq. (1.1), even with gravity absent.

and because the proper time uncertainty is just

$$\Delta\tau \sim T\Delta v^2/c^2, \tag{1.23}$$

Eq. (1.1) follows, where $\Delta\tau$ refers to time as read by a clock on a particle in the beam.

In this experiment, we can determine m very accurately. The price we pay for this is that Δv and Δp are very large after the experiment, so that we lose all further knowledge of the trajectory of the particle, and therefore τ.

This loss of knowledge of τ is a general feature of mass determinations made in nongravitational external fields. We can approximate this situation by the equations

$$\Delta m \sim 0, \quad \Delta\tau \sim \infty, \quad \Delta x \sim 0, \quad \Delta v \sim \infty,$$
$$\Delta p \sim \infty. \tag{1.24}$$

In words, an accurate mass determination precludes an accurate knowledge of the subsequent trajectory, as Δx and Δv cannot both be small. Therefore, $\Delta\tau$ is large.

More specifically, in the special case of an electromagnetic field, the different components of the 4-velocity do not commute,

$$[u_\mu, u_\nu] \propto F_{\mu\nu}, \tag{1.25}$$

from which it follows that τ cannot be accurately determined. For, in a magnetic field, we cannot know all the components of the velocity, and therefore the trajectory, accurately, so that τ is uncertain. And in an electric field, we cannot know both v and γ, so again τ is uncertain.

The situation in an external gravitational field is very different. Here the motion in the field gives no knowledge concerning the mass of the particle, because of equivalence, and we can use this to determine τ very accurately.

As an example, consider a particle released from rest in an external gravitational field. If we arrange the initial situation such that approximately

$$\Delta m \sim \infty, \quad \Delta\tau \sim 0, \quad \Delta x \sim 0, \quad \Delta v \sim 0,$$
$$\Delta p \sim \infty, \tag{1.26}$$

then the trajectory $x(t)$ can be calculated exactly even though the mass is unknown. Then, since the potential $\varphi(x)$ will also be known, a laboratory observer can calculate τ for the particle.

This type of experiment, where $\Delta m \sim \infty$, $\Delta\tau \sim 0$, can always be done in gravitational fields. Another example would be a planet moving around the sun in a circular orbit, for which the relation

$$\omega^2R^3 = GM_{\text{sun}} \tag{1.27}$$

allows one to determine τ by computation from the

earth-laboratory period, though the mass of the planet is completely undetermined.

The opposite set of conditions (1.24) and (1.26) on m and τ which pertain to nongravitational and gravitational fields, respectively, are brought about by the equivalence principle, which we believe provides an important clue to the quantum behavior of systems, which will be examined further in Sec. 3, even though we show in the next section that equivalence has no meaning for low-lying quantum states.

The conditions (1.26) are realized only in an *external* gravitational field. If the particle can interact with the source of the field, as in the scattering experiment described at the beginning of this section, then of course the experiment goes beyond equivalence, and then the mass of the particle can be determined, to within the limits determined by Eq. (1.1).

2. EQUIVALENCE AND QUANTUM MECHANICS—MACRO-EQUIVALENCE

Within the framework of ordinary quantum mechanics, the principle of equivalence has no unambiguous meaning for low-lying quantum states,[6] no matter how important equivalence may be in classical gravitational theory. In this section, we briefly recapitulate some of the arguments for this.

The (weak) equivalence principle asserts that any particle released in an external gravitational field with a given initial position $\mathbf{r}_0$ and velocity $\mathbf{v}_0$ will follow the identical trajectory, regardless of its mass. However, when we quantize such a system, even if we consider mass to be a fixed parameter, we find that for low-lying quantum states, radii, frequencies, accelerations, etc., depend on the mass of the particle. For example, a particle of mass m bound to the gravitational potential GmM/r, will have quantized average orbits, frequencies, and accelerations

$$\langle r\rangle_n = \frac{\hbar^2 n^2}{GMm^2}, \quad \langle\omega\rangle_n = \frac{(GM)^2m^3}{\hbar^3 n^3},$$
$$\langle a\rangle_n = \langle\omega^2 r\rangle_n = \frac{(GM)^3m^4}{n^4\hbar^4}. \tag{2.1}$$

The reason for this is dimensional, and quite general. Bohr orbits are defined by the relation

$$\oint p\,dq = nh, \tag{2.2}$$

so that velocities and radii, which classically would be mass independent, are quantized in units of

$$\oint v\,dq = nh/m. \tag{2.3}$$

This functional dependence can be seen in Eqs. (2.1).

The way in which the mass disappears in the limit of high orbits is given by the recipe that, for high n, n is proportional to m. In other words, if a particle of mass m_1 and another of mass $m_2 = Km_1$ are confined to the same region Δr, with the same velocity $\langle v\rangle$ and velocity spread Δv, then the heavier one, m_2, will have more momentum $\langle p_2\rangle = K\langle p_1\rangle$ and a greater momentum spread $\Delta p_2 = K\Delta p_1$. Also, since $\Delta r_2 = \Delta r_1$, then if $\Delta p_1 \cdot \Delta r = n\hbar$, it follows that $\Delta p_2 \cdot \Delta r = Kn\hbar$. It is easy to show in detail that all these relations are simultaneously satisfied by the recipe

$$\text{for} \quad n \gg 1, \quad m_2 = Km_1 \quad \text{implies} \quad n_2 = Kn_1, \tag{2.4}$$

and the whole wavepacket representing particle 2 is scaled up in momentum space accordingly. Specifically, for a potential of the form $V = m\varphi(r)$, the wavefunctions

$$\psi_1 = \psi(m_1, r) = \sum_n a_n u_n(m_1, r), \quad \bar{n} \gg \Delta n \gg 1, \tag{2.5}$$

and

$$\psi_2 = \psi(Km_1, r) = \sum_n a_n u_{Kn}(Km_1, r), \tag{2.6}$$

where the u_n are the eigenfunctions of the Hamiltonian, have the properties that

$$\langle r\rangle_1 = \langle r\rangle_2, \qquad \Delta r_1 = \Delta r_2,$$
$$\langle p\rangle_2 = K\langle p\rangle_1, \quad \Delta p_2 = K\Delta p_1. \tag{2.7}$$

This is how equivalence enters in the classical limit for wavefunctions.

However, for low-lying states $\bar{n} \sim 1$, the above recipe breaks down and, for "minimal" states with

$$\Delta p \cdot \Delta r \sim \hbar, \tag{2.8}$$

it is impossible to satisfy equivalence, as the velocity spread $\Delta v = \Delta p/m$ will then be mass dependent, if Δr is not. Also, such states do not travel in well-defined trajectories, so that the conditions required for classical equivalence are not unambiguously established. (There are also other arguments, given in Ref. 6, which we do not go into.)

The above arguments are presented under the assumption that mass is not a variable. If the mass is considered to be a variable, in the sense of this paper, then one can go somewhat further. In that case, one can construct states with large Δm, but small Δv and Δr, so that trajectories are well defined in the classical sense, and these states obey equivalence—however, they also are superpositions of states with large n—so that here too, states obeying equivalence have

$n \gg 1$. This is because $\Delta r \sim a$, the size of the system, for states with $n \sim 1$. To construct a wavepacket with a well-defined trajectory, then $\Delta r \ll a$, for which one needs a superposition of many states (in fact, approximately $a/\Delta r$ of them).

To sum up, regardless of whether mass is considered a dynamical variable or not, to construct states with well-defined trajectories, one must have $n \gg 1$. In this classical limit, one can satisfy the equivalence principle. However, for bound states with $n \sim 1$, there is no analog of equivalence, and radii, etc., are mass dependent. For this reason, it was proposed in Ref. 6 that the equivalence principle be called "macro-equivalence."

3. AN ALTERNATIVE QUANTIZATION SCHEME FOR GRAVITY MICRO — EQUIVALENCE

Quantum mechanics was developed with the laws of electrodynamics in mind, but there is no reason to believe that it is less applicable to strong and weak interactions. However, in the case of gravity, while there is no evidence that quantum mechanics does not apply, there are circumstances that make it fair to raise the question of whether it can be expected to apply unaltered, or will instead have to be modified.

We have seen that standard quantum mechanics forces upon us the view that the weak equivalence principle has no applicability for low-lying quantum states. This view is certainly self-consistent—however, it leaves one with the unpleasant feeling that equivalence is then merely a "classical accident." Because equivalence is the basis for the entire philosophy of the geometrization of space and time, and specifically of general relativity, it raises the question of whether gravity has any geometrical implications in the microscopic domain, or is in fact "just another force."

This is certainly possible. However, if one accepts the possibility that mass is an independent degree of freedom, then there arises quite naturally a second way to quantize a system in an external gravitational field—a way which is in some sense compatible with equivalence on the microscopic level. We call this alternate quantization scheme "micro-equivalence."

From our point of view, the usual quantum mechanics would hold in nongravitational fields, while the new scheme would hold in purely gravitational fields. We cannot yet present a theory covering the entire range of possibilities, when both gravitational and nongravitational forces are present; however, the two extreme situations form the opposite poles of a continuum of situations, which we can help place into perspective.

We have seen in Sec. 1 that, in an external gravitational field, no information is available concerning the mass of the particle; however, the trajectory, and the proper time along it, are determinable, i.e., $\Delta m \sim \infty$, $\Delta\tau \sim 0$. In an external electromagnetic field, on the other hand, masses can be determined, while trajectories and therefore proper times along them cannot be, i.e., time measurements are confined to the laboratory system, and $\Delta m \sim 0$, $\Delta\tau \sim \infty$.

We would suggest that these two extremes define a situation of complementarity between classical electromagnetic and gravitational fields in much the same way that the extremes of $\Delta p = 0$ and $\Delta x = 0$ define complementarity between classical wave and particle descriptions.[10] And just as one cannot simultaneously determine the particle and wave properties of a system, so one cannot simultaneously determine m and τ, and to the extent that Δm is neither 0 nor ∞, but $0 \ll \Delta m \ll \infty$, one cannot separately isolate the electromagnetic and gravitational properties of an external classical field. This would tend to imply that these two classical fields, electromagnetic and gravitational, form extreme projections of a more complicated unified field that can *only* be understood in full on a quantum level, and one should realize the unique role played by the equivalence principle in creating this interpretation. Thus, the proposal we are about to make for altering quantum mechanics should be taken, not as contradicting quantum mechanics, but rather as complementing it when applied to gravitational fields.

To begin with, while it is true that there is no evidence that the usual quantum mechanics fails to hold in a gravitational field, it is also true that there is no evidence that it does hold. Furthermore, the numbers that the usual quantization scheme yields for microscopic particles are rather absurd. For example, the lowest Bohr orbit for two gravitationally bound neutrons is about 10^{26} cm from Eq. (2.1), which is roughly the size of the universe. The energy is about 10^{-69} eV. Even if such a bound system existed, were it to decay from its first excited state to its ground state, the neutron would have to travel for 10^{9} years (at the speed of light, not at the incredibly small speed it actually has) just to locate its new orbit. While such numbers may merely indicate that we are unlikely to identify such states experimentally, they also tend to undermine the credibility of the theory, as well as raise important epistemological questions concerning its interpretation.

Because the motion of a particle in an external gravitational field is independent of its mass, the whole classical formalism can be rewritten so that the mass

does not enter. If the potential is of the form

$$V(r) = m\varphi(r), \tag{3.1}$$

where φ is independent of the mass, then we can define a canonical velocity

$$v_i \equiv p_i/m, \tag{3.2}$$

and a "reduced" Hamiltonian

$$\mathcal{H} \equiv H/m = \tfrac{1}{2}v^2 + \varphi(r) = \mathcal{E}. \tag{3.3}$$

Both v and $\mathcal{H}$ $(= \mathcal{E})$ are independent of the mass. Hamilton's equations become

$$\dot{x}_i = \frac{\partial \mathcal{H}}{\partial v_i}, \quad \dot{v}_i = -\frac{\partial \mathcal{H}}{\partial x_i}, \tag{3.4}$$

and we can introduce a "reduced Poisson bracket,"

$$\{x_i, v_j\} \equiv \sum_k \left[\left(\frac{\partial x_i}{\partial x_k}\right)\left(\frac{\partial v_j}{\partial v_k}\right) - \left(\frac{\partial v_j}{\partial x_k}\right)\left(\frac{\partial x_i}{\partial v_k}\right)\right] = \delta_{ij}. \tag{3.5}$$

Thus, the entire formalism exactly parallels the usual one, except that the mass never enters. Here the velocity plays the role of a generator of displacements, and the adiabatic invariants are the integrals of the form

$$J_i = \int v_i \, dx_i. \tag{3.6}$$

However, while the classical theory is mass independent, the usual quantized theory *is mass dependent* because the mass enters through the commutation rules

$$[p_i, x_i] = \hbar/i, \tag{3.7}$$

for if we define the operator

$$(v_i)_{\text{op}} \equiv (p_i)_{\text{op}}/m, \tag{3.8}$$

then we have

$$[v_i, x_i] = \hbar/im. \tag{3.9}$$

Thus, it is only at the stage of quantizing the theory that the mass enters.

But may we not ask whether we can carry our classical mass-independent formalism just one step further and introduce a quantum scheme that is also mass independent? For this we need a new fundamental constant, of dimension $\hbar/m$, which we write as $c\lambda_0$ so that the theory automatically introduces a scale λ_0 into physics,[11] which plays the same role here as the fundamental action does in the usual quantum mechanics. Then, as suggested by Eqs. (3.5) and (3.6), we have

$$[v_i, x_i] = c\lambda_0/i, \tag{3.10}$$

and the entire quantum formalism, as well as the classical one, is mass independent, and the justification for Eq. (3.10) in a gravitational field is certainly no weaker than the usual law which quantizes the action in a nongravitational field.

As to the size of the fundamental length λ_0, we have as yet no idea. From the other physical constants it is possible to construct a "length"

$$r_0 = (G\hbar/c^3)^{\frac{1}{2}} \sim 10^{-32} \text{ cm}, \tag{3.11}$$

but there is no reason to expect that λ_0 will be of this magnitude. Using the mass of the neutron, another length from the other physical constants is the "classical radius of the neutron,"

$$r_1 = e^2/mc^2 \sim 10^{-16} \text{ cm}, \tag{3.12}$$

about which the same caution should be exercised. To drive home the point that extreme caution is needed in anticipating numerical constants, we might try to guess the speed of light c' by recombining these constants into a "fundamental velocity." One good attempt would be

$$c' = Gm^2/\hbar \sim 10^{-28} \text{ cm/sec}, \tag{3.13}$$

which turns out to be much closer to the speed of darkness!

The proposal (3.10) or its semiclassical analog

$$J_i = \int v_i \, dx_i = nc\lambda_0, \tag{3.14}$$

should be taken as a suggestion, rather than a unique quantization scheme, in the absence of an exact theory. For example, the proposal

$$J_i' = c^2 \int \frac{p}{E} \, dx = nc\lambda_0, \tag{3.15}$$

would also fulfill our requirements, and reduce to (3.14) for a free particle. At this stage, we would only request an open mind on the subject.

Even without a detailed theory, however, there are certain experimentally observable conclusions which can be drawn concerning such a theory. One is that the phase factor $\exp(-iEt/\hbar)$ of the usual quantization scheme is mass dependent, while that of the new scheme $\exp(-i\delta t/c\lambda_0)$ would not be. This means that in a gravitational interference experiment, while the usual theory predicts that the center of the beam will follow the classical trajectory, (i.e., will be mass independent) it also predicts that interference effects will be mass dependent. With the new theory, all these effects will be mass independent, which is why the proposal is called "microequivalence" (although an exact microscopic trajectory is still not defined).

One way to observe these effects would be to perform a Stern–Gerlach experiment, splitting a beam of particles with spin in an inhomogeneous magnetic field and then coherently recombining it, and observing the effect of the earth's gravitational field while the beam was split. The magnitude of the effect is surprisingly large (from the usual theory) and such an experiment is actually being prepared at this university with the aid of Professor K. Rubin. If the experiment is done with K^{39}, one can use the large electronic magnetic moment to split the beam, while monitoring the gravitational interference effect on the much smaller hyperfine structure. If the two beams of K^{39} are split coherently by $z \sim 10^{-4}$ cm in a strong magnetic field of about 10^3 G, the frequency corresponding to the gravitational difference is $\omega_g = mgz/\hbar \sim 7 \times 10^3$ rad/sec. This is much smaller than the $I \cdot J$ hyperfine splitting, $\omega_{hyp} \sim 10^9$ rad/sec, and also smaller than the rate of nuclear precession in a field of 10^3 G, $\omega_n \sim 2 \times 10^6$ rad/sec. However, if the inhomogeneity of the splitting field is about 10^3 G/cm, then the two beams will be in H fields that differ by about 1/10 G, so that their relative frequency will be only $\Delta\omega_n \sim 200$ rad/sec, which is smaller than the gravitational effect. The experiment must be done so as only to see the relative frequency, rather than the much larger precessional frequencies themselves. The details of the experiment, together with a more detailed discussion of microequivalence, will be presented elsewhere.

In conclusion, we would like to reiterate our belief that the principle of equivalence contains considerably more physics than has been already exploited. Besides being the take-off point for relativity, it can provide the basis for a classical theory containing proper time as a new degree of freedom, all the conceptual features of which are capable of experimental verification.

At any rate, one should not be surprised that, if there exists an ultimate structure of space–time, characterized by a fundamental length, this should show up in a gravitational theory, and be related to equivalence. For the very fact that this length and any related phenomena are mass independent is an indication that they transcend any particular dynamical theory and are providing clues to the underlying geometry and topology of space itself.

[1] D. M. Greenberger, J. Math. Phys. **11**, 2329 (1970), hereafter referred to as Paper I.

[2] For the standard interpretation of this equation, see, for example, the text of A. Messiah, *Quantum Mechanics* (Wiley, New York, 1962).

[3] See Bohr's discussion in *Albert Einstein—Philosopher, Scientist*, P. A. Schlipp, Ed. (Tudor, New York, 1951).

[4] This was Bohr's interpretation of the experiment. He did not discuss Eq. I.1.

[5] More correctly, the relation for products of independent events involves the squares of these quantities. However, the results are identical.

[6] See D. M. Greenberger, Ann. Phys. (N.Y.) **47**, 116 (1968). A relevant publication, using a special wavepacket calculation (Ref. 7), as well as other examples of the gravitational Bohm–Aharanov effect (Refs. 8, 9), also exist.

[7] S. Epstein, Phys. Letters **11**, 233 (1964).

[8] J. S. Dowker, Nuovo Cimento **52B**, 129 (1967).

[9] Y. Aharanov and D. Visnivesky, Ann. Phys. (N.Y.) **45**, 479 (1967).

[10] A classic treatment of complementarity is W. Heisenberg, *Physical Principles of the Quantum Theory* (Dover, New York, 1930). See also D. Bohm, *Quantum Theory* (Prentice Hall, Englewood Cliffs, N.J., 1951).

[11] Other theories have been proposed introducing a fundamental length, usually with the hope of eliminating divergences in field theories. A recent attempt, which does not use a discrete space–time is Tung-Mow Yan, Phys. Rev. **160**, 1182 (1967); K. Ford, Phys. Rev. **175**, 2048 (1968).

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Moments and Correlation Functions of Solutions of a Stochastic Differential Equation

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This paper shows how to obtain exact, closed-form expressions for various moments and correlation functions of the solutions of the stochastic, ordinary differential equation

$$\frac{d^2u}{dz^2} + \beta_0^2[1 + \eta T(z)]u = 0,$$

where $T(z)$ is the so-called "random telegraph" wave and β_0^2 and η are positive real constants. These moments and correlation functions are calculated by two different methods, one a phase space method and the other a matrix method familiar from optics. It is found that the moments are sums of exponentials. The first-order moments decay exponentially but the second-order moments grow exponentially. The correlation functions are also sums of exponentials and show that the solutions do not form a stationary process. An important application of these results is obtained in the problem of a plane electromagnetic wave normally incident on a randomly stratified dielectric plate. It is shown that, if $\mathcal{C}$ is the amplitude transmission coefficient of the plate, then $\langle 1/\mathcal{C}\mathcal{C}^* \rangle$ can be expressed in terms of the second-order moments of the solutions and derivatives of solutions of the stochastic differential equation.

1. INTRODUCTION

This paper shows how to obtain exact, closed form expressions for various moments and correlation functions of the solutions of the stochastic, ordinary differential equation

$$\frac{d^2u}{dz^2} + \beta_0^2[1 + \eta T(z)]u = 0, \tag{1.1}$$

where $T(z)$ is the so-called "random telegraph" wave[1] and β_0^2 and η are positive real constants.

Equation (1.1) is interesting for a number of reasons. In the first place, several problems in the propagation of electromagnetic waves through a randomly stratified dielectric medium can be reduced to a solution of (1.1). These problems include the effect of the random stratification of the dielectric constant on the modes in a dielectric waveguide and on the transmission coefficient for a plane wave normally incident on a dielectric slab. Equation (1.1) also describes a harmonic oscillator with a spring constant which varies randomly. The slab problem will be carefully formulated in Sec. 2 of this paper. We will show that $\langle 1/\mathcal{C}\mathcal{C}^* \rangle$ can be expressed exactly in terms of various second-order moments of the solutions of (1.1), where $\mathcal{C}$ is the amplitude transmission coefficient of the slab and $\langle\ \rangle$ denotes the stochastic average. The slab problem has been the subject of numerous investigations,[2-4] but we believe the results presented here are new. The formula for $\langle 1/\mathcal{C}\mathcal{C}^* \rangle$ is important, for it suggests experiments from which the correlation length of the random irregularities of the dielectric can be estimated.

Since we can calculate exactly various moments and correlation functions of the solutions of (1.1), the equation provides a valuable model on which various approximate methods of solution can be tested. We are especially interested in using this equation to test the "smoothing method"[5] for obtaining approximate solutions of stochastic equations. This technique has been exploited in the study of wave-propagation problems by Keller,[6-9] and has been studied extensively by a number of other authors.[10] In particular, Bourret[11-13] has shown indirectly by diagram techniques that, if the method of smoothing is applied to (1.1) to calculate $\langle u(z) \rangle$, the answer obtained is exact. However, some care must be applied in calculating higher-order moments and correlation functions of (1.1) by the smoothing method, since wrong answers can easily be obtained, as we show in a separate paper,[14] in which we consider some of the problems of applying the method of smoothing to (1.1) wherein $T(z)$ is an arbitrary, stationary process.

In Sec. 2 we will define the random telegraph process, describe carefully the mathematical problem, and derive the relationship between $\langle 1/\mathcal{C}\mathcal{C}^* \rangle$ and various second-order moments of initial value solutions of (1.1).

The remainder of the paper will be devoted to calculating the first- and second-order moments and the correlation functions of the initial-value solutions of (1.1) by two different methods. In Secs. 3 and 4 we show how phase-space methods can be used to solve the problem, and we give some of the details of the calculations in Appendices A–C. In Secs. 5 and 6

we briefly show how the same results can be obtained by matrix methods, and we give some of the details of the calculations in Appendix D.

2. FORMULATION OF THE PROBLEM

The random telegraph process is an ensemble of functions $\{T(z)\}$ defined as follows[1,11–13]: A given function of the ensemble, $T(z)$, can assume only the values ± 1, and as a function of z it makes independent random traversals from one value to another. For fixed z, a sample function chosen at random will equal 1 or -1 with probability $\frac{1}{2}$. The probability that a given sample function makes n traversals in an interval of length z is given by the Poisson distribution

$$p(n, z) = [(bz)^n/n!]e^{-bz}, \quad n = 0, 1, 2, \cdots, \tag{2.1}$$

where b is the average number of traversals per unit length. In all that follows, $T(z)$ will always denote a sample function of the random telegraph process.

A straightforward calculation yields[1]

$$\langle T(z)\rangle = 0, \quad \langle T(y)T(z)\rangle = e^{-2b|y-z|}, \tag{2.2}$$

where here and in all that follows $\langle\ \rangle$ denotes the ensemble average. It follows that $\{T(z)\}$ is a wide sense stationary Markov process. From the expression (2.2) for the autocorrelation function, we see that the correlation length l is

$$l = 1/(2b). \tag{2.3}$$

Each sample function $T(z)$ defines on $0 \leq z < \infty$ two new real functions $u_m(z)$, $m = 1, 2$, which are the linearly independent solutions of

$$\frac{d^2u_m}{dz^2} + \beta_0^2[1 + \eta T(z)]u_m = 0 \tag{2.4}$$

which satisfy the nonstochastic initial conditions

$$u_1(0) = u_2'(0) = 1, \quad u_1'(0) = u_2(0) = 0, \tag{2.5}$$

where β_0 and η are fixed, positive constants. The ensembles of functions $\{u_m(z)\}$, $m = 1, 2$, form two random processes which are the subject of this paper. Throughout this paper we will use the notation

$$v_m(z) = u_m'(z) = \frac{du_m(z)}{dz}, \quad m = 1, 2, \tag{2.6}$$

and

$$\beta_\pm^2 = \beta_0^2(1 \pm \eta). \tag{2.7}$$

To motivate our interest in these random processes, we consider the important physical problem of computing the average reflection and transmission coefficients of an ensemble of randomly stratified dielectric slabs.[2–4] Each slab occupies the region $-\infty < x, y < \infty$, $0 \leq z \leq L$, and its dielectric constant is

$$K(z) = n_0^2[1 + \eta T(z)], \tag{2.8}$$

where we assume $0 < \eta < 1$. The mean and autocorrelation function of the ensemble $\{K(z)\}$ are

$$\langle K(z)\rangle = n_0^2, \quad \langle K(y)K(z)\rangle = n_0^4(1 + \eta^2 e^{-2b|y-z|}). \tag{2.9}$$

Thus each slab can be thought of as formed by a stack of plates having alternately the dielectric constants $n_0^2(1 \pm \eta)$, where the number and thickness of the plates is determined by the sample function $T(z)$. The regions $z < 0$ and $z > L$ are filled with uniform dielectric media having the dielectric constants n_1^2 and n_2^2, respectively.

Let a plane, monochromatic, electromagnetic wave, polarized in the y direction and propagating in the positive z direction, be normally incident on the slab from the left. Part of this incident wave will be reflected and part transmitted. If we denote the amplitude reflection and transmission coefficients by $\mathcal{R}$ and $\mathcal{T}$, respectively, and suppress the common time factor $e^{i\omega t}$, then the total electric field in $z \leq 0$ is

$$e_y = e^{-i\beta_1 z} + \mathcal{R}e^{i\beta_1 z}, \tag{2.10}$$

in $z \geq L$ is

$$e_y = \mathcal{T}e^{-i\beta_2(z-L)}, \tag{2.11}$$

and in $0 \leq z \leq L$ is

$$e_y = A_1u_1(z) + A_2u_2(z). \tag{2.12}$$

In these expressions

$$\beta_j = k_0n_j, \quad j = 0, 1, 2, \tag{2.13}$$

where

$$k_0 = \omega(\mu_0\epsilon_0)^{\frac{1}{2}} \tag{2.14}$$

is the free-space wavenumber. Equation (2.12) holds since the spatial part of the electric field must satisfy (2.4) with β_0 given by (2.13).

The electromagnetic boundary conditions require that e_y and de_y/dz be continuous at $z = 0$ and $z = L$. Applying these conditions, we obtain four linear equations from which the unknowns A_1, A_2, $\mathcal{T}$, and $\mathcal{R}$ can be determined. The power transmission coefficient is found to be

$$\mathcal{T}\mathcal{T}^* = 4\beta_1^2\{2\beta_1\beta_2 + v_1^2(L) + [\beta_2^2u_1^2(L) + \beta_1^2v_2^2(L)] + \beta_1^2\beta_2^2u_2^2(L)\}^{-1}, \tag{2.15}$$

and the power reflection coefficient is related to this by

$$\beta_1\mathcal{R}\mathcal{R}^* + \beta_2\mathcal{T}\mathcal{T}^* = \beta_1. \tag{2.16}$$

In deriving (2.15) we have made use of the fact that the Wronskian of (2.4) is identically 1:

$$u_1(z)v_2(z) - v_1(z)u_2(z) \equiv 1. \tag{2.17}$$

In Eq. (3.10) we will introduce a joint probability density function $p(u_1, v_1, u_2, v_2, z)$ which is given in terms of the solutions of a pair of first-order partial differential equations. In terms of this density function we have

$$\langle \mathcal{C}\mathcal{C}^* \rangle = \int_{-\infty}^{\infty} \mathcal{C}\mathcal{C}^* p(u_1, v_1, u_2, v_2, L)\, du_1\, dv_1\, du_2\, dv_2, \tag{2.18}$$

but we have been unable to calculate p explicitly. However, from (2.15) we do have the relationship

$$4\beta_1^2\langle 1/\mathcal{C}\mathcal{C}^* \rangle = 2\beta_1\beta_2 + \langle v_1^2(L)\rangle + \beta_2^2\langle u_1^2(L)\rangle + \beta_1^2\langle v_2^2(L)\rangle + \beta_1^2\beta_2^2\langle u_2^2(L)\rangle, \tag{2.19}$$

and all the second-order moments appearing in (2.19) can be calculated explicitly.

In fact, we will show in Sec. 3 by a phase space method that each second-order moment of the form $\langle u_j(z)u_k(z)\rangle$, $\langle u_j(z)v_k(z)\rangle$, and $\langle v_j(z)v_k(z)\rangle$, $j, k = 1, 2$, can be written as $\sum_{p=0}^{6} c_p e^{s_p z}$. Here the c_p, $p = 0, \cdots, 6$, are constants, $s_0 = 0$, and the remaining s_p are the roots of the equation $\Delta(s) = 0$, where $\Delta(s)$ is a sixth-degree polynomial given in (A14). The constants c_p are not given explicitly, but a simple prescription is given for their calculation. For small enough η, one of the s_p has a positive real part. In particular, this implies that $\lim \langle 1/\mathcal{C}\mathcal{C}^* \rangle = \infty$, as $L \to \infty$.

In Sec. 4 we show by the phase-space method and in Sec. 6 by the matrix method that each correlation function of the form $\langle u_j(z + \zeta)u_k(z)\rangle$, etc., $j, k = 1, 2$, where $z, \zeta \geq 0$, can be written as

$$\sum_{p=0}^{6}\sum_{r=1}^{4} c_{p,r} e^{s_p z + \sigma_r \zeta}.$$

Here the $c_{r,p}$ are constants and the σ_r are the roots of the equation $d(\sigma) = 0$, where $d(\sigma)$ is a fourth degree polynomial given in (C17). Again the $c_{p,r}$ are not given explicitly, but can be simply calculated. For $0 < \eta < 1$, all the σ_r have negative real parts. From these expressions, it can be seen that the processes $u_m(z)$ and $v_m(z)$ are neither stationary nor wide-sense stationary.

Section 5 is devoted to calculating the moments $\langle u_j(z)\rangle$ and $\langle v_j(z)\rangle$ $j = 1, 2$, by the matrix method. The results (which have been obtained earlier by Bourret[11–13]) show that each first-order moment is of the form $\sum_{r=1}^{4} a_r e^{\sigma_r z}$.

The striking difference between the growth behavior of the first- and second-order moments as $z \to \infty$ can be explained on the basis of phase cancellation. For each choice of sample function $T(z)$, the solutions of (1.1) will be oscillatory with either bounded or unbounded amplitude as $z \to \infty$. However, on taking the stochastic average of all these solutions, cancellations occur between oscillatory solutions which are out of phase, and so the average decays exponentially as $z \to \infty$. However, if these solutions are squared before averaging, the cancellations cannot take place, and so the average of the squares increases exponentially as $z \to \infty$.

3. MOMENTS BY THE PHASE-SPACE METHOD

In this section we show how phase space methods developed by Frisch and Lloyd[15] in their study of electron levels in a 1-dimensional random lattice can be used to calculate various moments of the solutions of (2.4). We remark that the combined process $[u_m(z), v_m(z), T(z), m = 1, 2]$ is a Markoff process, since a knowledge of $u_m(z_0)$, $v_m(z_0)$, $m = 1, 2$, and $T(z_0)$ determines the process for all $z \geq z_0$ via the differential equation and the fact that $T(z)$ itself is a Markoff process. However, $T(z)$ is not a diffusion process but a jump process; hence, the joint process $[u_m(z), v_m(z), T(z)]$ is not a diffusion process and so cannot be described by a Fokker–Planck equation.

We define the conditional probability density functions

$$\begin{aligned} &p_k(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2 \\ &\quad = \text{Prob}\ \{u_m \leq u_m(z) \leq u_m + du_m, \\ &\qquad v_m \leq v_m(z) \leq v_m + dv_m, \\ &\qquad (m = 1, 2) \mid T(z) = (-1)^{k-1}\}, \end{aligned} \tag{3.1}$$

with $k = 1, 2$. We derive a pair of partial differential equations which p_1 and p_2 satisfy. Let there be a small decrement δz in z, and consider the conservation of points in phase. Let us assume that $T(z) = +1$. Then there are three possibilities to be considered. (i) With probability $1 - b\delta z + o(\delta z)$, $T(z - \delta z) = +1$, and T does not change in the interval $(z - \delta z, z)$. In this case, from (2.4)

$$\begin{aligned} u_m(z - \delta z) &= u_m(z) - v_m(z)\delta z + o(\delta z), \\ v_m(z - \delta z) &= v_m(z) + \beta_+^2 u_m(z)\delta z + o(\delta z), \end{aligned} \tag{3.2}$$

and, in particular,

$$\frac{\partial(u_m(z - \delta z), v_m(z - \delta z))}{\partial(u_m(z), v_m(z))} = 1 + o(\delta z). \tag{3.3}$$

(ii) With probability $b\delta z + o(\delta z)$, $T(z - \delta z) = -1$, and there is just one change in T in the interval $(z - \delta z, z)$. In this case,

$$\begin{aligned} u_m(z - \delta z) &= u_m(z) + O(\delta z), \\ v_m(z - \delta z) &= v_m(z) + O(\delta z), \end{aligned} \tag{3.4}$$

and

$$\frac{\partial(u_m(z-\delta z), v_m(z-\delta z))}{\partial(u_m(z), v_m(z))} = 1 + O(\delta z). \quad (3.5)$$

(iii) With probability $o(\delta z)$ there is more than one change in T in the interval $(z-\delta z, z)$.

By combining these three cases and dividing by $du_1\, dv_1\, du_2\, dv_2$, it follows that

$$\begin{aligned} p_1(u_1, v_1, u_2, v_2, z) &= (1 - b\delta z)p_1(u_1 - v_1\delta z, v_1 + \beta_+^2 u_1\delta z, \\ &\qquad u_2 - v_2\delta z, v_2 + \beta_+^2 u_2\delta z, z - \delta z) \\ &\quad + b\delta z p_2(u_1, v_1, u_2, v_2, z) + o(\delta z). \end{aligned} \quad (3.6)$$

Subtracting $p_1(u_1, v_1, u_2, v_2, z)$ from each side of (3.6), dividing by δz, and letting $\delta z \to 0$, we find that[16]

$$\frac{\partial p_1}{\partial z} + v_1\frac{\partial p_1}{\partial u_1} + v_2\frac{\partial p_1}{\partial u_2} - \beta_+^2\left(u_1\frac{\partial p_1}{\partial v_1} + u_2\frac{\partial p_1}{\partial v_2}\right) + b(p_1 - p_2) = 0. \quad (3.7)$$

Similarly,

$$\frac{\partial p_2}{\partial z} + v_1\frac{\partial p_2}{\partial u_1} + v_2\frac{\partial p_2}{\partial u_2} - \beta_-^2\left(u_1\frac{\partial p_2}{\partial v_1} + u_2\frac{\partial p_2}{\partial v_2}\right) + b(p_2 - p_1) = 0. \quad (3.8)$$

The initial conditions, from (2.5) and (3.1), are

$$p_k(u_1, v_1, u_2, v_2, 0) = \delta(u_1 - 1)\delta(v_1)\delta(u_2)\delta(v_2 - 1), \quad k = 1, 2. \quad (3.9)$$

Now, let

$$p(u_1, v_1, u_2, v_2, z) = \tfrac{1}{2}\sum_{k=1}^{2} p_k(u_1, v_1, u_2, v_2, z). \quad (3.10)$$

Then, from (3.1), since $T(z) = \pm 1$ with probability $\frac{1}{2}$ for each sign,

$$\begin{aligned} &p(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2 \\ &\quad = \text{Prob}\{u_m \le u_m(z) \le u_m + du_m, \\ &\qquad v_m \le v_m(z) \le v_m + dv_m, (m = 1, 2)\}. \end{aligned} \quad (3.11)$$

We have been unable to solve these equations explicitly for $p_k(u_1, v_1, u_2, v_2, z)$, $k = 1, 2$, but (3.7) and (3.8) have the remarkable property that from them one can derive finite systems of constant coefficient, first-order, ordinary differential equations for the moments which can be solved explicitly. To define the moments, let

$$\mathbf{F}(z) = \begin{pmatrix} u_1(z) & u_2(z) \\ v_1(z) & v_2(z) \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} u_1 & u_2 \\ v_1 & v_2 \end{pmatrix}, \quad (3.12)$$

and denote by $\mathbf{A}^{(r)}$ the r fold Kronecker product of the matrix $\mathbf{A}$ with itself.[17] Then, in matrix form, the rth-order moments of p_k are given by

$$\langle \mathbf{F}(z)^{(r)} \rangle_k = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathbf{F}^{(r)} p_k(u_1, v_1, u_2, v_2, z) \times du_1\, dv_1\, du_2\, dv_2, \quad (3.13)$$

and the moments of p are defined analogously. Thus, from (3.10), we have

$$\langle \mathbf{F}(z)^{(r)} \rangle = \tfrac{1}{2}\sum_{k=1}^{2} \langle \mathbf{F}(z)^{(r)} \rangle_k. \quad (3.14)$$

[Some of the elements of $\mathbf{F}(z)^{(r)}$ are equal to each other, but this is still a convenient way to define all the moments.] The equations for the rth-order moments are obtained by multiplying (3.7) and (3.8) by the elements of $\mathbf{F}^{(r)}$ and integrating with respect to u_1, v_1, u_2, v_2 from $-\infty$ to ∞. Because of the homogeneity of (3.7) and (3.8) in the u's and v's, the equations for the rth-order moments are uncoupled from the equations for different order moments.

The details of the calculation for the second-order moments are given in the Appendices, but the technique can be applied to moments of all orders. There are twenty second-order moments in all, but there is considerable uncoupling of the equations. Equations are first given in Appendix A for $\langle u_m^2(z)\rangle_k$, $\langle u_m(z)v_m(z)\rangle_k$, and $\langle v_m^2(z)\rangle_k$. The equations for $m = 1$ are uncoupled from those for $m = 2$, and both are uncoupled from the equations for $\langle u_1(z)u_2(z)\rangle_k$, $\langle u_1(z)v_2(z)\rangle_k$, $\langle v_1(z)u_2(z)\rangle_k$, and $\langle v_1(z)v_2(z)\rangle_k$, as is evident from (3.7) and (3.8). The equations in Appendix A are solved by means of Laplace transforms. We denote the Laplace transform of $f(z)$ by

$$\mathfrak{L}(f) = \int_0^{\infty} e^{-sz} f(z)\, dz. \quad (3.15)$$

Expressions are derived for $\mathfrak{L}(\langle u_m^2\rangle)$, $\mathfrak{L}(\langle u_m v_m\rangle)$, and $\mathfrak{L}(\langle v_m^2\rangle)$, for $m = 1, 2$, and are given by (A15)–(A17), (A22), (A25), and (A27), where Δ is given by (A14). Note that, from (A22),

$$\langle u_1^2(z)\rangle = \langle v_2^2(z)\rangle. \quad (3.16)$$

Also, from (A16) and (A24),

$$\frac{d}{dz}\langle u_2^2(z)\rangle = 2\langle u_2(z)v_2(z)\rangle, \quad \frac{d}{dz}\langle u_1^2(z)\rangle = 2\langle u_1(z)v_1(z)\rangle, \quad (3.17)$$

since, from (2.5),

$$\langle u_m^2(0)\rangle = \delta_{m,1}. \quad (3.18)$$

Since $v_m(z) = du_m/dz$, the results of (3.17) are not surprising.

Coupled equations are given in Appendix B for the quantities $\langle u_1(z)u_2(z)\rangle_k$, $\langle u_1(z)v_2(z)\rangle_k$, $\langle v_1(z)u_2(z)\rangle_k$, and $\langle v_1(z)v_2(z)\rangle_k$. These equations are also solved by means of Laplace transforms and expressions for $\mathfrak{L}(\langle u_1v_2\rangle)$ and $\mathfrak{L}(\langle v_1u_2\rangle)$ are given in (B25) and (B26). From the first equation in (B24) it follows that

$$\langle u_1(z)v_2(z)\rangle + \langle v_1(z)u_2(z)\rangle = \frac{d}{dz}\langle u_1(z)u_2(z)\rangle, \quad (3.19)$$

since, from (2.5), $\langle u_1(0)u_2(0)\rangle = 0$. Again, this is not a surprising result in view of the definition of $v_m(z)$. The second equation of (B24) is a consequence of the Wronskian of the solutions of (2.4), i.e., (2.17). Finally, from (B18) and (B21), it follows that

$$\begin{aligned}\langle u_1(z)u_2(z)\rangle &= \langle u_2(z)v_2(z)\rangle,\\ \langle v_1(z)v_2(z)\rangle &= \langle u_1(z)v_1(z)\rangle.\end{aligned} \quad (3.20)$$

We can summarize these results by writing

$$\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_k = \sum_{p=0}^{6} \mathbf{C}_{p,k}e^{s_pz}, \quad (3.21)$$

where the $\mathbf{C}_{p,k}$, $p = 0, \cdots, 6$, $k = 1, 2$, are constant 4×4 matrices, the s_p, $p = 1, \cdots, 6$, are the six roots of $\Delta(s) = 0$, with $\Delta(s)$ given in (A14), and $s_0 = 0$. We have not evaluated the matrices $\mathbf{C}_{p,k}$ explicitly. They are calculated from the residues of the Laplace transforms of the moments at the roots of $s\Delta(s) = 0$. It is easily verified that for small η, $\Delta(s) = 0$ has one root with a positive real part, so that the second moments grow exponentially[18] as $z \to \infty$. This is in marked contrast to the first-order moments which, as we shall see in Sec. 4, all decay exponentially as $z \to \infty$, for $\eta < 1$.

4. CORRELATION FUNCTIONS BY THE PHASE-SPACE METHOD

We now turn our attention to the use of phase-space methods to calculate the correlation functions of the solutions and the derivatives of the solutions of (2.4). For this purpose, we define the conditional probability density functions, with $m, j, k = 1, 2$,

$$\begin{aligned}&Q_{m,jk}(U, V, \zeta \mid z)\, dU\, dV\\ &\quad = Q_{m,jk}(U, V, \zeta \mid u_1, v_1, u_2, v_2, z)\, dU\, dV\\ &\quad = \text{Prob}\,\{U \le u_m(z+\zeta) \le U + dU,\\ &\qquad V \le v_m(z+\zeta) \le V + dV,\\ &\qquad T(z+\zeta) = (-1)^{j-1} \mid u_l(z), v_l(z),\\ &\qquad\qquad (l = 1, 2),\ T(z) = (-1)^{k-1}\},\end{aligned} \quad (4.1)$$

where we assume that $\zeta \ge 0$. Then, since the events $T(z+\zeta) = \pm 1$ are mutually exclusive,

$$\begin{aligned}&\text{Prob}\,\{U \le u_m(z+\zeta) \le U + dU,\\ &\quad V \le v_m(z+\zeta) \le V + dV \mid u_l(z), v_l(z), (l = 1, 2),\\ &\qquad\qquad T(z) = (-1)^{k-1}\}\\ &\qquad = \sum_{j=1}^{2} Q_{m,jk}(U, V, \zeta \mid z)\, dU\, dV.\end{aligned} \quad (4.2)$$

Hence, from the definition of $p_k(u_1, v_1, u_2, v_2, z)$ in (3.1), we have

$$\begin{aligned}&\text{Prob}\,\{U \le u_m(z+\zeta) \le U + dU,\\ &\quad V \le v_m(z+\zeta) \le V + dV,\\ &\qquad u_l \le u_l(z) \le u_l + du_l,\ v_l \le v_l(z) \le v_l + dv_l,\\ &\qquad\qquad (l = 1, 2)\}\\ &\quad = \tfrac{1}{2}\sum_{k=1}^{2}\sum_{j=1}^{2} Q_{m,jk}(U, V, \zeta \mid z)\\ &\qquad \times p_k(u_1, v_1, u_2, v_2, z)\, dU\, dV\, du_1\, dv_1\, du_2\, dv_2,\end{aligned} \quad (4.3)$$

since $T(z) = \pm 1$ with probability $\frac{1}{2}$ for each sign. This result enables us to obtain the correlation functions.

Thus, we define the first-order moments of $Q_{m,jk}(U, V, \zeta \mid z)$ as

$$\langle U_m(\zeta) \mid z\rangle_{jk} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} UQ_{m,jk}(U, V, \zeta \mid z)\, dU\, dV, \quad (4.4)$$

$$\langle V_m(\zeta) \mid z\rangle_{jk} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} VQ_{m,jk}(U, V, \zeta \mid z)\, dU\, dV. \quad (4.5)$$

As is evident from (4.1), these moments depend on $u_l(z)$ and $v_l(z)$, $l = 1, 2$. Let

$$\langle \mathbf{\Phi}(\zeta) \mid z\rangle_{jk} = \begin{pmatrix} \langle U_1(\zeta) \mid z\rangle_{jk} & \langle U_2(\zeta) \mid z\rangle_{jk} \\ \langle V_1(\zeta) \mid z\rangle_{jk} & \langle V_2(\zeta) \mid z\rangle_{jk} \end{pmatrix}. \quad (4.6)$$

Then, from (3.12) and (4.3)–(4.6), we can write the correlation matrix as

$$\begin{aligned}&\langle \mathbf{F}(z+\zeta) \times \mathbf{F}(z)\rangle\\ &\quad = \tfrac{1}{2}\sum_{k=1}^{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\sum_{j=1}^{2}\langle \mathbf{\Phi}(\zeta) \mid z\rangle_{jk} \times \mathbf{F}\right)\\ &\qquad \times p_k(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2.\end{aligned} \quad (4.7)$$

For fixed m and k, the conditional probabilities $Q_{m,jk}$, $j = 1, 2$, satisfy two coupled, first-order partial differential equations which are very similar to Eqs. (3.7) and (3.8) satisfied by the p_k. These equations are given in Appendix C. We have been unable to solve them explicitly, but these equations again have the property that from them one can derive finite systems of first-order, constant-coefficient, ordinary differential equations for the moments which can be solved

explicitly. These equations, satisfied by $\langle U_m(\zeta) \mid z\rangle_{jk}$ and $\langle V_m(\zeta) \mid z\rangle_{jk}$, are also derived in Appendix C. The equations for these latter quantities are solved by means of Laplace transforms. The Laplace transform of a matrix $\mathbf{A}(\zeta)$ is denoted by

$$\Lambda[\mathbf{A}] = \int_0^\infty e^{-\sigma\zeta}\mathbf{A}(\zeta)\, d\zeta. \tag{4.8}$$

It follows from (C14) that

$$\langle \mathbf{\Phi}(\zeta) \mid z\rangle_{jk} = \langle \mathbf{\Phi}(\zeta) \mid 0\rangle_{jk}\mathbf{F}(z). \tag{4.9}$$

Hence, from (3.13), (4.7), and (4.9),

$$\langle \mathbf{F}(z+\zeta) \times \mathbf{F}(z)\rangle = \tfrac{1}{2}\sum_{k=1}^{2}\left[\left(\sum_{j=1}^{2}\langle \mathbf{\Phi}(\zeta) \mid 0\rangle_{jk} \times \mathbf{I}\right)\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_k\right]. \tag{4.10}$$

Expressions for $\Lambda[\langle \mathbf{\Phi}(\zeta) \mid 0\rangle_{jk}]$ follow from (C13), (C15), and (C17)–(C19). In view of (3.12), expressions for the elements of $\mathfrak{L}(\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_k)$ may be deduced from (A9), (A13), (A18), and (A19) and (B10), (B11), (B16), (B19), (B22), wherein **S**, **B**, and **E** are given by (A8).

Let us now consider the meaning of the elements of

$$\sum_{j=1}^{2}\langle \mathbf{\Phi}(\zeta) \mid 0\rangle_{jk},$$

i.e., of

$$\sum_{j=1}^{2}\langle U_m(\zeta) \mid 0\rangle_{jk} \quad \text{and} \quad \sum_{j=1}^{2}\langle V_m(\zeta) \mid 0\rangle_{jk},$$

as defined by (4.4) and (4.5), with $z = 0$. But

$$\sum_{j=1}^{2} Q_{m,jk}(U, V, \zeta \mid 0)$$

is given by (4.2), with $z = 0$. Since $u_l(0) = \delta_{l,1}$ and $v_l(0) = \delta_{l,2}$, $l = 1, 2$, are prescribed in any event, it follows that

$$\begin{aligned}\sum_{j=1}^{2}\langle U_m(\zeta) \mid 0\rangle_{jk} &= \langle u_m(\zeta) \mid T(0) = (-1)^{k-1}\rangle,\\ \sum_{j=1}^{2}\langle V_m(\zeta) \mid 0\rangle_{jk} &= \langle v_m(\zeta) \mid T(0) = (-1)^{k-1}\rangle.\end{aligned} \tag{4.11}$$

From (4.11) we see that we have obtained the first moments as a by-product of the correlation function calculation, since

$$\begin{aligned}\langle u_m(\zeta)\rangle &= \tfrac{1}{2}\sum_{k=1}^{2}\langle u_m(\zeta) \mid T(0) = (-1)^{k-1}\rangle\\ &= \tfrac{1}{2}\sum_{k=1}^{2}\sum_{j=1}^{2}\langle U_m(\zeta) \mid 0\rangle_{jk},\\ \langle v_m(\zeta)\rangle &= \tfrac{1}{2}\sum_{k=1}^{2}\langle v_m(\zeta) \mid T(0) = (-1)^{k-1}\rangle\\ &= \tfrac{1}{2}\sum_{k=1}^{2}\sum_{j=1}^{2}\langle V_m(\zeta) \mid 0\rangle_{jk}.\end{aligned} \tag{4.12}$$

Thus, from (3.12) and (4.6), it follows that

$$\langle \mathbf{F}(\zeta)\rangle = \tfrac{1}{2}\sum_{j=1}^{2}\sum_{k=1}^{2}\langle \mathbf{\Phi}(\zeta) \mid 0\rangle_{jk}. \tag{4.13}$$

To illustrate these results more clearly, from the results of Appendix C, we write

$$\langle \mathbf{\Phi}(\zeta) \mid 0\rangle_{jk} = \sum_{r=1}^{4}\mathbf{A}_{r,jk}e^{\sigma_r\zeta}, \tag{4.14}$$

where the $\mathbf{A}_{r,jk}$ are constant 2×2 matrices and the σ_r, $r = 1, \cdots, 4$, are the four roots of the equation $d(\sigma) = 0$ given in (C17). We have not evaluated the matrices $\mathbf{A}_{r,jk}$ explicitly, but they are the residues of the matrices given in (C18) and (C19) at the roots of $d(\sigma)$. The polynomial $d(\sigma)$ is a biquadratic in $\sigma + b$ and $d(\sigma) = 0$ can be solved easily, so that it can be shown explicitly that $\mathrm{Re}\,(\sigma_r) < 0$ for $r = 1, 2, 3, 4$, as long as $\eta < 1$. Thus the first moments all decay exponentially.

By employing (3.21), (4.10), and (4.14), we can write

$$\langle \mathbf{F}(z+\zeta) \times \mathbf{F}(z)\rangle = \tfrac{1}{2}\sum_{j=1}^{2}\sum_{k=1}^{2}\sum_{p=0}^{6}\sum_{r=1}^{4}(\mathbf{A}_{r,jk} \times \mathbf{I})\mathbf{C}_{p,k}e^{s_p z + \sigma_r\zeta}. \tag{4.15}$$

The processes $u_m(z)$ and $v_m(z)$ are not stationary or wide-sense stationary.

5. FIRST-ORDER MOMENTS BY MATRIX METHOD

In the previous two sections we have shown how various moments and correlation functions of the processes $u_m(z)$ and $v_m(z)$ can be calculated by phase-space methods. In this section we show that matrix methods commonly used to study wave propagation in stratified media[19] can be used to calculate the expected value of the fundamental solution matrix (3.12) corresponding to (2.4) and (2.5). The procedure is to write down the fundamental matrix for a given sample function of the ensemble $\{T(z)\}$, and then to directly average over the ensemble.

Since $T(z) = \pm 1$, (2.4) is an equation with constant coefficients in any interval in which $T(z)$ does not change sign. It is a straightforward matter to show that in such an interval the fundamental solution matrix satisfies

$$\mathbf{F}(z) = \mathbf{N}_\pm(z - z_0)\mathbf{F}(z_0), \tag{5.1}$$

where z_0 is in the interval and

$$\mathbf{N}_\pm(z) = \begin{pmatrix} \cos(\beta_\pm z) & (\beta_\pm)^{-1}\sin(\beta_\pm z)\\ -\beta_\pm \sin(\beta_\pm z) & \cos(\beta_\pm z)\end{pmatrix}, \tag{5.2}$$

according as $T(z) = \pm 1$. Now $\mathbf{F}(z)$ is continuous at the points of discontinuity of $T(z)$. It follows that, if there are n crossings of $T(z')$ in the interval $0 \leq z' \leq z$, at the points z_m, $1 \leq m \leq n$, with $0 < z_1 < z_2 \cdots < z_n < z$, then

$$\mathbf{F}(z) = \mathbf{N}_{(-1)^{n+k-1}}(z - z_n) \times \mathbf{N}_{(-1)^{n+k-2}}(z_n - z_{n-1}) \cdots \mathbf{N}_{(-1)^{k-1}}(z_1), \quad \text{if } T(0) = (-1)^{k-1}, \tag{5.3}$$

since, from (2.5), (2.6), and (3.12), $\mathbf{F}(0) = \mathbf{I}$.

We first calculate the conditional expectation value of $\mathbf{F}(z)$ given that there are n crossings in $(0, z)$ and $T(0) = (-1)^{k-1}$. Since the joint distribution of the n random points, ordered as above, has a uniform density distribution[20] $n!\, z^{-n}\, dz_1 \cdots dz_n$, this conditional expectation value is just

$$\mathfrak{F}_{n,k}(z) = \frac{n!}{z^n} \int_0^z \int_0^{z_n} \cdots \int_0^{z_2} \mathbf{N}_{(-1)^{n+k-1}}(z - z_n) \times \mathbf{N}_{(-1)^{n+k-2}}(z_n - z_{n-1}) \cdots \mathbf{N}_{(-1)^{k-1}}(z_1) \times dz_1 \cdots dz_{n-1}\, dz_n. \tag{5.4}$$

The integral in (5.4) is a multiple convolution and, following Darling,[20] we take the Laplace transform of $z^n \mathfrak{F}_{n,k}(z)$, as in (3.15). Then,

$$\mathfrak{L}[z^n \mathfrak{F}_{n,k}(z)] = n!\, \boldsymbol{\eta}_{(-1)^{n+k-1}}(s) \boldsymbol{\eta}_{(-1)^{n+k-2}}(s) \cdots \boldsymbol{\eta}_{(-1)^{k-1}}(s), \tag{5.5}$$

where

$$\boldsymbol{\eta}_{\pm}(s) = \mathfrak{L}[\mathbf{N}_{\pm}(z)] = \frac{1}{(s^2 + \beta_{\pm}^2)} \begin{pmatrix} s & 1 \\ -\beta_{\pm}^2 & s \end{pmatrix}. \tag{5.6}$$

Now, the probability that $T(z')$ has n crossings in the interval $0 \leq z' \leq z$ is $p(n, z)$, as given by (2.1). Also, $T(0) = \pm 1$ with probability $\frac{1}{2}$ for each sign. Hence, the average value of $\mathbf{F}(z)$ over the ensemble is

$$\langle \mathbf{F}(z) \rangle = \tfrac{1}{2} \sum_{k=1}^{2} \sum_{n=0}^{\infty} \frac{(bz)^n}{n!} e^{-bz} \mathfrak{F}_{n,k}(z). \tag{5.7}$$

For $j = 1, 2$ and $k = 1, 2$, we define

$$\langle \mathbf{F}(z) \rangle_{jk} = e^{-bz} \sum_{r=0}^{\infty} \frac{(bz)^{2r+|j-k|}}{(2r + |j-k|)!} \mathfrak{F}_{2r+|j-k|,k}(z). \tag{5.8}$$

Then,

$$\langle \mathbf{F}(z) \rangle = \tfrac{1}{2} \sum_{k=1}^{2} \sum_{j=1}^{2} \langle \mathbf{F}(z) \rangle_{jk}. \tag{5.9}$$

We shall see shortly that

$$\langle \mathbf{F}(\zeta) \rangle_{jk} = \langle \boldsymbol{\Phi}(\zeta) \mid 0 \rangle_{jk}, \tag{5.10}$$

where $\langle \boldsymbol{\Phi}(\zeta) \mid 0 \rangle_{jk}$ is given by (4.1) and (4.4)–(4.6). This result is consistent with (4.13) and (5.9).

Now, from (5.5) and (5.8), it follows that

$$\mathfrak{L}(\langle \mathbf{F} \rangle_{11}) = \sum_{r=0}^{\infty} \boldsymbol{\eta}_+(s+b)[b^2 \boldsymbol{\eta}_-(s+b)\boldsymbol{\eta}_+(s+b)]^{+r} = \boldsymbol{\eta}_+(s+b)[\mathbf{I} - b^2 \boldsymbol{\eta}_-(s+b)\boldsymbol{\eta}_+(s+b)]^{-1}. \tag{5.11}$$

Similarly,

$$\mathfrak{L}(\langle \mathbf{F} \rangle_{22}) = \boldsymbol{\eta}_-(s+b) \times [\mathbf{I} - b^2 \boldsymbol{\eta}_+(s+b)\boldsymbol{\eta}_-(s+b)]^{-1}, \tag{5.12}$$

and

$$\mathfrak{L}(\langle \mathbf{F} \rangle_{12}) = b\boldsymbol{\eta}_+(s+b)\boldsymbol{\eta}_-(s+b) \times [\mathbf{I} - b^2 \boldsymbol{\eta}_+(s+b)\boldsymbol{\eta}_-(s+b)]^{-1}, \tag{5.13}$$

$$\mathfrak{L}(\langle \mathbf{F} \rangle_{21}) = b\boldsymbol{\eta}_-(s+b)\boldsymbol{\eta}_+(s+b) \times [\mathbf{I} - b^2 \boldsymbol{\eta}_-(s+b)\boldsymbol{\eta}_+(s+b)]^{-1}. \tag{5.14}$$

Let

$$\mathfrak{D}_{\pm} = [\boldsymbol{\eta}_{\pm}(s+b)]^{-1} = \begin{pmatrix} (s+b) & -1 \\ \beta_{\pm}^2 & (s+b) \end{pmatrix}, \tag{5.15}$$

from (5.6). It should be noted that $\mathfrak{D}_{\pm}$ is just $\mathbf{D}_{\pm}$ of (C11) evaluated at $\sigma = s$. From (5.11)–(5.15),

$$\mathfrak{L}\begin{pmatrix} \langle \mathbf{F} \rangle_{11} & \langle \mathbf{F} \rangle_{12} \\ \langle \mathbf{F} \rangle_{21} & \langle \mathbf{F} \rangle_{22} \end{pmatrix} = \begin{pmatrix} \mathfrak{D}_-(\mathfrak{D}_+\mathfrak{D}_- - b^2\mathbf{I})^{-1} & b(\mathfrak{D}_-\mathfrak{D}_+ - b^2\mathbf{I})^{-1} \\ b(\mathfrak{D}_+\mathfrak{D}_- - b^2\mathbf{I})^{-1} & \mathfrak{D}_+(\mathfrak{D}_-\mathfrak{D}_+ - b^2\mathbf{I})^{-1} \end{pmatrix}. \tag{5.16}$$

It is now seen, from (4.8), (C11), (C13), (C15), (3.15), (5.15), and (5.16), that (5.10) holds.

We return to the definition of $\langle \boldsymbol{\Phi}(\zeta) \mid 0 \rangle_{jk}$, as given by (4.6) with $z = 0$, and show by a simple probability argument why (5.10) should hold. Thus, from (4.1) and (4.4), since $u_l(0)$ and $v_l(0)$ are prescribed in any event,

$$\begin{aligned} \langle U_m(\zeta) \mid 0 \rangle_{jk} &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U \text{ Prob}\{U \leq u_m(\zeta) \leq U + dU, \\ &\quad V \leq v_m(\zeta) \leq V + dV, \\ &\quad T(\zeta) = (-1)^{j-1} \mid T(0) = (-1)^{k-1}\}\, dU\, dV \\ &= \sum_{r=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U \text{ Prob}\{U \leq u_m(\zeta) \leq U + dU, \\ &\quad V \leq v_m(\zeta) \leq V + dV, (2r + |j-k|) \\ &\quad \text{crossings in } (0, \zeta) \mid T(0) = (-1)^{k-1}\}\, dU\, dV. \end{aligned} \tag{5.17}$$

An analogous result holds for $\langle V_m(\zeta) \mid 0\rangle_{jk}$. But

$$\begin{aligned}\text{Prob}\{&U \le u_m(\zeta) \le U + dU,\ V \le v_m(\zeta) \le V + dV,\\ &(2r + |j-k|) \text{ crossings in } (0,\zeta) \mid T(0) = (-1)^{k-1}\}\\ = \text{Prob}\{&U \le u_m(\zeta) \le U + dU,\ V \le v_m(\zeta)\\ &\le V + dV \mid (2r + |j-k|) \text{ crossings in } (0,\zeta),\\ &T(0) = (-1)^{k-1}\}p(2r + |j-k|, \zeta), \quad (5.18)\end{aligned}$$

where $p(n, \zeta)$ is the probability of n crossings in $(0, \zeta)$. However, $\mathcal{F}_{n,k}(\zeta)$ is just the expectation value of $\mathbf{F}(\zeta)$, given that there are n crossings in $(0, \zeta)$ and $T(0) = (-1)^{k-1}$. Hence, from (2.1), (3.12), (4.6), (5.8), (5.17), and (5.18), the relationship (5.10) follows.

6. CORRELATION FUNCTIONS BY MATRIX METHOD

We now consider the calculation of the correlation function by the matrix method. Thus, suppose that there are $n + m$ crossings of $T(z')$ in the interval $0 \le z' \le z + \zeta$, at the points z_p, $1 \le p \le m + n$, where

$$\begin{aligned}0 < z_1 < \cdots < z_n < z \le z_{n+1}\\ < \cdots < z_{n+m} < z + \zeta. \quad (6.1)\end{aligned}$$

Then the fundamental solution matrix, evaluated at z, is given by (5.3) and, evaluated at $z + \zeta$, is given by

$$\begin{aligned}\mathbf{F}(z + \zeta) = \mathbf{N}_{(-1)^{n+m+k-1}}(z + \zeta - z_{n+m}) \cdots\\ \mathbf{N}_{(-1)^{n+k-1}}(z_{n+1} - z)\mathbf{F}(z), \quad (6.2)\end{aligned}$$

if $T(0) = (-1)^{k-1}$. Let

$$\mathbf{N}_{\pm}(\mathbf{z}) \times \mathbf{N}_{\pm}(\mathbf{z}) = \mathbf{N}^{(2)}_{\pm}(\mathbf{z}). \quad (6.3)$$

Then, with $F(z)$ and $F(z + \zeta)$ given by (5.3) and (6.2), it follows, on rearranging the Kronecker products, that

$$\begin{aligned}\mathbf{F}(z + \zeta) \times \mathbf{F}(z)\\ = \{[\mathbf{N}_{(-1)^{n+m+k-1}}(z + \zeta - z_{n+m}) \cdots\\ \mathbf{N}_{(-1)^{n+k-1}}(z_{n+1} - z)] \times \mathbf{I}\}\\ \times \{\mathbf{N}^{(2)}_{(-1)^{n+k-1}}(z - z_n)\\ \times \mathbf{N}^{(2)}_{(-1)^{n+k-2}}(z_n - z_{n-1}) \cdots \mathbf{N}^{(2)}_{(-1)^{k-1}}(z_1)\}. \quad (6.4)\end{aligned}$$

We first calculate the expectation value of $\mathbf{F}(z + \zeta) \times \mathbf{F}(z)$ over the positions of $n + m$ crossings. Now the distribution of the n random points z_p, $1 \le p \le n$, is independent of the distribution of the m random points z_{n+q}, $1 \le q \le m$. The uniform density distribution of the n points is $n!\, z^{-n}\, dz_1 \cdots dz_n$, and that of the m points is $m!\, \zeta^{-m}\, dz_{n+1} \cdots dz_{n+m}$. In carrying out the integration of the expression in (6.4) over the m points, the change of variables $z_{n+q} = z + \zeta_q$, $1 \le q \le m$, is made. This leads to the expectation value as the product of an m-fold integral and an n-fold integral, namely $[\mathcal{F}_{m,n+k}(\zeta) \times \mathbf{I}]\mathfrak{E}_{n,k}(z)$, where $\mathcal{F}_{n,k}(z)$ is given by (5.4) and

$$\begin{aligned}\mathfrak{E}_{n,k}(z) = \frac{n!}{z^n}\int_0^z\int_0^{z_n}\cdots\int_0^{z_2}\mathbf{N}^{(2)}_{(-1)^{n+k-1}}(z - z_n)\\ \times \mathbf{N}^{(2)}_{(-1)^{n+k-2}}(z_n - z_{n-1}) \cdots\\ \times \mathbf{N}^{(2)}_{(-1)^{k-1}}(z_1)\, dz_1 \cdots dz_n. \quad (6.5)\end{aligned}$$

Now, the probability that $T(z')$ has n crossings in the interval $0 \le z' \le z$ and m crossings in the interval $z \le z' \le z + \zeta$ is $p(n, z)p(m, \zeta)$, where $p(n, z)$ is given by (2.1). Also, $T(0) = \pm 1$ with probability $\frac{1}{2}$ for each sign. Hence the average value of $\mathbf{F}(z + \zeta) \times \mathbf{F}(z)$ over the ensemble is

$$\begin{aligned}\langle \mathbf{F}(z + \zeta) \times \mathbf{F}(z)\rangle = \tfrac{1}{2}\sum_{k=1}^{2}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(b\zeta)^m}{m!}e^{-b\zeta}\frac{(bz)^n}{n!}\\ \times e^{-bz}[\mathcal{F}_{m,n+k}(\zeta) \times \mathbf{I}]\mathfrak{E}_{n,k}(z). \quad (6.6)\end{aligned}$$

In particular,

$$\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle = \tfrac{1}{2}\sum_{k=1}^{2}\sum_{n=0}^{\infty}\frac{(bz)^n}{n!}e^{-bz}\mathfrak{E}_{n,k}(z). \quad (6.7)$$

For $j = 1, 2$ and $k = 1, 2$ we define

$$\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_{jk} = e^{-bz}\sum_{r=0}^{\infty}\frac{(bz)^{2r+|j-k|}}{(2r + |j-k|)!}\mathfrak{E}_{2r+|j-k|,k}(z). \quad (6.8)$$

Then,

$$\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle = \tfrac{1}{2}\sum_{k=1}^{2}\sum_{j=1}^{2}\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_{jk}. \quad (6.9)$$

We proceed to simplify the expression in (6.6). First note, from (5.4), that

$$\mathcal{F}_{m,2r+|j-k|+k}(\zeta) = \mathcal{F}_{m,j}(\zeta), \quad (6.10)$$

since $2r + |j-k| + (k-j)$ is even. Also, from (5.8),

$$\sum_{i=1}^{2}\langle \mathbf{F}(\zeta)\rangle_{ij} = e^{-b\zeta}\sum_{m=0}^{\infty}\frac{(b\zeta)^m}{m!}\mathcal{F}_{m,j}(\zeta), \quad j = 1, 2. \quad (6.11)$$

Hence, from (6.6), (6.8), (6.10), and (6.11),

$$\begin{aligned}\langle F(z + \zeta) \times F(z)\rangle\\ = \tfrac{1}{2}\sum_{k=1}^{2}\sum_{m=0}^{\infty}\sum_{j=1}^{2}\sum_{r=0}^{\infty}\frac{(b\zeta)^m}{m!}\\ \times e^{-b\zeta}[\mathcal{F}_{m,j}(\zeta) \times \mathbf{I}]\frac{(bz)^{2r+|j-k|}}{(2r + |j-k|)!}e^{-bz}\mathfrak{E}_{2r+|j-k|,k}(z)\\ = \tfrac{1}{2}\sum_{j=1}^{2}\left(\sum_{i=1}^{2}\langle \mathbf{F}(\zeta)\rangle_{ij} \times \mathbf{I}\right)\left(\sum_{k=1}^{2}\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_{jk}\right). \quad (6.12)\end{aligned}$$

But we have already established the relationship (5.10). Hence for the consistency of (4.10) and (6.12) it remains to show that

$$\sum_{k=1}^{2}\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_{jk} = \langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_j, \quad j = 1, 2, \tag{6.13}$$

where, from (3.13),

$$\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_j = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(\mathbf{F} \times \mathbf{F}) \times p_j(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2, \tag{6.14}$$

with p_j defined by (3.1) and $\mathbf{F}$ given by (3.12). Note that (6.9) and (6.13) are consistent with (3.14).

In Appendix D we establish (6.13) and also derive expressions for the Laplace transforms of

$$\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_{jk},$$

which are given by (D9), subject to (D7).

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APPENDIX A

With the definitions of (3.12) and (3.13), it follows from (3.7) and (3.8), after some integrations by parts, that

$$\frac{d\langle u_m^2\rangle_1}{dz} - 2\langle u_m v_m\rangle_1 + b(\langle u_m^2\rangle_1 - \langle u_m^2\rangle_2) = 0, \tag{A1}$$

$$\frac{d\langle u_m^2\rangle_2}{dz} - 2\langle u_m v_m\rangle_2 + b(\langle u_m^2\rangle_2 - \langle u_m^2\rangle_1) = 0, \tag{A2}$$

$$\frac{d\langle u_m v_m\rangle_1}{dz} - \langle v_m^2\rangle_1 + \beta_+^2\langle u_m^2\rangle_1 + b(\langle u_m v_m\rangle_1 - \langle u_m v_m\rangle_2) = 0, \tag{A3}$$

$$\frac{d\langle u_m v_m\rangle_2}{dz} - \langle v_m^2\rangle_2 + \beta_-^2\langle u_m^2\rangle_2 + b(\langle u_m v_m\rangle_2 - \langle u_m v_m\rangle_1) = 0, \tag{A4}$$

$$\frac{d\langle v_m^2\rangle_1}{dz} + 2\beta_+^2\langle u_m v_m\rangle_1 + b(\langle v_m^2\rangle_1 - \langle v_m^2\rangle_2) = 0, \tag{A5}$$

$$\frac{d\langle v_m^2\rangle_2}{dz} + 2\beta_-^2\langle u_m v_m\rangle_2 + b(\langle v_m^2\rangle_2 - \langle v_m^2\rangle_1) = 0. \tag{A6}$$

From (3.9), the initial conditions are

$$\langle u_m^2(0)\rangle_k = \delta_{m,1}, \quad \langle u_m(0)v_m(0)\rangle_k = 0, \quad \langle v_m^2(0)\rangle_k = \delta_{m,2}. \tag{A7}$$

We take Laplace transforms, as in (3.15), of (A1)–(A6), and use (A7). It is convenient to introduce the matrices

$$\mathbf{S} = \begin{pmatrix}(s+b) & -b\\ -b & (s+b)\end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix}\beta_+^2 & 0\\ 0 & \beta_-^2\end{pmatrix}, \quad \mathbf{E} = \begin{pmatrix}1\\ 1\end{pmatrix}, \tag{A8}$$

and

$$\mathbf{X}_m = \begin{pmatrix}\mathfrak{L}(\langle u_m^2\rangle_1)\\ \mathfrak{L}(\langle u_m^2\rangle_2)\end{pmatrix}, \quad \mathbf{Y}_m = \begin{pmatrix}\mathfrak{L}(\langle u_m v_m\rangle_1)\\ \mathfrak{L}(\langle u_m v_m\rangle_2)\end{pmatrix}, \quad \mathbf{Z}_m = \begin{pmatrix}\mathfrak{L}(\langle v_m^2\rangle_1)\\ \mathfrak{L}(\langle v_m^2\rangle_2)\end{pmatrix}. \tag{A9}$$

Then, the transformed equations for $m = 1$ can be written as

$$\mathbf{SX}_1 - 2\mathbf{Y}_1 = \mathbf{E}, \quad \mathbf{BX}_1 + \mathbf{SY}_1 - \mathbf{Z}_1 = \mathbf{0}, \quad 2\mathbf{BY}_1 + \mathbf{SZ}_1 = \mathbf{0}, \tag{A10}$$

and those for $m = 2$ can be written as

$$\mathbf{SX}_2 - 2\mathbf{Y}_2 = \mathbf{0}, \quad \mathbf{BX}_2 + \mathbf{SY}_2 - \mathbf{Z}_2 = \mathbf{0}, \quad 2\mathbf{BY}_2 + \mathbf{SZ}_2 = \mathbf{E}. \tag{A11}$$

From (3.12), (3.14), and (A9), we have

$$\mathfrak{L}(\langle u_m^2\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{X}_m, \quad \mathfrak{L}(\langle u_m v_m\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{Y}_m, \quad \mathfrak{L}(\langle v_m^2\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{Z}_m, \tag{A12}$$

where $\mathbf{E}'$ is the transpose of $\mathbf{E}$.

We first consider the case $m = 2$. Then, from (A11), it follows that

$$\mathbf{Y}_2 = \tfrac{1}{2}\mathbf{SX}_2, \quad \mathbf{Z}_2 = (\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)\mathbf{X}_2, \quad (\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)\mathbf{X}_2 = \mathbf{E}. \tag{A13}$$

The calculation of $(\mathbf{BS} + \mathbf{SB} + \frac{1}{2}\mathbf{S}^3)^{-1}$ is straightforward, but tedious, and we omit the details. Letting $\Delta = \det[2(\mathbf{BS} + \mathbf{SB}) + \mathbf{S}^3]$, we find, using (2.7), that

$$\Delta \equiv \Delta(s) = \{s(s+2b)(s^2 + 4\beta_0^2)[(s+2b)^2 + 4\beta_0^2] - 16\eta^2\beta_0^4(s+b)^2\}. \tag{A14}$$

Then, from (A12) and (A13), it is found, after some reductions that

$$\mathfrak{L}(\langle u_2^2\rangle) = (2/\Delta)(s+2b)[(s+2b)^2 + 4\beta_0^2], \tag{A15}$$

$$\mathfrak{L}(\langle u_2 v_2\rangle) = (s/\Delta)(s+2b)[(s+2b)^2 + 4\beta_0^2] = \tfrac{1}{2}s\mathfrak{L}(\langle u_2^2\rangle), \tag{A16}$$

and

$$\mathfrak{L}(\langle v_2^2\rangle) = (1/\Delta)\{(s+2b)(s^2+2\beta_0^2)[(s+2b)^2+4\beta_0^2] - 8\eta^2\beta_0^4(s+b)\}. \quad \text{(A17)}$$

Now consider the case $m = 1$. From (A10), we have

$$\mathbf{Y}_1 = \tfrac{1}{2}(\mathbf{SX} - \mathbf{E}), \quad \mathbf{Z}_1 = [(\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)\mathbf{X}_1 - \tfrac{1}{2}\mathbf{SE}] \quad \text{(A18)}$$

and

$$(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)\mathbf{X}_1 = (\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)\mathbf{E}. \quad \text{(A19)}$$

Thus,

$$\mathbf{E}'\mathbf{X}_1 = \mathbf{E}'(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)^{-1}(\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)\mathbf{E}. \quad \text{(A20)}$$

But **B** and **S** are symmetric matrices. Hence, transposing the product of matrices on the right-hand side of (A20), which is scalar, we find that

$$\mathbf{E}'\mathbf{X}_1 = \mathbf{E}'(\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)^{-1}\mathbf{E}' = \mathbf{E}'\mathbf{Z}_2, \quad \text{(A21)}$$

from (A13). Thus, from (A12),

$$\mathfrak{L}(\langle u_1^2\rangle) = \mathfrak{L}(\langle v_2^2\rangle). \quad \text{(A22)}$$

From (A18), since, from (A8),

$$\mathbf{E}'\mathbf{S} = s\mathbf{E}', \quad \mathbf{E}'\mathbf{E} = 2, \quad \text{(A23)}$$

it follows that

$$2\mathfrak{L}(\langle u_1 v_1\rangle) = s\mathfrak{L}(\langle u_1^2\rangle) - 1. \quad \text{(A24)}$$

Thus, from (A14), (A17), (A22), and (A24),

$$\mathfrak{L}(\langle u_1 v_1\rangle) = (\beta_0^2/\Delta)(s+2b)\{4\eta^2\beta_0^2(s+b) - s[(s+2b)^2+4\beta_0^2]\}. \quad \text{(A25)}$$

Finally, from (A18) and (A19),

$$\mathbf{Z}_1 = (\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)^{-1} \times (\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2)\mathbf{E} - \tfrac{1}{2}\mathbf{SE}. \quad \text{(A26)}$$

After some reductions, the details of which we omit, it is found, from (A12), that

$$\mathfrak{L}(\langle v_1^2\rangle) = (2/\Delta)\beta_0^4(s+2b)\{[(s+2b)^2+4\beta_0^2] + \eta^2[s(s+2b) - 4\beta_0^2]\}. \quad \text{(A27)}$$

APPENDIX B

With the definitions of (3.12) and (3.13), it follows from (3.7) and (3.8), after some integrations by parts, that

$$\frac{d\langle u_1u_2\rangle_1}{dz} - \langle v_1u_2\rangle_1 - \langle u_1v_2\rangle_1 + b(\langle u_1u_2\rangle_1 - \langle u_1u_2\rangle_2) = 0, \quad \text{(B1)}$$

$$\frac{d\langle u_1u_2\rangle_2}{dz} - \langle v_1u_2\rangle_2 - \langle u_1v_2\rangle_2 + b(\langle u_1u_2\rangle_2 - \langle u_1u_2\rangle_1) = 0, \quad \text{(B2)}$$

$$\frac{d\langle u_1v_2\rangle_1}{dz} - \langle v_1v_2\rangle_1 + \beta_+^2\langle u_1u_2\rangle_1 + b(\langle u_1v_2\rangle_1 - \langle u_1v_2\rangle_2) = 0, \quad \text{(B3)}$$

$$\frac{d\langle u_1v_2\rangle_2}{dz} - \langle v_1v_2\rangle_2 + \beta_-^2\langle u_1u_2\rangle_2 + b(\langle u_1v_2\rangle_2 - \langle u_1v_2\rangle_1) = 0, \quad \text{(B4)}$$

$$\frac{d\langle v_1u_2\rangle_1}{dz} - \langle v_1v_2\rangle_1 + \beta_+^2\langle u_1u_2\rangle_1 + b(\langle v_1u_2\rangle_1 - \langle v_1u_2\rangle_2) = 0, \quad \text{(B5)}$$

$$\frac{d\langle v_1u_2\rangle_2}{dz} - \langle v_1v_2\rangle_2 + \beta_-^2\langle u_1u_2\rangle_2 + b(\langle v_1u_2\rangle_2 - \langle v_1u_2\rangle_1) = 0, \quad \text{(B6)}$$

$$\frac{d\langle v_1v_2\rangle_1}{dz} + \beta_+^2\langle u_1v_2\rangle_1 + \beta_+^2\langle v_1u_2\rangle_1 + b(\langle v_1v_2\rangle_1 - \langle v_1v_2\rangle_2) = 0, \quad \text{(B7)}$$

$$\frac{d\langle v_1v_2\rangle_2}{dz} + \beta_-^2\langle u_1v_2\rangle_2 + \beta_-^2\langle v_1u_2\rangle_2 + b(\langle v_1v_2\rangle_2 - \langle v_1v_2\rangle_1) = 0. \quad \text{(B8)}$$

From (3.9) the initial conditions are

$$\langle u_1(0)u_2(0)\rangle_k = 0, \quad \langle u_1(0)v_2(0)\rangle_k = 1,$$
$$\langle v_1(0)u_2(0)\rangle_k = 0, \quad \langle v_1(0)v_2(0)\rangle_k = 0. \quad \text{(B9)}$$

We take Laplace transforms of (B1)–(B8) and use (B9). Let

$$\mathbf{G} = \begin{pmatrix}\mathfrak{L}(\langle u_1u_2\rangle_1)\\ \mathfrak{L}(\langle u_1u_2\rangle_2)\end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix}\mathfrak{L}(\langle u_1v_2\rangle_1)\\ \mathfrak{L}(\langle u_1v_2\rangle_2)\end{pmatrix}, \quad \text{(B10)}$$

$$\mathbf{J} = \begin{pmatrix}\mathfrak{L}(\langle v_1u_2\rangle_1)\\ \mathfrak{L}(\langle v_1u_2\rangle_2)\end{pmatrix}, \quad \mathbf{K} = \begin{pmatrix}\mathfrak{L}(\langle v_1v_2\rangle_1)\\ \mathfrak{L}(\langle v_1v_2\rangle_2)\end{pmatrix}. \quad \text{(B11)}$$

Then, with **S**, **B**, and **E** as defined in (A8), the transformed equations can be written as

$$\mathbf{SG} - (\mathbf{H} + \mathbf{J}) = \mathbf{0}, \quad \mathbf{BG} + \mathbf{SH} - \mathbf{K} = \mathbf{E},$$
$$\mathbf{BG} + \mathbf{SJ} - \mathbf{K} = \mathbf{0}, \quad \mathbf{B}(\mathbf{H} + \mathbf{J}) + \mathbf{SK} = \mathbf{0}. \quad \text{(B12)}$$

Also, from (3.12), (3.14), (B10), and (B11),

$$\mathfrak{L}(\langle u_1u_2\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{G}, \quad \mathfrak{L}(\langle u_1v_2\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{H} \quad \text{(B13)}$$

and

$$\mathfrak{L}(\langle v_1u_2\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{J}, \quad \mathfrak{L}(\langle v_1v_2\rangle) = \tfrac{1}{2}\mathbf{E}'\mathbf{K}. \quad \text{(B14)}$$

Eliminating **H** and **J** from (B12),we obtain

$$(2\mathbf{B} + \mathbf{S}^2)\mathbf{G} - 2\mathbf{K} = \mathbf{E}, \quad \mathbf{BSG} + \mathbf{SK} = \mathbf{0}. \quad \text{(B15)}$$

Hence,

$$[2(\mathbf{BS} + \mathbf{SB}) + \mathbf{S}^3]\mathbf{G} = \mathbf{SE}. \quad \text{(B16)}$$

Thus, we have

$$\mathbf{E}'\mathbf{G} = \mathbf{E}'[2(\mathbf{BS} + \mathbf{SB}) + \mathbf{S}^3]^{-1}\mathbf{SE} = \mathbf{E}'\mathbf{S}[2(\mathbf{BS} + \mathbf{SB}) + \mathbf{S}^3]^{-1}\mathbf{E} = \mathbf{E}'\mathbf{Y}_2, \quad \text{(B17)}$$

transposing and using (A13). It follows from (A12) and (B13) that

$$\mathfrak{L}(\langle u_1u_2\rangle) = \mathfrak{L}(\langle u_2v_2\rangle). \quad \text{(B18)}$$

Next, from (B15) and (B16),

$$\mathbf{K} = -\mathbf{S}^{-1}\mathbf{BS}[2(\mathbf{BS} + \mathbf{SB}) + \mathbf{S}^3]^{-1}\mathbf{SE}. \quad \text{(B19)}$$

But, from (A18) and (A19), we have

$$\mathbf{E}'\mathbf{Y}_1 = \tfrac{1}{2}\mathbf{E}'[\mathbf{S}(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)^{-1}(\mathbf{B} + \tfrac{1}{2}\mathbf{S}^2) - \mathbf{I}]\mathbf{E} = -\tfrac{1}{2}\mathbf{E}'\mathbf{S}(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)^{-1}\mathbf{SBS}^{-1}\mathbf{E} = -\tfrac{1}{2}\mathbf{E}'\mathbf{S}^{-1}\mathbf{BS}(\mathbf{BS} + \mathbf{SB} + \tfrac{1}{2}\mathbf{S}^3)^{-1}\mathbf{SE} = \mathbf{E}'\mathbf{K}, \quad \text{(B20)}$$

transposing and using (B19). Thus, from (A12) and (B14),

$$\mathfrak{L}(\langle v_1v_2\rangle) = \mathfrak{L}(\langle u_1v_1\rangle). \quad \text{(B21)}$$

Finally, from (B12),

$$(\mathbf{H} + \mathbf{J}) = \mathbf{SG}, \quad \mathbf{S}(\mathbf{H} - \mathbf{J}) = \mathbf{E}. \quad \text{(B22)}$$

Hence, multiplying both equations by $\mathbf{E}'$ and using (A23), we obtain

$$\mathbf{E}'(\mathbf{H} + \mathbf{J}) = s\mathbf{E}'\mathbf{G}, \quad s\mathbf{E}'(\mathbf{H} - \mathbf{J}) = 2. \quad \text{(B23)}$$

It follows from (B13) and (B14) that

$$\mathfrak{L}(\langle u_1v_2\rangle + \langle v_1u_2\rangle) = s\mathfrak{L}(\langle u_1u_2\rangle),$$
$$\mathfrak{L}(\langle u_1v_2\rangle - \langle v_1u_2\rangle) = 1/s. \quad \text{(B24)}$$

Then, from (A14), (A16), (B18), and (B24),

$$\mathfrak{L}(\langle u_1v_2\rangle) = (1/s\Delta)\{s(s + 2b)(s^2 + 2\beta_0^2) \times [(s + 2b)^2 + 4\beta_0^2] - 8\eta^2\beta_0^4(s + b)^2\}, \quad \text{(B25)}$$

and

$$\mathfrak{L}(\langle v_1u_2\rangle) = (2\beta_0^2/s\Delta)\{4\eta^2\beta_0^2(s + b)^2 - s(s + 2b) \times [(s + 2b)^2 + 4\beta_0^2]\}. \quad \text{(B26)}$$

A straightforward calculation shows that the determinant $\mathfrak{D}(s)$ of the coefficient matrix in Eqs. (B12) is

$$\mathfrak{D}(s) = s(s + 2b)\Delta(s). \quad \text{(B27)}$$

However, we now show that the factor $s + 2b$ does not appear in the denominator of the expression for $\mathbf{G}$, $\mathbf{H}$, $\mathbf{J}$, and $\mathbf{K}$. First, from (B16) we see that only $\Delta(s)$ occurs in the denominator of $\mathbf{G}$. Then, from (B22), $\mathbf{H} + \mathbf{J}$ has the same denominator as $\mathbf{G}$, and

$$\mathbf{H} - \mathbf{J} = \mathbf{S}^{-1}\mathbf{E} = s^{-1}\mathbf{E}. \quad \text{(B28)}$$

Finally, from (B12) it is clear that $s + 2b$ does not appear in the denominator of $\mathbf{K}$.

APPENDIX C

We first give the equations satisfied by

$$Q_{m,jk}(U, V, \zeta \mid z).$$

We omit the derivation, since it is similar to that in Sec. 3 for $p_k(u_1, v_1, u_2, v_2, z)$, but simpler. It is found that

$$\frac{\partial Q_{m,1k}}{\partial \zeta} + V\frac{\partial Q_{m,1k}}{\partial U} - \beta_+^2 U\frac{\partial Q_{m,1k}}{\partial V} + b(Q_{m,1k} - Q_{m,2k}) = 0 \quad \text{(C1)}$$

and

$$\frac{\partial Q_{m,2k}}{\partial \zeta} + V\frac{\partial Q_{m,2k}}{\partial U} - \beta_-^2 U\frac{\partial Q_{m,2k}}{\partial V} + b(Q_{m,2k} - Q_{m,1k}) = 0. \quad \text{(C2)}$$

From (4.1) the initial conditions are

$$Q_{m,11}(U, V, 0 \mid z) = \delta[U - u_m(z)]\delta[V - v_m(z)] = Q_{m,22}(U, V, 0 \mid z) \quad \text{(C3)}$$

and

$$Q_{m,12}(U, V, 0 \mid z) = 0 = Q_{m,21}(U, V, 0 \mid z) \quad \text{(C4)}$$

since $T(z)$ is not equal to $+1$ and -1 simultaneously.

From (4.4), (4.5), and (C1)–(C4) it follows, after some integrations by parts, that

$$\frac{d\langle U_m\rangle_{1k}}{d\zeta} - \langle V_m\rangle_{1k} + b(\langle U_m\rangle_{1k} - \langle U_m\rangle_{2k}) = 0, \quad \text{(C5)}$$

$$\frac{d\langle U_m\rangle_{2k}}{d\zeta} - \langle V_m\rangle_{2k} + b(\langle U_m\rangle_{2k} - \langle U_m\rangle_{1k}) = 0, \quad \text{(C6)}$$

$$\frac{d\langle V_m\rangle_{1k}}{d\zeta} + \beta_+^2\langle U_m\rangle_{1k} + b(\langle V_m\rangle_{1k} - \langle V_m\rangle_{2k}) = 0, \quad \text{(C7)}$$

$$\frac{d\langle V_m\rangle_{2k}}{d\zeta} + \beta_-^2\langle U_m\rangle_{2k} + b(\langle V_m\rangle_{2k} - \langle V_m\rangle_{1k}) = 0, \quad \text{(C8)}$$

with initial conditions

$$\langle U_m(0) \mid z\rangle_{11} = u_m(z) = \langle U_m(0) \mid z\rangle_{22},$$
$$\langle V_m(0) \mid z\rangle_{11} = v_m(z) = \langle V_m(0) \mid z\rangle_{22}, \quad \text{(C9)}$$
$$\langle U_m(0) \mid z\rangle_{12} = 0 = \langle U_m(0) \mid z\rangle_{21},$$
$$\langle V_m(0) \mid z\rangle_{12} = 0 = \langle V_m(0) \mid z\rangle_{21}. \quad \text{(C10)}$$

We take Laplace transforms, as in (4.8), of (C5)–(C8) and use (C9) and (C10). It is convenient to

introduce the matrices

$$\mathbf{D}_{\pm} = \begin{pmatrix} (\sigma + b) & -1 \\ \beta_{\pm}^2 & (\sigma + b) \end{pmatrix}. \tag{C11}$$

Then, from (3.12) and (4.6),

$$\begin{pmatrix} \mathbf{D}_+ & -b\mathbf{I} \\ -b\mathbf{I} & \mathbf{D}_- \end{pmatrix} \Lambda \begin{pmatrix} \langle \mathbf{\Phi} \mid z \rangle_{11} & \langle \mathbf{\Phi} \mid z \rangle_{12} \\ \langle \mathbf{\Phi} \mid z \rangle_{21} & \langle \mathbf{\Phi} \mid z \rangle_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{F}(z) & \mathbf{0} \\ \mathbf{0} & \mathbf{F}(z) \end{pmatrix}. \tag{C12}$$

But, from (2.5) and (3.12), $\mathbf{F}(0) = \mathbf{I}$. Hence

$$\Lambda \begin{pmatrix} \langle \mathbf{\Phi} \mid 0 \rangle_{11} & \langle \mathbf{\Phi} \mid 0 \rangle_{12} \\ \langle \mathbf{\Phi} \mid 0 \rangle_{21} & \langle \mathbf{\Phi} \mid 0 \rangle_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{D}_+ & -b\mathbf{I} \\ -b\mathbf{I} & \mathbf{D}_- \end{pmatrix}^{-1}. \tag{C13}$$

Thus, from (C12) and (C13),

$$\begin{pmatrix} \langle \mathbf{\Phi}(\zeta) \mid z \rangle_{11} & \langle \mathbf{\Phi}(\zeta) \mid z \rangle_{12} \\ \langle \mathbf{\Phi}(\zeta) \mid z \rangle_{21} & \langle \mathbf{\Phi}(\zeta) \mid z \rangle_{22} \end{pmatrix} = \begin{pmatrix} \langle \mathbf{\Phi}(\zeta) \mid 0 \rangle_{11} & \langle \mathbf{\Phi}(\zeta) \mid 0 \rangle_{12} \\ \langle \mathbf{\Phi}(\zeta) \mid 0 \rangle_{21} & \langle \mathbf{\Phi}(\zeta) \mid 0 \rangle_{22} \end{pmatrix} \begin{pmatrix} \mathbf{F}(z) & \mathbf{0} \\ \mathbf{0} & \mathbf{F}(z) \end{pmatrix}. \tag{C14}$$

Now,

$$\begin{pmatrix} \mathbf{D}_+ & -b\mathbf{I} \\ -b\mathbf{I} & \mathbf{D}_- \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{D}_-(\mathbf{D}_+\mathbf{D}_- - b^2\mathbf{I})^{-1} & b(\mathbf{D}_-\mathbf{D}_+ - b^2\mathbf{I})^{-1} \\ b(\mathbf{D}_+\mathbf{D}_- - b^2\mathbf{I})^{-1} & \mathbf{D}_+(\mathbf{D}_-\mathbf{D}_+ - b^2\mathbf{I})^{-1} \end{pmatrix}. \tag{C15}$$

We note that

$$\begin{aligned} \mathbf{D}_+(\mathbf{D}_-\mathbf{D}_+ - b^2\mathbf{I})^{-1} &= (\mathbf{D}_- - b^2\mathbf{D}_+^{-1})^{-1} \\ &= (\mathbf{D}_+\mathbf{D}_- - b^2\mathbf{I})^{-1}\mathbf{D}_+, \\ \mathbf{D}_-(\mathbf{D}_+\mathbf{D}_- - b^2\mathbf{I})^{-1} &= (\mathbf{D}_+ - b^2\mathbf{D}_-^{-1})^{-1} \\ &= (\mathbf{D}_-\mathbf{D}_+ - b^2\mathbf{I})^{-1}\mathbf{D}_-. \end{aligned} \tag{C16}$$

It is a straightforward matter to calculate the matrix elements on the right-hand side of (C15); thus we omit the details. Let

$$d(\sigma) = (\sigma + b)^4 + 2(\beta_0^2 - b^2)(\sigma + b)^2 + (b^2 + \beta_+^2)(b^2 + \beta_-^2). \tag{C17}$$

It is found that

$$(\mathbf{D}_{\pm}\mathbf{D}_{\mp} - b^2\mathbf{I})^{-1} = \frac{1}{d(\sigma)} \begin{pmatrix} [\sigma(\sigma + 2b) - \beta_{\pm}^2] & 2(\sigma + b) \\ -2\beta_0^2(\sigma + b) & [\sigma(\sigma + 2b) - \beta_{\mp}^2] \end{pmatrix}, \tag{C18}$$

and

$$\mathbf{D}_{\mp}(\mathbf{D}_{\pm}\mathbf{D}_{\mp} - b^2\mathbf{I})^{-1} = \frac{1}{d(\sigma)} \begin{pmatrix} (\sigma + b)[\sigma(\sigma + 2b) + \beta_{\mp}^2] & [(\sigma + b)^2 + b^2 + \beta_{\mp}^2] \\ -[\beta_+^2\beta_-^2 + \beta_{\pm}^2(\sigma + b)^2 + \beta_{\mp}^2 b^2] & (\sigma + b)[\sigma(\sigma + 2b) + \beta_{\mp}^2] \end{pmatrix}. \tag{C19}$$

APPENDIX D

We first show by a simple probability argument why (6.13) should hold. Accordingly, we introduce the conditional probability density functions

$$\begin{aligned} &q_{jk}(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2 \\ &\quad = \text{Prob}\{u_m \le u_m(z) \le u_m + du_m, \\ &\qquad v_m \le v_m(z) \le v_m + dv_m, (m = 1, 2), \\ &\qquad T(z) = (-1)^{j-1} \mid T(0) = (-1)^{k-1}\}, \end{aligned} \tag{D1}$$

with $j = 1, 2$, and $k = 1, 2$. Proceeding as at the end of Sec. 5, we may rewrite (D1) in the form

$$\begin{aligned} &q_{jk}(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2 \\ &\quad = \sum_{r=0}^{\infty} \text{Prob}\{u_m \le u_m(z) \le u_m + du_m, \\ &\qquad v_m \le v_m(z) \le v_m + dv_m, (m = 1, 2), \\ &\qquad \mid (2r + \mid j - k\mid) \text{ crossings in } (0, z), \\ &\qquad T(0) = (-1)^{k-1}\} p(2r + \mid j - k\mid, z), \end{aligned} \tag{D2}$$

where $p(n, z)$ is the probability of n crossings in $(0, z)$. But $\mathfrak{E}_{n,k}(z)$ is just the expectation value of $\mathbf{F}(z) \times \mathbf{F}(z)$, given that there are n crossings in $(0, z)$ and $T(0) = (-1)^{k-1}$, as is seen from (5.3), (6.3), and (6.5). Hence, from (2.1), (6.8), and (D2),

$$\begin{aligned} &\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (\mathbf{F} \times \mathbf{F}) \\ &\qquad \times q_{jk}(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2 \\ &\qquad = \langle \mathbf{F}(z) \times \mathbf{F}(z) \rangle_{jk}. \end{aligned} \tag{D3}$$

But, $T(0) = \pm 1$ with probability $\frac{1}{2}$ for each sign. Hence, from (D1)

$$\begin{aligned} &\tfrac{1}{2}\sum_{k=1}^{2} q_{jk}(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2 \\ &\quad = \text{Prob}\{u_m \le u_m(z) \le u_m + du_m, \\ &\qquad v_m \le v_m(z) \le v_m + dv_m, (m = 1, 2,) \\ &\qquad T(z) = (-1)^{j-1}\} \\ &\quad = \tfrac{1}{2} p_j(u_1, v_1, u_2, v_2, z)\, du_1\, dv_1\, du_2\, dv_2, \end{aligned} \tag{D4}$$

from (3.1), since $T(z) = (-1)^{j-1}$ with probability $\frac{1}{2}$. Thus, from (6.14), (D3), and (D4), the relationship (6.13) follows.

We now consider the determination of the quantities $\langle \mathbf{F}(z) \times \mathbf{F}(z) \rangle_{jk}$. Proceeding as in Sec. 3, we find that the pair of functions (q_{1k}, q_{2k}), for $k = 1$ and $k = 2$, satisfy the same partial differential equations as the pair of functions (p_1, p_2), as given by (3.7) and (3.8). The initial conditions, however, differ in that,

from (2.5), (2.6), and (D1),

$$q_{11}(u_1, v_1, u_2, v_2, 0) = \delta(u_1 - 1)\delta(v_1)\delta(u_2)\delta(v_2 - 1) = q_{22}(u_1, v_1, u_2, v_2, 0), \quad \text{(D5)}$$

but

$$q_{12}(u_1, v_1, u_2, v_2, 0) = 0 = q_{21}(u_1, v_1, u_2, v_2, 0). \quad \text{(D6)}$$

Ordinary differential equations, with constant coefficients, are obtained for $\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle_{jk}$ from (D3) and the equations for q_{jk}. The initial conditions follow from (D5) and (D6). The equations are solved by means of Laplace transforms, but we omit the details and give the results.

Let

$$\mathfrak{C}_\pm = \begin{pmatrix} (s+b) & -1 & -1 & 0 \\ \beta_\pm^2 & (s+b) & 0 & -1 \\ \beta_\pm^2 & 0 & (s+b) & -1 \\ 0 & \beta_\pm^2 & \beta_\pm^2 & (s+b) \end{pmatrix} \quad \text{(D7)}$$

Then it is found that

$$\begin{pmatrix} \mathfrak{C}_+ & -b\mathbf{I} \\ -b\mathbf{I} & \mathfrak{C}_- \end{pmatrix} \mathfrak{L}\begin{pmatrix} \langle \mathbf{F}\times\mathbf{F}\rangle_{11} & \langle \mathbf{F}\times\mathbf{F}\rangle_{12} \\ \langle \mathbf{F}\times\mathbf{F}\rangle_{21} & \langle \mathbf{F}\times\mathbf{F}\rangle_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}. \quad \text{(D8)}$$

It follows that

$$\mathfrak{L}\begin{pmatrix} \langle \mathbf{F}\times\mathbf{F}\rangle_{11} & \langle \mathbf{F}\times\mathbf{F}\rangle_{12} \\ \langle \mathbf{F}\times\mathbf{F}\rangle_{21} & \langle \mathbf{F}\times\mathbf{F}\rangle_{22} \end{pmatrix} = \begin{pmatrix} \mathfrak{C}_-(\mathfrak{C}_+\mathfrak{C}_- - b^2\mathbf{I})^{-1} & b(\mathfrak{C}_-\mathfrak{C}_+ - b^2\mathbf{I})^{-1} \\ b(\mathfrak{C}_+\mathfrak{C}_- - b^2\mathbf{I})^{-1} & \mathfrak{C}_+(\mathfrak{C}_-\mathfrak{C}_+ - b^2\mathbf{I})^{-1} \end{pmatrix}. \quad \text{(D9)}$$

This result may also be obtained by the matrix method. Thus, if we take the Laplace transform of the expression in (6.8), using (6.5), we obtain expressions for $\mathfrak{L}(\langle \mathbf{F}\times\mathbf{F}\rangle_{jk})$ analogous to those obtained for $\mathfrak{L}(\langle \mathbf{F}\rangle_{jk})$ in (5.11)–(5.14), the only difference being that $\eta_\pm(s+b)$ is replaced by $\mathcal{M}_\pm(s+b)$, where

$$\mathcal{M}_\pm(s) = \mathfrak{L}[\mathbf{N}_\pm^{(2)}(z)] = \frac{1}{s(s^2+4\beta_\pm^2)} \begin{pmatrix} (s^2+2\beta_\pm^2) & s & s & 2 \\ -\beta_\pm^2 s & (s^2+2\beta_\pm^2) & -2\beta_\pm^2 & s \\ -\beta_\pm^2 s & -2\beta_\pm^2 & (s^2+2\beta_\pm^2) & s \\ 2\beta_\pm^4 & -\beta_\pm^2 s & -\beta_\pm^2 s & (s^2+2\beta_\pm^2) \end{pmatrix} \quad \text{(D10)}$$

from (5.2) and (6.3). The result in (D9) then follows from the fact that

$$\mathfrak{C}_\pm = [\mathcal{M}_\pm(s+b)]^{-1}. \quad \text{(D11)}$$

[1] W. B. Davenport, Jr., and W. L. Root, *Random Signals and Noise* (McGraw-Hill, New York, 1958), p. 61.
[2] I. Kay and R. A. Silverman, Nuovo Cimento, Suppl., **9**, 626 (1958).
[3] A. R. Hochstim and C. P. Martins, IDA Research Report P-316, 1967.
[4] M. Fibich and E. Helfand, Phys. Rev. **183**, 265 (1969).
[5] U. Frisch, in *Probabilistic Methods in Applied Mathematics*, A. T. Bharucha-Reid, Ed. (Academic, New York, 1968), p. 117.
[6] J. B. Keller, Proc. Symp. Appl. Math. **13** 227 (1962).
[7] J. B. Keller, Proc. Symp. Appl. Math. **16**, 145 (1964).
[8] F. C. Karal and J. B. Keller, J. Math. Phys. **5**, 537 (1964).
[9] J. B. Keller and F. C. Karal, J. Math. Phys. **7**, 661 (1966).
[10] See Ref. 5 for an extensive bibliography.
[11] R. C. Bourret, Phys. Letters, **12**, 323 (1964).
[12] R. C. Bourret, Can. J. Phys. **43**, 619 (1965).
[13] R. C. Bourret, Can. J. Phys. **44**, 2519 (1966).
[14] J. A. Morrison and J. McKenna, J. Math. Phys. **11**, 2361 (1970), following paper.
[15] H. L. Frisch and S. P. Lloyd, Phys. Rev. **120**, 1175 (1960).
[16] The authors are indebted to Dr. S. P. Lloyd for outlining the derivation of Eqs. (3.7) and (3.8).
[17] R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill, New York, 1960), p. 227.
[18] This is similar to the case where $\{T(z)\}$ is Gaussian. See Ref. 5, p. 139.
[19] M. Born and E. Wolf, *Principles of Optics* (Pergamon, London, 1959), p. 50.
[20] D. A. Darling, Ann. Math. Stat. **24**, 239 (1953).

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Application of the Smoothing Method to a Stochastic Ordinary Differential Equation

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We study the use of the "smoothing method" to calculate the second-order moments of solutions of stochastic, ordinary, linear differential equations. We consider in detail the equation

$$\frac{d^2u}{dz^2} + \beta_0^2[1 + \eta N(z)]u = 0,$$

where $N(z)$ is a real, zero mean, wide-sense stationary stochastic process and β_0 and $\eta \ll 1$ are positive constants. We show that, for one choice of $N(z)$, the conventional use of the smoothing method yields correct first-order moments of the solutions, but badly incorrect second-order moments. We develop what we believe is a better way to use the smoothing method to calculate second-order moments. For the special choice of $N(z)$, this method yields exact results. The method can be extended to the calculation of moments of all orders for arbitrary stochastic, ordinary, linear differential equations.

1. INTRODUCTION

In this paper, we investigate how the "smoothing method" can be used correctly to calculate second- and higher-order moments of the solutions of stochastic, ordinary differential equations. We do this by calculating approximately the various second-order moments associated with the solutions of a specific, stochastic, second-order, ordinary differential equation. However, the technique can be applied to the calculation of higher-order moments of ordinary, linear differential equations of any order.

Let $\{N(z)\}$ be a real, wide sense stationary stochastic process with

$$\langle N(z)\rangle = 0, \quad \langle N(y)N(z)\rangle = \Gamma(y - z), \quad (1.1)$$

where $\langle\ \rangle$ denotes the ensemble average. Each sample function $N(z)$ defines two new real functions $u_m(z)$, $m = 1, 2$, on $0 \leq z < \infty$, which are the linearly independent solutions of

$$\frac{d^2u_m}{dz^2} + \beta_0^2[1 + \eta N(z)]u_m = 0 \quad (1.2)$$

satisfying the nonstochastic initial conditions

$$u_1(0) = u_2'(0) = 1, \quad u_1'(0) = u_2(0) = 0, \quad (1.3)$$

where β_0 and $\eta \ll 1$ are positive constants. The ensembles of functions $\{u_m(z)\}$, $m = 1, 2$, form two real random processes which we study in this paper. We assume that almost all the sample functions $N(z)$ are smooth enough so that the solutions $u_m(z)$ of (1.2) exist. Throughout the paper, we use the notation

$$v_m(z) = \frac{du_m(z)}{dz} = u_m'(z), \quad m = 1, 2. \quad (1.4)$$

The smoothing method[1] for calculating various moments of the solutions of stochastic differential equations has been extensively developed by Keller[1–5] and Bourret,[6–10] and it has been used by a number of other authors.[11,12] We follow Keller and give an outline of the development of the technique in Sec. 2. We apply the smoothing technique to calculate $\langle u_m(z)\rangle$ and $\langle v_m(z)\rangle$, $m = 1, 2$. These results are not new; they have already been obtained by Bourret.[9] However, we show that the use of these first-order moments to calculate the second-order moments by a widely used technique can lead to an incorrect answer. We are able to do this because an exact solution of the second-order moments of the solutions of (1.2) is available when $\{N(z)\}$ is the random telegraph process.[13]

In Sec. 3, we apply the smoothing technique to a system of ordinary differential equations whose solutions are the products u_mu_n, u_mv_n, v_mv_n, $m, n = 1, 2$. For the case when $\{N(z)\}$ is the random telegraph process, this procedure yields the correct answer, regardless of the magnitude of η. This suggests that the method of using the smoothing technique presented here is the correct one. Keller has suggested using the smoothing method in a different fashion to calculate the second-order moments of solution of partial differential equations.[14–16]

As an application of the smoothing technique, we consider the interesting problem of calculating the average of the inverse of the power transmission coefficient of a randomly stratified dielectric slab. We assume that the dielectric slab fills the region $0 \leq z \leq L$ and that its dielectric constant is

$$K(z) = n_0^2[1 + \eta N(z)],$$

where $N(z)$ is a real stochastic process satisfying (1.1), n_0^2 is the average dielectric constant of the slab, and $0 < \eta \ll 1$ is constant. The regions $z < 0$ and $z > L$ are filled with nonstochastic dielectric media having the dielectric constants n_1^2 and n_2^2, respectively. Let a plane-polarized monochromatic electromagnetic wave of frequency ω be normally incident on the plate from the left. Then we have shown[13] that

$$4\beta_1^2\langle 1/\mathcal{T}\mathcal{T}^*\rangle = 2\beta_1\beta_2 + \langle v_1^2(L)\rangle + \beta_2^2\langle u_1^2(L)\rangle + \beta_1^2\langle v_2^2(L)\rangle + \beta_1^2\beta_2^2\langle u_2^2(L)\rangle, \quad (1.5)$$

where $\mathcal{T}$ is the amplitude transmission coefficient. In (1.5),

$$\beta_j = k_0 n_j, \quad j = 0, 1, 2, \quad (1.6)$$

where $k_0 = \omega(\mu_0\epsilon_0)^{\frac{1}{2}}$ is the free-space wavenumber, and u_m and v_m, $m = 1, 2$, are the solutions of the Eqs. (1.2)–(1.4). In Sec. 3, we use the smoothing method to calculate $\langle 1/\mathcal{T}\mathcal{T}^*\rangle$ to order η^2 for the case where $\Gamma(z) = e^{-2b|z|}$ and also to show that, for a large class of $\Gamma(z)$, the quantity $\langle 1/\mathcal{T}\mathcal{T}^*\rangle$ grows exponentially as $L \to \infty$ for small enough η.

2. THE SMOOTHING METHOD AND FIRST-ORDER MOMENTS

We begin this section with a brief review of Keller's formulation of the smoothing method.[3] Consider a linear, stochastic (ordinary or partial) differential operator M and the stochastic equation for u,

$$Mu = g, \quad (2.1)$$

where g is a known nonstochastic function. We assume that M has an expansion in powers of a small, positive parameter η, so that we can write (2.1) as

$$[L_0 + \eta L_1 + \eta^2 L_2 + O(\eta^3)]u = g, \quad (2.2)$$

where L_0 is a nonstochastic operator, while L_1 and L_2 are stochastic operators. We denote the stochastic average of u by $\langle u\rangle$, and we define the incoherent part of the solution $\mathsf{C}u\mathsf{D}$ by

$$\mathsf{C}u\mathsf{D} = u - \langle u\rangle. \quad (2.3)$$

An immediate consequence of definition (2.3) is

$$\langle \mathsf{C}u\mathsf{D}\rangle = 0. \quad (2.4)$$

Then the smoothing method yields the equation for the average solution[3]

$$\{L_0 + \eta\langle L_1\rangle + \eta^2[\langle L_1\rangle L_0^{-1}\langle L_1\rangle - \langle L_1 L_0^{-1} L_1\rangle + \langle L_2\rangle]\}\langle u\rangle = g, \quad (2.5)$$

where terms of order η^3 have been neglected and L_0^{-1} is the inverse operator to L_0. The incoherent part of the solution is related to the average solution by the relation[3]

$$\mathsf{C}u\mathsf{D} = -\eta L_0^{-1}\{L_1 - \langle L_1\rangle\}\langle u\rangle, \quad (2.6)$$

where terms of order η^2 have been neglected. This whole formalism is valid when M, u, and g are matrices. Finally, if $\langle u_n\rangle$ and $\mathsf{C}u_n\mathsf{D}$, $n = 1, 2$, are two solutions of (2.5) and (2.6) corresponding to the same inverse L_0^{-1}, one can use the identities

$$\langle u_n u_m\rangle = \langle u_n\rangle\langle u_m\rangle + \langle \mathsf{C}u_n\mathsf{D}\mathsf{C}u_m\mathsf{D}\rangle, \quad n, m = 1, 2, \quad (2.7)$$

to obtain the formula

$$\langle u_n u_m\rangle = \langle u_n\rangle\langle u_m\rangle + \eta^2\langle[L_0^{-1}\{L_1 - \langle L_1\rangle\}\langle u_n\rangle] \times [L_0^{-1}\{L_1 - \langle L_1\rangle\}\langle u_m\rangle]\rangle, \quad n, m = 1, 2. \quad (2.8)$$

In (2.8), the implication is that the second term is of order η^2 and only terms of order higher than η^2 have been neglected.

These equations, in one guise or another, have been widely used in the study of stochastic differential equations. Since all derivations of (2.5), (2.6), and (2.8) are strictly formal, considerable interest attaches to their validity. To gain some insight into this last consideration, we apply the smoothing method to the stochastic equation (1.2) with the boundary conditions (1.3).

In this case, we have

$$L_0 = \frac{d^2}{dz^2} + \beta_0^2, \quad L_1 = \beta_0^2 N(z),$$
$$\langle L_1\rangle = 0, \quad L_2 = 0, \quad g = 0. \quad (2.9)$$

From (1.3), we get the initial conditions

$$\langle u_m(0)\rangle = \delta_{m,1}, \quad \langle u_m'(0)\rangle = \delta_{m,2}, \quad (2.10)$$

$$\mathsf{C}u_m(0)\mathsf{D} = \mathsf{C}u_m'(0)\mathsf{D} = 0, \quad m = 1, 2, \quad (2.11)$$

where $\delta_{m,n}$ is the Kronecker δ. The inverse operator L_0^{-1} is given by means of a Green's function $g(z, \zeta)$ satisfying

$$\frac{d^2 g}{dz^2} + \beta_0^2 g = \delta(z - \zeta). \quad (2.12)$$

If $\mathsf{C}u_m(z)\mathsf{D}$ given by (2.6) is to satisfy the initial conditions (2.11), then we must have

$$g(0, \zeta) = \frac{dg(0, \zeta)}{dz} = 0. \quad (2.13)$$

The solution of (2.12) satisfying (2.13) is

$$g(z, \zeta) = 0, \quad 0 \le z \le \zeta,$$
$$= \beta_0^{-1}\sin\beta_0(z - \zeta), \quad \le z. \quad (2.14)$$

Equation (2.5) now becomes

$$\left(\frac{d^2}{dz^2} + \beta_0^2\right)\langle u_m(z)\rangle = \eta^2\beta_0^3\int_0^z \sin\beta_0(z-\zeta)\Gamma(z-\zeta)\langle u_m(\zeta)\rangle\, d\zeta, \quad m = 1, 2, \quad (2.15)$$

while (2.6) becomes

$$\subset u_m(z)\supset = -\eta\beta_0\int_0^z \sin\beta_0(z-\zeta)N(\zeta)\langle u_m(\zeta)\rangle\, d\zeta, \quad m = 1, 2. \quad (2.16)$$

As Bourret[9] has shown, the Laplace transforms of the solutions of (2.15) are readily obtained. We define

$$\mathfrak{L}(f) = \int_0^\infty e^{-sz} f(z)\, dz \quad (2.17)$$

and

$$\gamma(s) = \mathfrak{L}(\Gamma). \quad (2.18)$$

Then it follows directly from (2.15) that

$$\{s^2 + \beta_0^2 - (\eta^2\beta_0^3/2i)[\gamma(s - i\beta_0) - \gamma(s + i\beta_0)]\}\mathfrak{L}(\langle u_m\rangle) = s^{2-m}, \quad m = 1, 2. \quad (2.19)$$

It is also true that

$$\mathfrak{L}(\langle v_m\rangle) = s\mathfrak{L}(\langle u_m\rangle) - \delta_{m,1}, \quad m = 1, 2. \quad (2.20)$$

We now consider in more detail the important case where

$$\Gamma(z) = e^{-2b|z|}. \quad (2.21)$$

In this case,

$$\gamma(s) = (s + 2b)^{-1} \quad (2.22)$$

and

$$\mathfrak{L}(\langle u_m\rangle) = s^{2-m}[(s + 2b)^2 + \beta_0^2]/d(s), \quad (2.23)$$

where

$$d(s) = (s^2 + \beta_0^2)[(s + 2b)^2 + \beta_0^2] - \eta^2\beta_0^4. \quad (2.24)$$

It follows that

$$\langle u_m(z)\rangle = \sum_{j=1}^4 a_{m,j}e^{\sigma_j z}, \quad m = 1, 2, \quad (2.25)$$

where the σ_j are the four roots of the equation $d(s) = 0$ and the $a_{m,j}$ are the residues of the rational functions defining $\mathfrak{L}(\langle u_m\rangle)$ at $s = \sigma_j$.

Now, if $N(z)$ is the random telegraph process,[8,10,17] it has zero mean and its correlation function is given by (2.21). But it was shown generally by Bourret[10] that, for the random telegraph process, the smoothing method gives the exact result, and this is borne out by (2.23), (2.24), and our exact calculations.[13] It can be shown by standard methods[18] that, if $0 < \eta < 1$, all the roots of $d(s)$ have negative real parts, so that $\langle u_m(z)\rangle$ as given in (2.25) decays exponentially as $z \to \infty$.

We now turn to the calculation of $\langle u_m(z)u_n(z)\rangle$ by means of (2.8) for the special case when $\Gamma(z)$ is given by (2.21). The second term on the right of (2.8) is now

$$\eta^2\beta_0^2\sum_{j=1}^4\sum_{k=1}^4 a_{m,j}a_{n,k}\int_0^z\int_0^z \sin\beta_0(z-\zeta) \times \sin\beta_0(z-\xi)e^{-2b|\zeta-\xi|+\sigma_j\zeta+\sigma_k\xi}\, d\xi\, d\zeta. \quad (2.26)$$

The evaluation of the integrals in (2.26) is elementary but laborious, and we omit writing down the answer. However, the moment $\langle u_m(z)u_n(z)\rangle$ calculated in this fashion is a sum of the form $\sum_{p=0}^{18} A_p e^{r_p z}$, where $r_0 = 0$ and the remaining r_p take on the values $\sigma_j + \sigma_k$, $\pm i\beta_0 - 2b + \sigma_j$, $j, k = 1, 2, 3, 4$. Now, in the case where $N(z)$ is the random telegraph wave, the second-order moments have been calculated exactly,[13] and they all turn out to be of the form $\sum_{j=0}^6 B_j e^{s_j z}$. Here also, $s_0 = 0$, but none of the remaining exponents s_j, $1 \le j \le 6$, can be approximated to order η^2 by any of the r_p. In fact, one of the s_j has a positive real part for small enough η, while for $0 < \eta < 1$ all the r_p have negative real parts. Thus, we have an example where the smoothing method yields the first-order moments exactly, but a straightforward application of the method to calculate the second-order moments by means of (2.8) gives an incorrect answer.

Correlation functions of the form $\langle u_m(z)u_n(z + \zeta)\rangle$ have also been calculated exactly when $N(z)$ is the random telegraph process, and again it can be shown that the use of Eq. (2.8) yields badly incorrect answers.

Additional examples have been studied by Samuels and Eringen,[19] Stratonovich,[20] Khas'minskii,[21] Frisch,[22] and Papanicolaou.[23] They have shown that, in these cases also, the second-order moments grow exponentially with z. Thus the standard use of the smoothing method to calculate second-order moments fails here, too.

A close examination of the integrals appearing in (2.26) shows that they are of order η^{-2} when $z = O(\eta^{-2})$ so that the whole term in (2.26) is $O(1)$ instead of $O(\eta^2)$. This is due to the fact that, in the evaluation of the integrals in (2.26), terms such as

$$(\sigma_j + \sigma_k)^{-1}(e^{(\sigma_j+\sigma_k)z} - 1) \quad (2.27)$$

and similar terms appear and, for appropriate choice of j and k, $\sigma_j + \sigma_k = O(\eta^2)$.

The striking difference between the growth behavior of the first- and second-order moments is discussed further in Ref. 13.

3. SECOND-ORDER MOMENTS

The results of Sec. 2 strongly suggest that the use of (2.8) to calculate second-order moments by the smoothing method is suspect in general. However, they also suggest that a better way to get approximate expressions for higher-order moments is to find a

differential equation whose solutions include the products whose stochastic average is desired and to apply the smoothing technique directly to this equation.

In applying this idea to (1.2) to calculate second-order moments, we first derived a linear, third-order equation whose solutions were u_1^2, u_1u_2, and u_2^2. Then, following a suggestion of Papanicolaou, we have found it better to use Kronecker products[23,24] to derive a system of first-order, ordinary differential equations whose solutions are the products $u_n(z)u_m(z)$, $u_n(z)v_m(z)$, and $v_n(z)v_m(z)$, $m, n = 1, 2$. We then apply the smoothing technique to this set of equations. This method can clearly be extended to the calculation of moments of arbitrary-order of the solutions of any linear, ordinary differential equation.

For the case when $N(z)$ is the random telegraph process, this method yields the exact answer. This is not surprising in the light of Bourret's results.[10] It will also be shown that under quite general conditions on $N(z)$, the second-moments calculated in this way grow exponentially as $z \to \infty$.

We first rewrite (1.2) in matrix form. Thus, we define

$$\mathbf{F}(z) = \begin{pmatrix} u_1(z) & u_2(z) \\ v_1(z) & v_2(z) \end{pmatrix}, \tag{3.1}$$

where $v_m(z)$, $m = 1, 2$, is given by (1.4), and let

$$\mathbf{A} = \begin{pmatrix} 0 & -1 \\ \beta_0^2 & 0 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.2}$$

Then, from (1.2) and (1.3), we find that

$$\frac{d\mathbf{F}}{dz} + [\mathbf{A} + \eta\beta_0^2 N(z)\mathbf{C}]\mathbf{F} = \mathbf{0}, \quad \mathbf{F}(0) = \mathbf{I}. \tag{3.3}$$

From (3.3), we obtain an equation for the Kronecker product of $\mathbf{F}$ with itself in the form

$$(\mathbf{L}_0 + \eta\mathbf{L}_1)(\mathbf{F} \times \mathbf{F}) = 0, \quad \mathbf{F}(0) \times \mathbf{F}(0) = \mathbf{I} \times \mathbf{I}, \tag{3.4}$$

where

$$\mathbf{L}_0(z) \equiv (\mathbf{I} \times \mathbf{I})\frac{d}{dz} + [(\mathbf{A} \times \mathbf{I}) + (\mathbf{I} \times \mathbf{A})] \tag{3.5}$$

and

$$\mathbf{L}_1(z) \equiv \beta_0^2 N(z)[(\mathbf{C} \times \mathbf{I}) + (\mathbf{I} \times \mathbf{C})]. \tag{3.6}$$

We now apply the smoothing method to (3.4). The Green's function corresponding to the inverse of $\mathbf{L}_0$ satisfies

$$\mathbf{L}_0(z)\mathbf{G}(z, \zeta) = \delta(z - \zeta)(\mathbf{I} \times \mathbf{I}), \quad \mathbf{G}(0, \zeta) = \mathbf{0}, \quad \zeta > 0. \tag{3.7}$$

The boundary condition on $\mathbf{G}$ is a consequence of (2.6) and the nonstochastic initial value of $\mathbf{F} \times \mathbf{F}$, so that

$$\subset \mathbf{F}(0) \times \mathbf{F}(0) \supset = \mathbf{0}. \tag{3.8}$$

From (3.5) and (3.7), it follows that

$$\begin{aligned} \mathbf{G}(z, \zeta) &= 0, && 0 \le z < \zeta, \\ &= [\mathbf{E}(z - \zeta) \times \mathbf{E}(z - \zeta)], && z > \zeta, \end{aligned} \tag{3.9}$$

where

$$\frac{d\mathbf{E}}{dz} + \mathbf{A}\mathbf{E} = \mathbf{0}, \quad \mathbf{E}(0) = \mathbf{I}. \tag{3.10}$$

We may verify, using (3.2), that

$$\mathbf{E}(z) = \begin{pmatrix} \cos\beta_0 z & \beta_0^{-1}\sin\beta_0 z \\ -\beta_0 \sin\beta_0 z & \cos\beta_0 z \end{pmatrix}. \tag{3.11}$$

From (1.1), (2.5), (3.2), (3.5), (3.6), (3.9), and (3.11), we obtain the equation for the average of $\mathbf{F} \times \mathbf{F}$, namely,

$$\frac{d}{dz}\langle \mathbf{F} \times \mathbf{F}\rangle + [(\mathbf{A} \times \mathbf{I}) + (\mathbf{I} \times \mathbf{A})]\langle \mathbf{F}(z) \times \mathbf{F}(z)\rangle$$

$$= \eta^2\beta_0^2 \int_0^z \begin{pmatrix} 0 & 0 & 0 & 0 \\ \beta_0 \sin 2\beta_0(z-\zeta) & \sin^2\beta_0(z-\zeta) & \sin^2\beta_0(z-\zeta) & 0 \\ \beta_0 \sin 2\beta_0(z-\zeta) & \sin^2\beta_0(z-\zeta) & \sin^2\beta_0(z-\zeta) & 0 \\ 2\beta_0^2 \cos 2\beta_0(z-\zeta) & \beta_0 \sin 2\beta_0(z-\zeta) & \beta_0 \sin 2\beta_0(z-\zeta) & 0 \end{pmatrix} \Gamma(z - \zeta)\langle \mathbf{F}(\zeta) \times \mathbf{F}(\zeta)\rangle \, d\zeta. \tag{3.12}$$

Also, from (3.4), we have

$$\langle \mathbf{F}(0) \times \mathbf{F}(0)\rangle = (\mathbf{I} \times \mathbf{I}). \tag{3.13}$$

Expressions are derived in the Appendix for the Laplace transform of $\langle \mathbf{F} \times \mathbf{F}\rangle$, that is, from (3.1), for

$$\mathfrak{L}(\langle \mathbf{F} \times \mathbf{F}\rangle) = \mathfrak{L}\begin{pmatrix} \langle u_1^2\rangle & \langle u_1u_2\rangle & \langle u_2u_1\rangle & \langle u_2^2\rangle \\ \langle u_1v_1\rangle & \langle u_1v_2\rangle & \langle u_2v_1\rangle & \langle u_2v_2\rangle \\ \langle v_1u_1\rangle & \langle v_1u_2\rangle & \langle v_2u_1\rangle & \langle v_2u_2\rangle \\ \langle v_1^2\rangle & \langle v_1v_2\rangle & \langle v_2v_1\rangle & \langle v_2^2\rangle \end{pmatrix}. \tag{3.14}$$

An expression for $\mathfrak{L}(\langle \mathbf{F} \times \mathbf{F}\rangle)$ is given in (A5), the quantities occurring therein being given by (A6), (A9), and (A17)–(A21), with $\gamma(s)$ as in (2.18). From (A10), it follows that

$$\begin{aligned} \langle u_1^2(z)\rangle &= \langle v_2^2(z)\rangle, \\ \langle u_1(z)u_2(z)\rangle &= \langle u_2(z)v_2(z)\rangle, \\ \langle u_1(z)v_1(z)\rangle &= \langle v_1(z)v_2(z)\rangle. \end{aligned} \tag{3.15}$$

From (A11) and (A12), in view of the initial values in

(1.3), it follows that

$$\frac{d}{dz}\langle u_2^2(z)\rangle = 2\langle u_2(z)v_2(z)\rangle \tag{3.16}$$

$$\frac{d}{dz}\langle u_1(z)u_2(z)\rangle = \langle u_1(z)v_2(z)\rangle + \langle v_1(z)u_2(z)\rangle, \tag{3.17}$$

and

$$\frac{d}{dz}\langle u_1^2(z)\rangle = 2\langle u_1(z)v_1(z)\rangle, \tag{3.18}$$

which are not surprising results in view of (1.4). Finally, (A13) is a consequence of the Wronskian of the solutions of (1.2), namely,

$$u_1(z)v_2(z) - u_2(z)v_1(z) = 1. \tag{3.19}$$

We comment that it is possible to remove the redundancy that occurs in the Kronecker product $\mathbf{F} \times \mathbf{F}$. Thus, a first-order differential equation may be derived for the matrix

$$\mathbf{W} = \begin{pmatrix} u_1^2 & 2u_1u_2 & u_2^2 \\ u_1v_1 & (u_1v_2 + v_1u_2) & u_2v_2 \\ v_1^2 & 2v_1v_2 & v_2^2 \end{pmatrix}, \tag{3.20}$$

which is called a Kronecker power.[24] The determination of $\mathbf{W}$, together with the Wronskian (3.19), yields the ten distinct elements of $\mathbf{F} \times \mathbf{F}$. However, the use of Kronecker powers for higher-order moments would appear to be more involved than the use of Kronecker products.

Now consider the case in which (2.21) holds. The corresponding expressions for $\mathfrak{L}(\langle u_1^2\rangle)$, $\mathfrak{L}(\langle v_1^2\rangle)$, and $\mathfrak{L}(\langle u_2^2\rangle)$ are given in (A26)–(A28). The remaining elements in (3.14) are obtained by means of (A10)–(A13). These expressions for the elements in (3.14) agree with the exact results derived[13] for the random telegraph process.

As an application of these results, we calculate $\langle 1/\mathcal{C}\mathcal{C}^*\rangle$, as given in (1.5), to order η^2 when $\Gamma(z)$ is given by (2.21). Inversion of the Laplace transforms in (A26)–(A28) leads, from (1.5), to

$$4\beta_1^2\left\langle \frac{1}{\mathcal{C}\mathcal{C}^*}\right\rangle = 2\beta_1\beta_2 + \sum_{j=1}^{6} C_j(\eta^2)\exp[s_j(\eta^2)L]. \tag{3.21}$$

Here, the $s_j(\eta^2)$ are the six roots of the equation $\Delta(s) = 0$, where $\Delta(s)$ is given by (A25), and the $C_j(\eta^2)$ are evaluated from the residues of the expressions in (A26)–(A28). For $\eta^2 \ll 1$ and $\eta^2\beta_0 L \leq O(1)$, from (A30), (A31), and (A35), we have

$$\begin{aligned}\left(4\beta_1^2\left\langle \frac{1}{\mathcal{C}\mathcal{C}^*}\right\rangle - 2\beta_1\beta_2\right) &= \frac{[1 + O(\eta^2)]}{2\beta_0^2}\left\{(\beta_0^2 + \beta_1^2)(\beta_0^2 + \beta_2^2)\right. \\ &\times \exp\left(\frac{\eta^2\beta_0^2 bL}{2(b^2 + \beta_0^2)}\right) - (\beta_0^2 - \beta_1^2)(\beta_0^2 - \beta_2^2) \\ &\times \exp\left(-\frac{\eta^2\beta_0^2(b^2 + 2\beta_0^2)L}{4b(b^2 + \beta_0^2)}\right) \\ &\times \left.\cos\left[\left(2 - \frac{\eta^2\beta_0^2}{4(b^2 + \beta_0^2)}\right)\beta_0 L\right]\right\}.\end{aligned} \tag{3.22}$$

Returning to the general case, as in (1.1), it follows from results in the Appendix that, for $\eta^2 \ll 1$, $\langle 1/\mathcal{C}\mathcal{C}^*\rangle$ contains a term which grows exponentially with L, provided that

$$\int_{-\infty}^{\infty} e^{2i\beta_0 z}\Gamma(z)\,dz$$

does not vanish. This term arises from the root s_1 of $\Lambda(s) = 0$, as defined by (A9) and (A19), which is given approximately by (A37). From (1.5) and (A38)–(A40), it follows that the corresponding term in $\langle 1/\mathcal{C}\mathcal{C}^*\rangle$ is

$$\{[1 + O(\eta^2)]/2\beta_0^2\}(\beta_0^2 + \beta_1^2)(\beta_0^2 + \beta_2^2)e^{s_1 L}. \tag{3.23}$$

Note that the coefficient in (3.23) is, to lowest order in η^2, independent of $\gamma(s)$, which is assumed to be analytic at $s = 0$.

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APPENDIX

Here, we solve Eq. (3.12) for the average of $\mathbf{F} \times \mathbf{F}$, subject to the initial condition (3.13), by means of Laplace transforms. We define

$$\rho = \eta^2\beta_0^2\int_0^{\infty} e^{-sz}\sin^2(\beta_0 z)\Gamma(z)\,dz, \tag{A1}$$

$$\sigma = \eta^2\beta_0^3\int_0^{\infty} e^{-sz}\sin(2\beta_0 z)\Gamma(z)\,dz, \tag{A2}$$

and

$$\tau = 2\eta^2\beta_0^4\int_0^{\infty} e^{-sz}\cos(2\beta_0 z)\Gamma(z)\,dz. \tag{A3}$$

Then, from (2.17), (3.2), (3.12), and (3.13),

$$\begin{pmatrix} s & -1 & -1 & 0 \\ (\beta_0^2-\sigma) & (s-\rho) & -\rho & -1 \\ (\beta_0^2-\sigma) & -\rho & (s-\rho) & -1 \\ -\tau & (\beta_0^2-\sigma) & (\beta_0^2-\sigma) & s \end{pmatrix} \mathfrak{L}(\langle \mathbf{F}\times\mathbf{F}\rangle) = \begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{pmatrix} \tag{A4}$$

It follows from (A4) that

$$\mathfrak{L}(\langle \mathbf{F}\times\mathbf{F}\rangle) = \frac{1}{\Lambda}\begin{pmatrix} [(s^2+2\beta_0^2)-2\mu] & s & s & 2 \\ (\nu - s\beta_0^2) & [(s^2+2\beta_0^2)-\kappa/s] & (\kappa/s - 2\beta_0^2) & s \\ (\nu - s\beta_0^2) & (\kappa/s - 2\beta_0^2) & [(s^2+2\beta_0^2)-\kappa/s] & s \\ \lambda & (\nu - s\beta_0^2) & (\nu - s\beta_0^2) & [(s^2+2\beta_0^2)-2\mu] \end{pmatrix}, \tag{A5}$$

where

$$\lambda = 2(\beta_0^2-\sigma)^2 + \tau(s-2\rho) = 2[\beta_0^4 + (\sigma^2-\rho\tau)] + (s\tau - 4\beta_0^2\sigma), \tag{A6}$$

$$\mu = (s\rho+\sigma), \quad \nu = (s\sigma+\tau), \tag{A7}$$

$$\kappa = (s^2\rho + 2s\sigma + \tau) = (s\mu + \nu), \tag{A8}$$

and

$$\Lambda = \Lambda(s) \equiv [s(s^2+4\beta_0^2) - 2\kappa]. \tag{A9}$$

Note, from (3.14) and (A5), that

$$\mathfrak{L}(\langle u_1^2\rangle) = \mathfrak{L}(\langle v_2^2\rangle), \quad \mathfrak{L}(\langle u_1u_2\rangle) = \mathfrak{L}(\langle u_2v_2\rangle), \quad \mathfrak{L}(\langle u_1v_1\rangle) = \mathfrak{L}(\langle v_1v_2\rangle), \tag{A10}$$

and

$$s\mathfrak{L}(\langle u_2^2\rangle) = 2\mathfrak{L}(\langle u_2v_2\rangle), \quad s\mathfrak{L}(\langle u_1u_2\rangle) = \mathfrak{L}(\langle u_1v_2\rangle + \langle v_1u_2\rangle). \tag{A11}$$

Also, using (A8) and (A9), we find that

$$s\mathfrak{L}(\langle u_1^2\rangle) - 1 = 2\mathfrak{L}(\langle u_1v_1\rangle) \tag{A12}$$

and

$$\mathfrak{L}(\langle u_1v_2\rangle - \langle u_2v_1\rangle) = s^{-1}. \tag{A13}$$

Now, from (2.17), (2.18), and (A1)–(A3), we have

$$\rho = \tfrac{1}{4}\eta^2\beta_0^2[2\gamma(s) - \gamma(s-2i\beta_0) - \gamma(s+2i\beta_0)], \tag{A14}$$

$$\sigma = \tfrac{1}{2}i\eta^2\beta_0^3[\gamma(s+2i\beta_0) - \gamma(s-2i\beta_0)], \tag{A15}$$

and

$$\tau = \eta^2\beta_0^4[\gamma(s-2i\beta_0) + \gamma(s+2i\beta_0)]. \tag{A16}$$

Hence, from (A7) and (A8), we find

$$\mu = \tfrac{1}{4}\eta^2\beta_0^2[2s\gamma(s) - (s+2i\beta_0)\gamma(s-2i\beta_0) - (s-2i\beta_0)\gamma(s+2i\beta_0)], \tag{A17}$$

$$\nu = \tfrac{1}{2}i\eta^2\beta_0^3[(s-2i\beta_0)\gamma(s+2i\beta_0) - (s+2i\beta_0)\gamma(s-2i\beta_0)], \tag{A18}$$

and

$$\kappa = \tfrac{1}{4}\eta^2\beta_0^2[2s^2\gamma(s) - (s+2i\beta_0)^2\gamma(s-2i\beta_0) - (s-2i\beta_0)^2\gamma(s+2i\beta_0)]. \tag{A19}$$

Also,

$$(s\tau - 4\beta_0^2\sigma) = \eta^2\beta_0^4[(s+2i\beta_0)\gamma(s-2i\beta_0) + (s-2i\beta_0)\gamma(s+2i\beta_0)] \tag{A20}$$

and

$$(\sigma^2 - \rho\tau) = \tfrac{1}{2}\eta^2\beta_0^6\{2\gamma(s-2i\beta_0)\gamma(s+2i\beta_0) - \gamma(s)[\gamma(s-2i\beta_0) + \gamma(s+2i\beta_0)]\}. \tag{A21}$$

We now consider the particular case in which $\gamma(s)$ is given by (2.22). Then, from (A17)–(A21), it follows that

$$\mu = 4\eta^2\beta_0^4(s+b)/(s+2b)[(s+2b)^2+4\beta_0^2], \quad \nu = (s+2b)\mu, \quad \kappa = 2(s+b)\mu, \tag{A22}$$

and

$$(s\tau - 4\beta_0^2\sigma) = 2\eta^2\beta_0^4[s(s+2b) - 4\beta_0^2]/[(s+2b)^2+4\beta_0^2], \quad (\sigma^2-\rho\tau) = 0. \tag{A23}$$

Hence, from (A9), we have

$$\Lambda = \Delta/(s+2b)[(s+2b)^2+4\beta_0^2], \tag{A24}$$

where

$$\Delta = \Delta(s) \equiv \{s(s+2b)(s^2+4\beta_0^2)[(s+2b)^2+4\beta_0^2] - 16\eta^2\beta_0^4(s+b)^2\}. \tag{A25}$$

Thus, from (3.14), (A5), (A6), and (A22)–(A24), we find

$$\mathfrak{L}(\langle u_1^2\rangle) = (1/\Delta)\{(s+2b)(s^2+2\beta_0^2)[(s+2b)^2+4\beta_0^2] - 8\eta^2\beta_0^4(s+b)\} = \mathfrak{L}(\langle v_2^2\rangle), \tag{A26}$$

$$\mathfrak{L}(\langle v_1^2\rangle) = (2/\Delta)\beta_0^4(s+2b)\{[(s+2b)^2+4\beta_0^2] + \eta^2[s(s+2b) - 4\beta_0^2]\}, \tag{A27}$$

and

$$\mathfrak{L}(\langle u_2^2\rangle) = (2/\Delta)(s+2b)[(s+2b)^2+4\beta_0^2]. \tag{A28}$$

Now consider the equation $\Delta(s) = 0$, with roots $s_j, j = 1, \cdots, 6$. If s is a root, then so is $-(s + 2b)$. Hence, we may set

$$s_{q+3} = -(s_q + 2b), \quad q = 1, 2, 3. \tag{A29}$$

For $\eta^2 \ll 1$, we have the roots

$$s_1 = [\eta^2\beta_0^2 b/2(b^2 + \beta_0^2) + O(\eta^4)] \tag{A30}$$

and

$$s_2 = s_3^* = [2i\beta_0 - \eta^2\beta_0^2(b + 2i\beta_0)/4b(b + i\beta_0) + O(\eta^4)]. \tag{A31}$$

It follows, from (A29) and (A31), that, in (3.21),

$$C_3^*(\eta^2) = C_2(\eta^2), \quad C_6^*(\eta^2) = C_5(\eta^2). \tag{A32}$$

But for $\eta = 0$, from (A25)–(A28),

$$\mathfrak{L}(\langle v_1^2\rangle_0 + \beta_2^2\langle u_1^2\rangle_0 + \beta_1^2\langle v_2^2\rangle_0 + \beta_1^2\beta_2^2\langle u_2^2\rangle_0) = \frac{1}{2\beta_0^2}\left(\frac{1}{s}(\beta_0^2 + \beta_1^2)(\beta_0^2 + \beta_2^2) + \frac{(\beta_0^2 - \beta_1^2)(\beta_0^2 - \beta_2^2)}{(s^2 + 4\beta_0^2)}\right). \tag{A33}$$

Hence, from (1.5), (3.21), and (A29)–(A33),

$$C_1(0) = (1/2\beta_0^2)(\beta_0^2 + \beta_1^2)(\beta_0^2 + \beta_2^2), \quad C_4(0) = 0,$$
$$C_2(0) = (-1/4\beta_0^2)(\beta_0^2 - \beta_1^2)(\beta_0^2 - \beta_2^2), \quad C_5(0) = 0. \tag{A34}$$

Thus, for $\eta^2 \ll 1$, we have

$$[4\beta_1^2\langle 1/\mathcal{C}\mathcal{C}^*\rangle - 2\beta_1\beta_2] = \{[1 + O(\eta^2)]/2\beta_0^2\}\{(\beta_0^2 + \beta_1^2)(\beta_0^2 + \beta_2^2)\exp[s_1(\eta^2)L] - (\beta_0^2 - \beta_1^2)(\beta_0^2 - \beta_2^2) \times \exp(\mathrm{Re}\,[s_2(\eta^2)]L)\cos(\mathrm{Im}\,[s_2(\eta^2)]L)\}. \tag{A35}$$

Finally, we consider the equation $\Lambda(s) = 0$, where $\Lambda(s)$ is given by (A9) with κ as in (A19). We suppose that $\gamma(s)$ is sufficiently well behaved, in particular, at the origin. Denote the root of $\Lambda(s) = 0$ which vanishes for $\eta = 0$ by s_1. Then, for $\eta^2 \ll 1$, we have

$$s_1 \approx \tfrac{1}{2}\eta^2\beta_0^2[\gamma(-2i\beta_0) + \gamma(2i\beta_0)] = \tfrac{1}{2}\eta^2\beta_0^2\int_0^\infty (e^{2i\beta_0 z} + e^{-2i\beta_0 z})\Gamma(z)\,dz, \tag{A36}$$

using (2.17) and (2.18). But, from (1.1), $\Gamma(-z) = \Gamma(z)$. Hence,

$$s_1 \approx \tfrac{1}{2}\eta^2\beta_0^2\int_{-\infty}^{\infty} e^{2i\beta_0 z}\Gamma(z)\,dz \geq 0, \tag{A37}$$

by a well-known result.[25] From (3.14), (A5), (A6), (A9), (A17), and (A19)–(A21), we have

$$\lim_{s\to s_1}[(s - s_1)\mathfrak{L}(\langle u_1^2\rangle)] = \lim_{s\to s_1}[(s - s_1)\mathfrak{L}(\langle v_2^2\rangle)] = [\tfrac{1}{2} + O(\eta^2)], \tag{A38}$$

$$\lim_{s\to s_1}[(s - s_1)\mathfrak{L}(\langle u_2^2\rangle)] = \left(\frac{1}{2\beta_0^2} + O(\eta^2)\right), \tag{A39}$$

and

$$\lim_{s\to s}[(s - s_1)\mathfrak{L}(\langle v_1^2\rangle)] = [\tfrac{1}{2}\beta_0^2 + O(\eta^2)], \tag{A40}$$

assuming that $\gamma(s)$ is analytic at $s = 0$.

[1] U. Frisch, *Probabilistic Methods in Applied Mathematics*, A. T. Bharucha-Reid, Ed. (Academic, New York, 1968), p. 114. Throughout this paper, what we call the smoothing method, Frisch calls the first-order smoothing approximation.

[2] J. B. Keller, Proc. Symp. Appl. Math. **13**, 227 (1962).

[3] J. B. Keller, Proc. Symp. Appl. Math. **16**, 145 (1964).

[4] F. C. Karal and J. B. Keller, J. Math. Phys. **5**, 537 (1964).

[5] J. B. Keller and F. C. Karal, J. Math. Phys. **7**, 661 (1966).

[6] R. C. Bourret, Nuovo Cimento **26**, 1 (1962).

[7] R. C. Bourret, Can. J. Phys. **40**, 782 (1962).

[8] R. C. Bourret, Phys. Letters **13**, 323 (1964).

[9] R. C. Bourret, Can. J. Phys. **43**, 619 (1965).

[10] R. C. Bourret, Can. J. Phys. **44**, 2519 (1966).

[11] R. T. Aiken, Bell System Tech. J. **48**, 1129 (1969).

[12] See Ref. 1 for an extensive bibliography.

[13] J. McKenna and J. A. Morrison, J. Math. Phys. **11**, 2348 (1970), preceding paper.

[14] J. B. Keller, *Stochastic Equations and the Theory of Turbulence in Geophysical Fluid Dynamics* (Course Lectures and Seminars, Woods Hole, Mass., 1966), pp. 131–136.

[15] J. B. Keller, *Proceedings of the Symposium on Turbulence in Fluids and Plasmas* (Brooklyn Poly. Inst., Brooklyn, N.Y., 1968), pp. 131–142.

[16] J. B. Keller, *Contemporary Physics, Vol. I, Trieste Symposium, 1968* (International Atomic Energy Agency, Vienna, 1969), pp. 257–272.

[17] W. B. Davenport, Jr., and W. L. Root, *Random Signals and Noise* (McGraw-Hill, New York, 1968), p. 61.

[18] E. C. Titchmarsh, *The Theory of Functions* (Oxford U.P., London, 1949), p. 115.

[19] J. C. Samuels and A. C. Eringen, J. Math. & Phys. **38**, 83 (1959).

[20] R. L. Stratonovich, *Topics in the Theory of Random Noise* (Gordon & Breach, New York, 1963, 1967), Vols. I and II.

[21] R. Z. Khas'minskii, Theory Probability Appl. (USSR) **11**, 390 (1966).

[22] U. Frisch, Ref. 1, p. 139.

[23] G. Papanicolaou, Ph.D. thesis, New York University, 1969.

[24] R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill, New York, 1960), pp. 227, 228.

[25] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1966), Vol. II, p. 586.

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Canonical Unit Adjoint Tensor Operators in $U(n)$*

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A complete, fully explicit, and canonical determination of the matrix elements of all adjoint tensor operators in all $U(n)$ is presented. The class of adjoint tensor operators—those transforming as the IR $[1\ 0\ \cdots\ 0\ -1]$—is the first exhibiting a nontrivial multiplicity. It is demonstrated that the canonical resolution of this multiplicity possesses several compatible (or equivalent) properties: classification by null spaces, classification by degree in the Racah invariants, classification by limit properties, and the classification by conjugation parity. (The concepts in these various classification properties are developed in detail.) A systematic treatment is presented for the coupling of projective (tensor) operators. Six appendices treat in detail the explicit evaluation of all Gel'fand-invariant operators (I_k), the structural properties of Gram determinants formed of the I_k, the zeros of the norms of the adjoint operators, and the conjugation properties of the canonical adjoint tensor operators.

1. INTRODUCTION AND SUMMARY

Over the past few years, the problem of constructing for the unitary group $U(n)$ (n arbitrary but fixed) the analog—in so far as possible—to the Wigner–Racah angular-momentum calculus for $SU(2)$ has been a topic of considerable research interest. In a series of papers,[1–7] we have developed several general methods for attacking this problem and have, in particular, advocated the view that not only does there exist a generalization of the angular-momentum calculus for $U(n)$, but that this structure is canonical—that is to say, it is *unique*, to within equivalence. In Ref. 1, we have succeeded in proving that this is indeed the case for $U(3)$ and that accordingly the whole machinery of $U(3)$-Wigner and $U(3)$-Racah coefficients is now canonically defined.

One might summarize the content of our demonstration of a canonical structure for $U(3)$ by making an analogy to the Weyl branching theorem[8] [this theorem serves to classify canonically all states belonging to a given (unitary) irreducible representation of $U(n)$]. Our result for $U(3)$ establishes a branching law for tensor operators which thereby induces a complete operator classification. Expressed somewhat differently, this branching serves to establish a generalized Wigner–Eckart theorem for $U(3)$, *in which all quantum numbers for classifying tensor operators are uniquely, and intrinsically, specified.*[9]

The present paper is primarily concerned with the extension of our $U(3)$ results to $U(n)$; rather than attempting to discuss the complete problem, however, the present work is restricted to demonstrating a canonical classification of the class of unit adjoint tensor operators in $U(n)$—these are the tensor operators transforming as the $U(n)$ irreducible representation[10] $[1\ 0\ \cdots\ 0\ -1]$ {equivalent to

$$[2\ 1\ 1\ \cdots\ 1\ 0]$$

in $SU(n)$}.

The class of adjoint tensor operators is of considerable intrinsic interest in mathematical physics. This class includes the generators, whose matrix elements were first given, for all $U(n)$, by Gel'fand and Zetlin.[11] In the present paper, we give the explicit matrix elements of all unit adjoint tensor operators in all $U(n)$, classified canonically. [For $U(3)$, this has already been done in Ref. 5 (Paper V); for $U(2)$ the results are very well known, having been obtained in 1927 by Wigner.[12] The remaining results are new.]

As a by-product of this development, we also give explicitly the matrix elements of the (canonical) $U(n)$ Racah coefficients (for

$$[1\ 0\ \cdots\ 0] \times [0\ 0\ \cdots\ 0\ -1] \rightarrow [1\ 0\ \cdots\ 0\ -1]).$$

Although these explicit constructions are both interesting and new, they are not the principal result of the present paper. Rather, we are mainly concerned with discussing the resolution of the multiplicity for adjoint tensor operators as a specific nontrivial example to illuminate various aspects of the canonical approach. Our major result is the proposition that concludes Sec. 7, in which we demonstrate the equivalence of several properties of the canonical resolution: classification by null spaces (see Secs. 2 and 7), classification by degree in the Racah invariants (Sec. 5), classification by limit properties (also in Sec. 5), and the compatibility with the classification by conjugation parity (Appendix F).

One of the more vexing aspects of the whole problem of a general $U(n)$ operator calculus is that of devising an acceptable notation; operator labeling details that may appear horribly complicated are often structurally very elementary. We have attempted to solve this dilemma by generalizing on Gel'fand's ingenious notation. Without adequate discussion, these notational developments would render the present work needlessly inaccessible; accordingly, we include in Sec. 2 a fairly lengthy survey of both the technical background and these notational developments.

In Sec. 3, we discuss the problem of coupling projective operators (defined in Sec. 2), which forms a necessary technical development for the $U(n)$ calculus. Sections 4 and 5 are devoted to construction of the explicit matrix elements for the (canonical) adjoint (unit tensor) operators.

The calculus of projective operators is generalized in Sec. 6, and this "extended calculus" is demonstrated to comprise a significant structural link which emerges naturally from the calculus of projective operators in the limit of large (negative) quantum numbers. Finally, Sec. 7 contains a detailed discussion of the canonical labeling problem and concludes with a proof of the proposition mentioned earlier.

We have relegated many detailed calculations to various appendices. It is our belief, however, that much of this material is new (or at least unpublished). In particular, we would like to call attention to the general summation formulas (treated in Appendix A), the explicit eigenvalues of the general invariant operators I_k (treated in Appendix B), and the explicit construction of the null spaces of all adjoint Wigner operators (Appendix E). Appendices C, D, and E contain several general structural properties of Gram determinants formed from the invariants I_k.

2. NOTATIONAL CONVENTIONS AND RÉSUMÉ OF BASIC CONCEPTS

The purpose of this section is to state the notational conventions to be employed and to cite the basic theorems and concepts to be used in the constructions to follow. It is not our intention to make this résumé self-contained; rather, we seek only to give referencing and discussion adequate to elaborating the methods.

A. Irreducible Tensor Operators

Let U denote an $n \times n$ unitary matrix and let the correspondence $U \to \mathcal{O}_U$, $U \in U(n)$, be a representation of the group $U(n)$ by unitary operators on a Hilbert space over $\mathbf{C}$ (the field of complex numbers). Each invariant representation space with respect to which these operators are irreducible is spanned by a set of orthonormal vectors which are specified by a partition of integers $[m] = [m_{1n}\, m_{2n} \cdots m_{nn}]$, $m_{1n} \geq m_{2n} \geq \cdots \geq m_{nn}$, together with $\frac{1}{2}n(n-1)$ additional integers m_{ij}, $i \leq j = 1, 2, \cdots, n-1$, whose range of values enumerates the vectors in the basis. The set of $n(n+1)/2$ integers is arranged in a *Gel'fand pattern*, a triangular array of n rows, denoted by (m):

$$(m) = \begin{pmatrix} m_{1n} & & m_{2n} & & \cdots & & m_{n-1\,n} & & m_{nn} \\ & m_{1n-1} & & m_{2n-1} & & & & m_{n-1\,n-1} & \\ & & \cdot & & & & \cdot & & \\ & & & \cdot & & & \cdot & & \\ & & & & m_{12} & & m_{22} & & \\ & & & & & m_{11} & & & \end{pmatrix} \tag{2.1}$$

The integers m_{ij}, $i, j = 1, 2, \cdots, n-1$, run over all values consistent with the conditions

$$m_{i\,j+1} \geq m_{ij} \geq m_{i+1\,j+1}, \tag{2.2}$$

which are referred to as the "betweenness conditions."

A *vector* of the orthonormal Gel'fand basis is denoted by $|(m)\rangle$. When the need to indicate explicitly the partition labels $[m]$ arises, we use the notation[13]

$$\left|\begin{pmatrix}[m]\\(m)\end{pmatrix}\right\rangle \tag{2.3}$$

The number of orthonormal vectors in the space specified by $[m]$ [these labels are hereafter called "IR" (for irreducible representation) labels] is given by the Weyl dimension function[8]:

$$D([m]) \equiv \prod_{i<j=1}^{n} \frac{(p_{in} - p_{jn})}{1!\,2! \cdots (n-1)!}, \tag{2.4}$$

where the p_{in} are the *partial hooks* (for $j = n$) defined generally by

$$p_{ij} \equiv m_{ij} + j - i, \quad i \leq j = 1, 2, \cdots, n. \tag{2.5}$$

The vector $|(m)\rangle' = \mathcal{O}_U\,|(m)\rangle$ is given by

$$\mathcal{O}_U \left|\begin{pmatrix}[m]\\(m)\end{pmatrix}\right\rangle = \sum_{(m')} D^{[m]}_{(m')(m)}(U) \left|\begin{pmatrix}[m]\\(m')\end{pmatrix}\right\rangle, \tag{2.6}$$

and

$$U \to D^{[m]}(U) \tag{2.7}$$

is an irreducible representation of $U(n)$ by unitary matrices of dimension $D([m])$. We refer to the vectors (2.3) as "the state vectors for IR $[m]$ of $U(n)$" or as "$U(n)$ state vectors."

The significance of the betweenness conditions (2) and of the integers in the Gel'fand pattern (m) is readily understood as a geometrical realization of the Weyl branching law. The condition $m_{nn} = 0$ distinguishes $SU(n)$ IR's; in the general case, m_{nn} may be any integer (positive, zero, or *negative*). Each set of IR labels $[m]$ specifies an IR of $U(n)$, and the state vectors $|(m)\rangle$ specify the Gel'fand basis.

Consider next the concept of an irreducible tensor operator with respect to $U(n)$. An irreducible tensor operator T is a *set* of operators which is transformed linearly into itself under $\mathcal{O}_U$; furthermore, $\mathcal{O}_U$ is irreducible on this set.[14] This signifies that the set T can be assigned the labels $[M]$ of an IR of $U(n)$; we denote T by $T([M])$. Moreover, the operators in the set can be classified by the Gel'fand labels. The law of transformation is

$$\mathcal{O}_U T\begin{pmatrix}[M]\\(M)\end{pmatrix}\mathcal{O}_U{}^{-1} = \sum_{(M')} D^{[M]}_{(M')(M)}(U)\, T\begin{pmatrix}[M]\\(M')\end{pmatrix}. \tag{2.8}$$

This global definition is equivalent to the infinitesimal transformations

$$\left[E_{ij}, T\begin{pmatrix}[M]\\(M)\end{pmatrix}\right] = \sum_{(M')} \left\langle \begin{pmatrix}[M]\\(M')\end{pmatrix} \middle| E_{ij} \middle| \begin{pmatrix}[M]\\(M)\end{pmatrix} \right\rangle T\begin{pmatrix}[M]\\(M')\end{pmatrix}, \tag{2.9}$$

where the E_{ij}, $i, j = 1, 2, \cdots, n$, are the generators of the representation $U \to \mathcal{O}_U$.

The set of all irreducible tensor operators carrying IR labels $[M]$ is itself a vector space [of dimension $D([M])$] over the invariant functions as scalars. (The invariant functions are functions of the independent invariant operators $I_k^{(n)}$, $k = 1, 2, \cdots, n$. We shall need quite detailed information on these invariant operators and their eigenvalues, including some results not hitherto published. This material is developed and discussed in Appendices A and B.)

Our essential purpose is to characterize this space of irreducible tensor operators in explicit and complete detail. The first step in this characterization is, of course, to use the transformation properties, Eqs. (2.8) and (2.9), to assign the Gel'fand pattern labels (M). A physically motivated second step is to determine the *selection rules* obeyed by the tensor operator. In the language of $U(n)$, this step determines the changes in the IR labels of a *generic* state which are effected by the application of a tensor operator. [We insist on a generic state since, just as in $SU(2)$, the operator may annihilate particular states despite the selection rules. For example, the shift $\Delta J = -1$ cannot be effected by a dipole operator on states with $J = 0$.] For an operator $T([M])$, the "selection rules" are $[m] \to [m'] = [m] + [\Delta]$, where $[\Delta] = [\Delta_{in}]$ designates any *weight* associated with (operator) IR labels $[M]$ and $[\Delta]$ runs over all such weights.

In $SU(2)$, these two steps provide a complete classification, but, as is well known, this classification is incomplete in $SU(n)$ $(n > 2)$.

Given a tensor operator $T([M])$ which induces the particular transformation $[m] \to [m'] = [m] + [\Delta]$ ($[\Delta]$ a prescribed weight), the dimensionality of the associated (operator) space is known to be equal to the intertwining number of the three IR's involved, that is, $\mathfrak{I}([M], [m], [m']^*)$. The intertwining number is thus associated with a triple of IR labels; but *we wish to associate somehow this dimensionality with the operator itself.* With generic states, the maximum dimensionality is clearly an intrinsic property of the operator $T([M])$. This dimensionality has been shown (Ref. 5, Paper III) to be exactly the multiplicity of the weight $[\Delta]$ in $[M]$. In other words (letting $[\Delta]$ run over all weights), we define precisely $D([M])$ *independent tensor operators* which span the space of all tensor operators transforming as $[M]$. {*Each* of these tensor operators also has, of course, $D([M])$ components.} On *certain spaces* $|(m)\rangle$, some of these operators necessarily become dependent or, by using an orthogonal basis, *certain of the operators necessarily vanish.* Thus, each of the tensor operators in the set of $D([M])$ orthogonal operators carrying IR labels $[M]$ has associated with it a *null space* (the set of all vectors belonging to the various IR spaces annihilated by the particular operator). (A problem arises immediately: To what extent does the null space characterize the operator? This is discussed in detail in Sec. 7 for the adjoint tensor operators.)

We have dealt rather overlong on this concept of a tensor operator since it is a subject which is at once fundamental, yet frequently confused in the literature.

The essential purpose of the ideas discussed above has been to extend results—well defined by particular matrix elements—to the concept of a unique tensor operator defined on *all* states. Norming this operator to unity (on all states *not* in the null space) leads to unit tensor operators or—as they are also called—Wigner operators. The set of all Wigner operators is an orthonormal basis, over the invariant functions, for all tensor operators.

1. Notation

A unit tensor operator is denoted by

$$\left\langle \begin{matrix} (\Gamma) \\ [M] \\ (M) \end{matrix} \right\rangle \tag{2.10}$$

The lower pattern is the Gel'fand pattern assigned by the transformation property (2.8). The upper pattern (Γ) enumerates the various—$D([M])$ in number—unit tensor operators in the basis. It also has the form of a Gel'fand pattern (inverted for notational convenience):

$$\begin{pmatrix} (\Gamma) \\ [M] \end{pmatrix} = \begin{pmatrix} & & & & \Gamma_{11} & & & \\ & & & \Gamma_{12} & & \Gamma_{22} & & \\ & & \cdot & & \cdot & & \cdot & \\ & \cdot & & \cdot & & \cdot & & \cdot \\ & & \cdot & & \cdot & & \cdot & \\ & & \Gamma_{1n-1} & & \cdots & & \Gamma_{n-1\,n-1} & \\ M_{1n} & & & M_{2n} & & \cdots & & M_{nn} \end{pmatrix} \tag{2.11}$$

The entries in the pattern (Γ) are also required to satisfy the betweenness conditions.

The significance of the labels (Γ)—called "upper pattern labels" or "operator patterns"—is very different from that of a Gel'fand pattern (M), since the latter are completely interpreted from the subgroup properties implied by the Weyl branching law. By contrast, the "operator patterns" are—until proven otherwise (see Sec. 7)—to be interpreted as mere labels.

The notation implies that one may associate a weight with the upper pattern (Γ); *this weight is the shift* $[\Delta]$ *induced by the tensor operator*—or, as we shall also call it, the Δ pattern of the operator (2.10). It is given explicitly by

$$[\Delta(\Gamma)] = [\Delta_{1n}(\Gamma)\, \Delta_{2n}(\Gamma) \cdots \Delta_{nn}(\Gamma)], \tag{2.12}$$

where

$$\Delta_{in}(\Gamma) = \sum_{j=1}^{i} \Gamma_{ji} - \sum_{j=1}^{i-1} \Gamma_{ji-1}. \tag{2.13}$$

2. Orthogonality and Completeness

The unit tensor operators of prescribed IR labels $[M]$ satisfy the equations as follows (the dagger denotes Hermitian conjugation):

$$\sum_{(M)} \left\langle \begin{matrix} (\Gamma) \\ [M] \\ (M) \end{matrix} \right\rangle \left\langle \begin{matrix} (\Gamma') \\ [M] \\ (M) \end{matrix} \right\rangle^{\dagger} = \delta_{(\Gamma)(\Gamma')} I_{(\Gamma)}, \tag{2.14}$$

$$\sum_{(\Gamma)} \left\langle \begin{matrix} (\Gamma) \\ [M] \\ (M) \end{matrix} \right\rangle^{\dagger} \left\langle \begin{matrix} (\Gamma) \\ [M] \\ (M') \end{matrix} \right\rangle = \delta_{(M)(M')}, \tag{2.15}$$

where $I_{(\Gamma)}$ is a function defined on the set of all $U(n)$ IR labels, $\{[m]_n\}$: It has value 0 whenever the $U(n)$ IR labels belong to the null space of

$$\left\langle \begin{matrix} (\Gamma) \\ [M] \\ \cdot \end{matrix} \right\rangle^{\dagger};$$

otherwise, it has value 1.

We are now able to state the selection rules more precisely: The matrix element of the unit tensor operator (2.10) between initial and final states $|(m)\rangle$ and $|(m')\rangle$, respectively, vanishes unless conditions (i)–(iv) below are met; that is, the matrix element

$$\left\langle \begin{pmatrix} [m']_n \\ (m')_{n-1} \end{pmatrix} \right| \left\langle \begin{matrix} (\Gamma)_{n-1} \\ [M]_n \\ (M)_{n-1} \end{matrix} \right\rangle \left| \begin{pmatrix} [m]_n \\ (m)_{n-1} \end{pmatrix} \right\rangle \tag{2.16}$$

vanishes unless:

(i) All patterns (Gel'fand and operator) are *lexical* (i.e., satisfy betweenness relations as well as the ordering imposed on IR labels);

(ii) $[m']_n = [m]_n + [\Delta(\Gamma)]_n$, i.e., $m'_{in} = m_{in} + \Delta_{in}(\Gamma)$;

(iii) for each $j = 1, 2, \cdots, n$, there exists at least one operator pattern of j rows $(\gamma)_j$ of the form

$$(\gamma)_j = \begin{pmatrix} [M]_j \\ (\gamma)_{j-1} \end{pmatrix},$$

where $[M]_j$ is row j of $(M)_n$, such that

$$[m']_j = [m]_j + [\Delta(\gamma)]_j$$

[statement (iii) is a consequence of subgroup properties to be discussed below];

(iv) $|(m)_n\rangle$ does not belong to the null space[15] of

$$\left\langle \begin{matrix} (\Gamma) \\ [M] \\ \cdot \end{matrix} \right\rangle$$

The essential content of the selection rule for a unit tensor operator is contained in statement (ii). It asserts that the effect of a unit tensor operator on the IR labels $[m]_n$ of a generic state vector is to effect the shift $[\Delta(\Gamma)]$. (Similar shifts are also effected on the subgroup labels $(m)_{n-1}$ in accordance with the subgroup reduction properties discussed below.)

The Δ pattern associated with a prescribed set of IR labels $[M]$ can be used to partition the set of Wigner operators (2.10) into subsets possessing a common Δ pattern:

$$\left\{ \left| \begin{matrix} (\Gamma) \\ [M] \\ (M) \end{matrix} \right\rangle : (\Gamma) = (\Gamma'), (\Gamma''), \cdots \text{ such that } [\Delta(\Gamma')] = [\Delta(\Gamma'')] = \cdots \right\}. \tag{2.17}$$

The number of operators in this set is called *the multiplicity of the Wigner operators having the prescribed Δ pattern.* If the multiplicity is 1, then that Wigner operator is *unique.*[16] In this paper, we extend this uniqueness to the adjoint Wigner operators of arbitrary $U(n)$.

It is important to understand the significance of the nonzero matrix elements (2.16) in a familiar context: *The matrices of the unit tensor operators are the coupling coefficients of $U(n)$.* This means, for example, that we can couple two kinematically independent[17] state vectors $|(m)\rangle_1$ and $|(M)\rangle_2$ to obtain coupled state vectors which are again the Gel'fand basis vectors for an IR of $U(n)$ in the direct product space:

$$\left| \begin{pmatrix} [m] + [\Delta(\Gamma)] \\ (m') \end{pmatrix}; (\Gamma) \right\rangle = \sum_{(M)(m)} \left\langle \begin{pmatrix} [m] + [\Delta(\Gamma)] \\ (m') \end{pmatrix} \middle| \left| \begin{matrix} (\Gamma) \\ [M] \\ (M) \end{matrix} \right\rangle \middle| \begin{pmatrix} [m] \\ (m) \end{pmatrix} \right\rangle \times \left| \begin{pmatrix} [M] \\ (M) \end{pmatrix} \right\rangle_2 \left| \begin{pmatrix} [m] \\ (m) \end{pmatrix} \right\rangle_1, \tag{2.18}$$

where the coupled vectors are orthonormal whenever they are nonzero, that is, whenever $|(m)\rangle$ does not belong to the null space of

$$\left| \begin{matrix} (\Gamma) \\ [M] \\ \cdot \end{matrix} \right\rangle,$$

$$\left\langle \begin{pmatrix} [m] + [\Delta(\Gamma)] \\ (m') \end{pmatrix}; (\Gamma) \middle| \begin{pmatrix} [m] + [\Delta(\Gamma')] \\ (m'') \end{pmatrix}; (\Gamma') \right\rangle = \delta_{(m')(m'')}\delta_{(\Gamma)(\Gamma')}. \tag{2.19}$$

Thus, the determination of the coefficients (2.16) constitutes the solution to the state vector coupling problem. [It is for this reason that we call these $U(n)$ coefficients *Wigner coefficients* and the unit tensor operators $U(n)$ *Wigner operators.*]

It is an immediate result that these Wigner coefficients are also the elements of the unitary matrix (real orthogonal) which reduces the direct product

$$D^{[m]}(U) \otimes D^{[M]}(U)$$

into its irreducible constituents.

B. Subgroup Reduction and Reduced Wigner Coefficients

The existence of subgroup properties is intrinsic in the definition of a $U(n)$ Wigner operator. The essential feature is that the $U(n)$ Wigner operator

$$\left| \begin{matrix} (\Gamma)_{n-1} \\ [M]_n \\ [M]_{n-1} \\ (M)_{n-2} \end{matrix} \right\rangle, \tag{2.20}$$

in which the $U(n-1)$ IR labels $[M]_{n-1}$ are fixed (in accordance with the betweenness conditions), is also an irreducible tensor operator with IR labels $[M]_{n-1}$ with respect to $U(n-1)$. But the set of $U(n-1)$ Wigner operators

$$\left\{ \left| \begin{matrix} (\gamma)_{n-2} \\ [M]_{n-1} \\ (M)_{n-2} \end{matrix} \right\rangle, \text{ all } (\gamma)_{n-2} \right\} \tag{2.21}$$

is a basis for all $U(n-1)$ irreducible tensor operators with IR labels $[M]_{n-1}$. These properties imply a relation between $U(n)$ and $U(n-1)$ Wigner coefficients which is explicitly stated as follows:

$$\left\langle \begin{pmatrix} [m]_n + [\Delta(\Gamma)]_n \\ (m')_{n-1} \end{pmatrix} \middle| \left| \begin{matrix} (\Gamma)_{n-1} \\ [M]_n \\ (M)_{n-1} \end{matrix} \right\rangle \middle| \begin{pmatrix} [m]_n \\ (m)_{n-1} \end{pmatrix} \right\rangle = \sum_{(\gamma)_{n-2}} \left\langle \begin{pmatrix} [m]_n + [\Delta(\Gamma)]_n \\ [m']_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \middle| \begin{pmatrix} [m]_n \\ [m]_{n-1} \end{pmatrix} \right\rangle \times \left\langle \begin{pmatrix} [m']_{n-1} \\ (m')_{n-2} \end{pmatrix} \middle| \left| \begin{matrix} (\gamma)_{n-2} \\ [M]_{n-1} \\ (M)_{n-2} \end{matrix} \right\rangle \middle| \begin{pmatrix} [m]_{n-1} \\ (m)_{n-2} \end{pmatrix} \right\rangle, \tag{2.22}$$

where $(\gamma)_{n-1}$ is the (lexical) operator pattern which has $[M]_{n-1}$ in row $n-1$ and $(\gamma)_{n-2}$ in the remaining $n-2$ rows [i.e., is the operator pattern of the $U(n-1)$ Wigner coefficient].

Let us consider the first of the two terms in the sum above. This quantity is the invariant [with respect to $U(n-1)$] which appears in the restriction of a $U(n)$ Wigner operator to a $U(n-1)$ tensor operator. Hence, it is independent of the $U(n-2)$ subgroup labels; it is therefore completely labeled by the "free" labels from the left-hand side together with the $U(n-1)$ IR labels and the summation pattern $(\gamma)_{n-2}$. These coefficients are called $U(n):U(n-1)$ *reduced Wigner coefficients* [these are the isoscalar factors[18] of $SU(3)$]. The "matrix element form" of the notation for these reduced Wigner coefficients, introduced in Eq. (2.22), is motivated by the fact that these coefficients then multiply (see Sec. 3) as the elements of a matrix or, in physical language,[19] as observables. [Observe that, for $n=2$, a $U(2):U(1)$ reduced Wigner coefficient is, in fact, a $U(2)$ Wigner coefficient.]

The $U(n):U(n-1)$ reduced Wigner coefficients

$$\left\langle \begin{pmatrix} [m']_n \\ [m']_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \middle| \begin{pmatrix} [m]_n \\ [m]_{n-1} \end{pmatrix} \right\rangle \tag{2.23}$$

are defined to be zero unless:

(i) All patterns are lexical (This means, in particular, that $[m]_{n-1}$ and $[m']_{n-1}$ must fulfill the betweenness conditions with $[m]_n$ and $[m']_n$, respectively.);

(ii) the initial and final labels are related by

$$[m']_n = [m]_n + [\Delta(\Gamma)]_n,$$
$$[m']_{n-1} = [m]_{n-1} + [\Delta(\gamma)]_{n-1};$$

(iii) the $U(n)$ IR labels $[m]_n$ do not belong to the null space of $\left\langle \begin{smallmatrix} (\Gamma)_{n-1} \\ [M]_n \\ \cdot \end{smallmatrix} \right\rangle$; the $U(n-1)$ IR labels $[m]_{n-1}$ do not belong to the null space of $\left\langle \begin{smallmatrix} (\gamma)_{n-2} \\ [\gamma]_{n-1} \\ \cdot \end{smallmatrix} \right\rangle$.

The coefficients (2.23) also satisfy orthogonality relations in consequence of the orthogonality relations for $U(n)$ *and* $U(n-1)$ Wigner coefficients. These properties are most concisely expressed through the notion of a $U(n):U(n-1)$ projective operator to which we now turn.

C. $U(n):U(n-1)$ Projective Operators

The concept of a $U(n):U(n-1)$ projective operator is abstracted from $U(n):U(n-1)$ Wigner coefficients in precisely the same way that a Wigner operator is abstracted from Wigner coefficients: Consider $U(n)$ state vectors $|(m)_n\rangle$ in which the $U(n-2)$ labels are taken to be *maximal*. We then define the unit $U(n):U(n-1)$ projective operator

$$\begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \tag{2.24}$$

to be that operator which effects the following transformation between maximal states in $U(n-2)$:

$$\begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \left| \begin{pmatrix} [m]_n \\ [m]_{n-1} \\ (\max) \end{pmatrix} \right\rangle$$
$$= \left\langle \begin{pmatrix} [m]_n + [\Delta(\Gamma)]_n \\ [m]_{n-1} + [\Delta(\gamma)]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \middle| \begin{pmatrix} [m]_n \\ [m]_{n-1} \end{pmatrix} \right\rangle$$
$$\times \left| \begin{pmatrix} [m]_n + [\Delta(\Gamma)]_n \\ [m]_{n-1} + [\Delta(\gamma)]_{n-1} \\ (\max) \end{pmatrix} \right\rangle . \tag{2.25}$$

The orthogonality relations referred to previously are simply the matrix element statements of the following operator equations:

$$\sum_{(\gamma)} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix} \begin{bmatrix} (\Gamma') \\ [M] \\ (\gamma) \end{bmatrix}^{\dagger} = \delta_{(\Gamma)(\Gamma')} I_{(\Gamma)}, \tag{2.26}$$

$$\sum_{(\Gamma)} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix}^{\dagger} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma') \end{bmatrix} = \delta_{(\gamma)(\gamma')} I'_{(\gamma)}, \tag{2.27}$$

where $I_{(\Gamma)}$ is the invariant function introduced in Eq. (2.14). $I'_{(\gamma)}$ is a function defined on the set of all $U(n-1)$ IR labels, $\{[m]_{n-1}\}$: It has value 0 whenever the $U(n-1)$ IR labels belong to the null space of

$$\left\langle \begin{smallmatrix} (\gamma)_{n-2} \\ [\gamma]_{n-1} \\ \cdot \end{smallmatrix} \right\rangle ;$$

otherwise, it has value 1.

Equations (2.26) and (2.27) are necessary properties which unit $U(n):U(n-1)$ projective operators must have in consequence of the orthogonality properties of $U(n)$ and $U(n-1)$ Wigner operators. It is the converse of this result which is important: Consider the set of $U(n-1)$ Wigner operators as known. *Then every set of unit* $U(n):U(n-1)$ *projective operators satisfying the orthogonality relations* (2.26) *and* (2.27) *defines a complete set of* $U(n)$ *Wigner operators through Eq.* (2.22). The problem of defining completely *all* Wigner operators has thus been reduced to the problem of defining completely the unit $U(n):U(n-1)$ projective operators for all n. *The basic structures to be studied in the Racah–Wigner calculus are therefore the unit projective operators.*

D. The Pattern Calculus Rules

It is a remarkable fact that the explicit matrix elements of all *extremal* unit $U(n):U(n-1)$ projective operators can be calculated from a few simple rules of the pattern calculus.[2] In particular, this class of explicitly known projective operators includes all *elementary* operators of the form $[\dot{1}_k \quad \dot{0}_{n-k}]$ and $[\dot{0}_{n-k} \quad -\dot{1}_k]$ (a dot over a numeral implies that the numeral is repeated a number of times equal to the subscript), which themselves are a basis for constructing all $U(n)$ tensor operators.

The pattern calculus proceeds by considering a given unit $U(n):U(n-1)$ projective operator

$$\begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix}.$$

To this operator we assign a Δ pattern of two rows, corresponding to the shifts $[\Delta(\Gamma)]_n$ and $[\Delta(\gamma)]_{n-1}$. From the Δ pattern, we construct an "arrow pattern" and write out the $U(n):U(n-1)$ reduced Wigner coefficient by the following rules.

The Arrow-Pattern Rules

Rule 1: Write out two rows of dots, as shown:

$$\begin{array}{ll} \cdots & \cdots \; n \text{ dots} \\ & \cdots \\ \cdots & \cdot\cdot \; n-1 \text{ dots.} \end{array}$$

Rule 2: Draw arrows between dots as follows: Select a dot i in row n and a dot j in row $n-1$. If $\Delta_{in}(\Gamma) > \Delta_{jn-1}(\gamma)$, draw $\Delta_{in}(\Gamma) - \Delta_{jn-1}(\gamma)$ arrows from dot i to dot j; if $\Delta_{jn-1}(\gamma) > \Delta_{in}(\Gamma)$, draw the arrows from dot j to dot i. Carry out this procedure for all dots in rows n and $n-1$. This yields a *numerator arrow pattern* with arrows going *between* rows.

Carry out this procedure for dots within row n and dots within row $n-1$. This yields a *denominator arrow pattern* with arrows going *within* rows.

Rule 3: In the arrow patterns, assign the partial hook p_{in} to dot i, $i = 1, 2, \cdots, n$, in row n and p_{jn-1} to dot j, $j = 1, 2, \cdots, n-1$, in row $n-1$. ($p_{ij} \equiv m_{ij} + j - i$.)

Rule 4: In general, there will be several arrows going between two dots in the arrow patterns. Assign to the first arrow the factor

$$p(\text{tail}) - p(\text{head}) + e(\text{tail}),$$

to the second arrow, the factor

$$p(\text{tail}) - p(\text{head}) + e(\text{tail}) + 1,$$

etc., until all arrows going between the same two dots have been counted:

$$e(\text{tail}) \equiv 1, \text{ if tail of arrow on row } n-1,$$
$$\equiv 0, \text{ if tail of arrow on row } n.$$

Rule 5: Write out the products

N^2 = product of all factors for numerator arrow pattern,
D^2 = product of all factors for denominator arrow pattern.

The net effect of these rules is to make the associations

$$\begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix} \leftrightarrow \Delta \text{ pattern} \leftrightarrow \begin{matrix} \text{arrow} \\ \text{pattern} \end{matrix} \leftrightarrow \begin{matrix} \text{algebraic} \\ \text{factor} \end{matrix} \equiv \left| \frac{N}{D} \right|.$$

The arrow-pattern rules clearly yield the same result if we effect an integral shift $\Delta_{in}(\Gamma) \to \Delta_{in}(\Gamma) + \lambda$, $i = 1, 2, \cdots, n$, $\Delta_{in-1}(\gamma) \to \Delta_{in-1}(\gamma) + \lambda$, $i = 1, 2, \cdots, n-1$. Thus, the rules apply to Δ patterns which contain negative integers. In particular, all operators of the form $[\dot{0}_k \quad -\dot{1}_{n-k}]$ are obtained from the rules above.

In the present work, we later need the $[1 \quad \dot{0}]$ and $[\dot{0} \quad -1]$ operators for which the following special notations are introduced:

$$\begin{bmatrix} \tau \\ [1 \quad \dot{0}] \\ \rho \end{bmatrix} \text{ and } \begin{bmatrix} \bar{\tau} \\ [\dot{0} \quad -1] \\ \bar{\rho} \end{bmatrix}, \quad \rho, \tau = 1, 2, \cdots, n, \tag{2.28}$$

where $\begin{pmatrix} [1 \quad \dot{0}] \\ \rho \end{pmatrix}$ denotes the (uniquely determined) operator pattern which has Δ pattern given by $\Delta_n(\rho) \equiv [0 \cdots 0 \; 1 \; 0 \cdots 0]$, where 1 stands in position ρ; similarly, $\begin{pmatrix} [\dot{0} \quad -1] \\ \bar{\rho} \end{pmatrix}$ denotes the operator pattern which has Δ pattern given by $-\Delta_n(\rho)$. The τ specifies the upper operator pattern. Let us note explicitly the phases of the projective operators (2.28):

$$\text{sign of } \begin{bmatrix} \tau \\ [1 \quad \dot{0}] \\ \rho \end{bmatrix} = S(\rho - \tau), \tag{2.29}$$

$$\text{sign of } \begin{bmatrix} \bar{\tau} \\ [\dot{0} \quad -1] \\ \bar{\rho} \end{bmatrix} = (-1)^{\rho-\tau} S(\rho - \tau), \tag{2.30}$$

where $S(\rho - \tau)$ is $+1$ for $\rho \geq \tau$ and -1 for $\rho < \tau$. The complete set of Wigner coefficients for $[1 \quad \dot{0}]$ and $[\dot{0} \quad -1]$ can now be set down.

We shall make use of the pattern calculus rules to *define* a "pattern calculus factor" for *arbitrary* Δ patterns for two rows.

E. The Factorization Lemma

The use of boson variables as a convenient realization for the carrier space of $U(n)$ is very familiar.[20] In order to realize all IR's of $U(n)$, it is necessary to assume n kinematically independent copies of an n-state boson variable; that is, one takes the variables a_j^i, $i,j = 1, 2, \cdots, n$, with the commutators

$$[\bar{a}_j^i, a_{j'}^{i'}] = \delta_i^{i'}\delta_j^{j'}, \tag{2.31}$$

all other commutators defined to be zero. The generators E_{ij} of the group $U(n)$ are defined by the mapping

$$E_{ij} \to \mathcal{E}_{ij} \equiv \sum_{k=1}^{n} a_i^k \bar{a}_j^k. \tag{2.32}$$

It is clear, however, that these boson variables admit also of a second, isomorphic, $U(n)$ group generated by the operator mapping

$$E^{ij} \to \mathcal{E}^{ij} \equiv \sum_{k=1}^{n} a_k^i \bar{a}_k^j, \tag{2.33}$$

and that, moreover, the two sets of operators $\{E_{ij}\}$ and $\{E^{ij}\}$ commute. Thus, this boson realization involves the direct product group $U_n \times U_n$.

In fact, one sees at once that this boson realization $\{a_j^i\}$ really involves the group U_{n^2} and all totally symmetric IR's thereof. This defines a canonical imbedding of $U(n)$ in the sequence of groups $U_{n^2} \supset U_n \times U_n \supset U_n$, in which, moreover, the IR labels of the two $U(n)$ groups in $U_n \times U_n$ *coincide* (we denote this by $U_n \star U_n$). This structure is precisely the analog to that exhibited by the tensor operators of $U(n)$, and Ref. 1 discusses this canonical embedding in detail, proving the factorization lemma to which we now turn.

Let

$$\left|\begin{pmatrix}(M')\\ [M]\\ (M)\end{pmatrix}\right\rangle \tag{2.34}$$

denote a normalized basis vector in $U_n \star U_n$. In this notation, the first $U(n)$ refers to the $U(n)$ group with generators E_{ij}, the second to the $U(n)$ group with generators E^{ij}. [These two $U(n)$ groups are isomorphic but distinct (and commuting); the placement of the indices is merely a reminder as to which group is which ("upper" vs "lower")—there is no implication as to metric in this placement of indices. The star signifies that the Casimir invariants of the IR's of these two groups coincide.] Hence, both

$$(M) = \begin{pmatrix}[M]\\ (M)\end{pmatrix} \quad \text{and} \quad (M') = \begin{pmatrix}(M')\\ [M]\end{pmatrix} \tag{2.35}$$

in Eq. (2.34) are Gel'fand patterns, the second one being inverted. The basis vector (2.34) may also be written in the form

$$\left|\begin{pmatrix}(M')\\ [M]\\ (M)\end{pmatrix}\right\rangle = \mathcal{M}([M])^{-\frac{1}{2}} \; B\begin{pmatrix}(M')\\ [M]\\ (M)\end{pmatrix}(A)\,|0\rangle, \tag{2.36}$$

where

$$B\begin{pmatrix}(M')\\ [M]\\ (M)\end{pmatrix}(A) \tag{2.37}$$

is an operator-valued polynomial[21] in the set of boson creation operators $\{a_j^i\}$, the symbol $|0\rangle$ denotes the vacuum ket, and $\mathcal{M}([M])$ is the measure of the highest weight tableau associated with $[M]$:

$$\mathcal{M}([M]) \equiv \frac{\prod_{i=1}^{n}(M_{in} + n - i)!}{\prod_{i<j=1}^{n}(M_{in} - M_{jn} + j - i)}. \tag{2.38}$$

The introduction of $\mathcal{M}^{-\frac{1}{2}}$ into Eq. (2.36) defines the manner in which the boson operators (2.37) are normalized: For example, if $(M')_n$ and $(M)_n$ are maximal, i.e.,

$$M'_{ij} = M_{in}, \quad M_{ij} = M_{in}, \text{ all } i,j, \tag{2.39a}$$

then

$$B\begin{pmatrix}\max\\ [M]_n\\ \max\end{pmatrix}(A) = \prod_{k=1}^{n}(a_{12\cdots k}^{12\cdots k})^{M_{kn}-M_{k+1n}}, \tag{2.39b}$$

where $a_{12\cdots k}^{12\cdots k}$ is the determinant formed from the k bosons a_j^i, $i,j \leq k$.

The boson operator (2.37) is clearly a tensor operator in either its lower or upper Gel'fand pattern with respect to transformations in the respective $U(n)$ subgroup of $U_n \star U_n$. As such, it must be bilinear in the canonical Wigner operators which are defined, respectively, on the two $U(n)$ groups. *The factorization lemma asserts that the precise form of this bilinear*

relation is

$$B\begin{pmatrix}(M')_{n-1}\\ [M]_n\\ (M)_{n-1}\end{pmatrix}(A) = \mathcal{M}^{\frac{1}{2}}\sum_{(\Gamma)_{n-1}}\left\langle\begin{matrix}(\Gamma)_{n-1}\\ [M]_n\\ (M)_{n-1}\end{matrix}\right\rangle_{\ell}\left\langle\begin{matrix}(\Gamma)_{n-1}\\ [M]_n\\ (M')_{n-1}\end{matrix}\right\rangle_{u}\mathcal{M}^{-\frac{1}{2}}, \quad (2.40)$$

where $\mathcal{M}$ is an invariant operator of $U_n \star U_n$ which has eigenvalue equal to the measure $\mathcal{M}([m])$ for an arbitrary vector with labels $[m]$. The indices ℓ and u designate the fact that the Wigner operators act, respectively, on the lower and upper Gel'fand patterns of an arbitrary vector of $U_n \star U_n$:

$$\left|\begin{pmatrix}(\mu)_{n-1}\\ [m]_n\\ (m)_{n-1}\end{pmatrix}\right\rangle = \left|\begin{matrix}\begin{pmatrix}(\mu)_{n-1}\\ [m]_n\end{pmatrix}\\ \cdots\cdots\cdots\\ \begin{pmatrix}[m]_n\\ (m)_{n-1}\end{pmatrix}\end{matrix}\right\rangle. \quad (2.41)$$

Note that when we apply the *individual* Wigner operators in Eq. (2.40) to an arbitrary basis vector (2.34), we should consider the common labels $[m]_n$ to be two identical sets of labels as indicated in Eq. (2.41). Note also that the two Wigner operators in Eq. (2.40) commute since they act in different spaces and that the application of a *single* Wigner operator carries a vector *outside* of $U_n \star U_n$, in the general case. [More precisely, these properties serve to *define* the meaning of the product of operators in Eq. (2.40).]

The work in Sec. 5 makes use of the following important special case of Eq. (2.40):

$$a_i^j = \mathcal{M}^{\frac{1}{2}}\left(\sum_{\tau=1}^{n}\left\langle\begin{matrix}\tau\\ [1\ \dot{0}]\\ i\end{matrix}\right\rangle_{\ell}\left\langle\begin{matrix}\tau\\ [1\ \dot{0}]\\ j\end{matrix}\right\rangle_{u}\right)\mathcal{M}^{-\frac{1}{2}}. \quad (2.42)$$

(This special case accounts for the term "boson factorization.")

The crucial importance of the factorization lemma in our work may not be clear from this brief summary. This importance rests primarily on the fact that the factorization lemma allows one to define *a general operator* from knowledge of *particular* matrix elements.

F. Coupling of Wigner Operators

It is well known in the Racah–Wigner angular-momentum calculus how to couple two irreducible tensor operators to form a third—one simply uses the coupling coefficients of the group. Here, we follow precisely this procedure, except that we are interested in coupling unit tensor operators:

$$\sum_{(M')(M)}\left\langle\begin{pmatrix}[M]+[\Delta(\Lambda)]\\ (M'')\end{pmatrix}\right|\left\langle\begin{matrix}(\Lambda)\\ [M']\\ (M')\end{matrix}\right\rangle\left|\begin{pmatrix}[M]\\ (M)\end{pmatrix}\right\rangle \times\left\langle\begin{matrix}(\Gamma')\\ [M']\\ (M')\end{matrix}\right\rangle\left\langle\begin{matrix}(\Gamma)\\ [M]\\ (M)\end{matrix}\right\rangle = \sum_{(\Gamma'')}\left\{\begin{pmatrix}[M]+[\Delta(\Lambda)]\\ (\Gamma'')\end{pmatrix}\begin{pmatrix}(\Lambda)\\ [M']\\ (\Gamma')\end{pmatrix}\begin{pmatrix}[M]\\ (\Gamma)\end{pmatrix}\right\} \times\left\langle\begin{matrix}(\Gamma'')\\ [M]+[\Delta(\Lambda)]\\ (M'')\end{matrix}\right\rangle. \quad (2.43)$$

The complicated appearing equation is the statement of a very simple fact. First, consider the left-hand side. When we examine the transformation properties of this sum of Wigner operators, we find that the object is an irreducible tensor operator with IR labels $[M]+[\Delta(\Lambda)]$:

$$T\begin{pmatrix}[M]+[\Delta(\Lambda)]\\ (M'')\end{pmatrix}.$$

But all such irreducible tensor operators are expressible as linear combinations (with invariant coefficients) of the Wigner operators appearing on the right-hand side of Eq. (2.43). The invariant coefficients are denoted by the notation

$$\left\{\begin{pmatrix}[M]+[\Delta(\Lambda)]\\ (\Gamma'')\end{pmatrix}\begin{pmatrix}(\Lambda)\\ [M']\\ (\Gamma')\end{pmatrix}\begin{pmatrix}[M]\\ (\Gamma)\end{pmatrix}\right\}, \quad (2.44)$$

which we now explain. The particular arrangement of operator patterns in this $U(n)$ invariant is not contrived arbitrarily, but rather to portray certain features that these invariants share with Wigner coefficients of the same labels—these properties will emerge later. For the moment, we justify the notation by noting that these invariant coefficients must be labeled by the free operator patterns appearing on the left-hand side as well as the summation operator pattern of the right-hand side. We have taken the liberty of arranging the operator patterns in the right to left order: initial, intermediate, final. The pattern (Λ) is assigned its position in accordance with its position in the Wigner coefficient and its role of relating the initial IR labels to the final ones.

The $U(n)$ invariants (2.44) are called (left) *Racah invariants* because, as will be seen, their eigenvalues on arbitrary state vectors are the Racah coefficients of the group. The first significant property of a Racah invariant is a consequence of the requirement that the Δ pattern of each side of Eq. (2.43) be the same (the Δ pattern of a product of Wigner operators is clearly the sum of individual Δ patterns). We arrive at the following rule. The Racah invariant

$$\left\{\begin{pmatrix}[M'']_n\\(\Gamma'')_{n-1}\end{pmatrix}\begin{pmatrix}(\Lambda)_{n-1}\\[M']_n\\(\Gamma')_{n-1}\end{pmatrix}\begin{pmatrix}[M]_n\\(\Gamma)_{n-1}\end{pmatrix}\right\} \tag{2.45}$$

is defined to be zero unless:

(i) All operator patterns are lexical (satisfy all betweenness conditions);

(ii) $[M'']_n = [M]_n + [\Delta(\Lambda)]_n$;

(iii) $[\Delta(\Gamma'')]_n = [\Delta(\Gamma')]_n + [\Delta(\Gamma)]_n$.

These conditions should be compared with the previous set of conditions on the Wigner coefficients. We can make no restriction for Racah invariants comparable to the previous condition (iii) of Eq. (2.16) because we have demonstrated no subgroup properties for operator patterns. [An interesting consequence of these properties is illustrated, for example, by the following Racah invariant from $U(3)$:

$$\left\{\begin{pmatrix}2&1&0\\&2&0\\&&1\end{pmatrix}\begin{pmatrix}&&&1\\&1&&0\\1&&0&0\\&0&&0\\&&0\end{pmatrix}\begin{pmatrix}1&1&0\\&1&1\\&&1\end{pmatrix}\right\}.$$

The Wigner coefficient having these same labels,

$$\left\langle\begin{pmatrix}2&1&0\\&2&0\\&&1\end{pmatrix}\middle|\left\langle\begin{pmatrix}&&&1\\&1&&0\\1&&0&0\\&0&&0\\&&0\end{pmatrix}\middle|\begin{pmatrix}1&1&0\\&1&1\\&&1\end{pmatrix}\right\rangle\right\rangle,$$

is automatically zero because we cannot obtain $\langle 2\ \ 0\rangle$ by coupling $\langle 0\ \ 0\rangle$ with $\langle 1\ \ 1\rangle$. There is, however, no reason for the Racah invariant to be zero.] Despite this dissimilarity in detail, we nonetheless emphasize below the close structural similarity that exists between Racah invariants and Wigner coefficients.

Next, we turn to the derivation of some properties which the Racah invariants (2.45) must have in consequence of their definition as the coefficients in Eq. (2.43). The following expression is an easy consequence of orthogonality relation (2.14)[22,23]:

$$\left\{\begin{pmatrix}[M]+[\Delta(\Lambda)]\\(\Gamma'')\end{pmatrix}\begin{pmatrix}(\Lambda)\\[M']\\(\Gamma')\end{pmatrix}\begin{pmatrix}[M]\\(\Gamma)\end{pmatrix}\right\}$$
$$=\sum_{(M'')(M')(M)}\left\langle\begin{pmatrix}[M]+[\Delta(\Lambda)]\\(M'')\end{pmatrix}\middle|\left\langle\begin{matrix}(\Lambda)\\[M']\\(M')\end{matrix}\right\rangle\middle|\begin{pmatrix}[M]\\(M)\end{pmatrix}\right\rangle$$
$$\times\left\langle\begin{matrix}(\Gamma')\\[M']\\(M')\end{matrix}\right\rangle\left\langle\begin{matrix}(\Gamma)\\[M]\\(M)\end{matrix}\right\rangle\left\langle\begin{matrix}(\Gamma'')\\[M]+[\Delta(\Lambda)]\\(M'')\end{matrix}\right\rangle^{\dagger}. \tag{2.46}$$

Equation (2.46) is the explicit expression of the (left) Racah invariants in terms of Wigner operators and Wigner coefficients.

Because the matrix elements of Wigner operators can be chosen real, the Racah invariants can be considered to be *Hermitian invariants*. This result, combined with Eq. (2.46) and the orthonormality relations (2.14) and (2.15), leads to the orthonormality relations for (left) Racah invariants:

$$\sum_{(\Gamma')(\Gamma)}\left\{\begin{pmatrix}[M]+[\Delta(\Lambda)]\\(\Gamma'')\end{pmatrix}\begin{pmatrix}(\Lambda)\\[M']\\(\Gamma')\end{pmatrix}\begin{pmatrix}[M]\\(\Gamma)\end{pmatrix}\right\}$$
$$\times\left\{\begin{pmatrix}[M]+[\Delta(\Lambda')]\\(\Gamma''')\end{pmatrix}\begin{pmatrix}(\Lambda')\\[M']\\(\Gamma')\end{pmatrix}\begin{pmatrix}[M]\\(\Gamma)\end{pmatrix}\right\}$$
$$=\delta_{(\Lambda)(\Lambda')}\delta_{(\Gamma'')(\Gamma''')}I_{(\Gamma'')}, \tag{2.47}$$

$$\sum_{(\Gamma'')(\Lambda'')}\left\{\begin{pmatrix}[M]+[\Delta(\Lambda'')]\\(\Gamma'')\end{pmatrix}\begin{pmatrix}(\Lambda'')\\[M']\\(\Gamma')\end{pmatrix}\begin{pmatrix}[M]\\(\Gamma)\end{pmatrix}\right\}$$
$$\times\left\{\begin{pmatrix}[M]+[\Delta(\Lambda'')]\\(\Gamma'')\end{pmatrix}\begin{pmatrix}(\Lambda'')\\[M']\\(\Lambda')\end{pmatrix}\begin{pmatrix}[M]\\(\Lambda)\end{pmatrix}\right\}$$
$$=\delta_{(\Gamma')(\Lambda')}\delta_{(\Gamma)(\Lambda)}I_{(\Gamma)(\Gamma')}, \tag{2.48}$$

where $I_{(\Gamma'')}$ is the function introduced in Eq. (2.14); $I_{(\Gamma)(\Gamma')}$ is a function which has value zero on the null space of the product

$$\left\langle\begin{matrix}(\Gamma)\\[M]\\.\end{matrix}\right\rangle^{\dagger}\left\langle\begin{matrix}(\Gamma')\\[M']\\.\end{matrix}\right\rangle^{\dagger},$$

and, otherwise, it has value one.

The *coupling law* for Wigner operators is now obtained by using the orthonormality relation (2.47) to move the Racah invariant to the left-hand side in Eq. (2.43). The result is

$$\delta_{(\Lambda')(\Lambda)}\left\langle \begin{matrix} (\Gamma'') \\ [M]+[\Delta(\Lambda)] \\ (M'') \end{matrix} \right\rangle = \sum_{\substack{(M')(M) \\ (\Gamma')(\Gamma)}} \left\langle \begin{pmatrix} [M]+[\Delta(\Lambda)] \\ (M'') \end{pmatrix} \middle| \left\langle \begin{matrix} (\Lambda) \\ [M'] \\ (M') \end{matrix} \right\rangle \middle| \begin{pmatrix} [M] \\ (M) \end{pmatrix} \right\rangle \times \left\{ \begin{pmatrix} [M]+[\Delta(\Lambda')] \\ (\Gamma'') \end{pmatrix} \begin{pmatrix} (\Lambda') \\ [M'] \\ (\Gamma') \end{pmatrix} \begin{pmatrix} [M] \\ (\Gamma) \end{pmatrix} \right\} \times \left\langle \begin{matrix} (\Gamma') \\ [M'] \\ (M') \end{matrix} \right\rangle \left\langle \begin{matrix} (\Gamma) \\ [M] \\ (M) \end{matrix} \right\rangle. \tag{2.49}$$

This form is very significant. It exhibits clearly the fact that Racah invariants play the same role with respect to operator patterns as do Wigner coefficients with respect to Gel'fand patterns. *Racah invariants are the coupling coefficients for operator patterns* (more precisely, the objects carrying these patterns). *To form a new Wigner operator from a given pair, we Wigner-couple its Gel'fand patterns and Racah-couple its operator patterns.* This important property is symbolized by writing

$$\left\langle \begin{matrix} \cdot \\ [M'] \\ \cdot \end{matrix} \right\rangle \begin{matrix} \textcircled{R} \\ \\ \textcircled{W} \end{matrix} \left\langle \begin{matrix} \cdot \\ [M] \\ \cdot \end{matrix} \right\rangle = \left\langle \begin{matrix} \cdot \\ [M''] \\ \cdot \end{matrix} \right\rangle. \tag{2.50}$$

An important special case results for $[M'] = [1 \quad \dot{0}]$:

$$\left\langle \begin{matrix} \cdot \\ [1 \quad \dot{0}] \\ \cdot \end{matrix} \right\rangle \begin{matrix} \textcircled{R} \\ \\ \textcircled{W} \end{matrix} \left\langle \begin{matrix} \cdot \\ [M] \\ \cdot \end{matrix} \right\rangle = \left\langle \begin{matrix} \cdot \\ [M]+\Delta_n(\rho) \\ \cdot \end{matrix} \right\rangle. \tag{2.51}$$

In this coupling, the fundamental Wigner operator and the fundamental Wigner coefficients (the lower-pattern coupling) are known explicitly. The upper-pattern coupling is effected by the *fundamental Racah invariants* (those having $[M'] = [1 \quad \dot{0}]$). We thus see that knowledge of the fundamental Racah invariants is equivalent to a complete solution to the problem—*all* Wigner operators could then be constructed from Eq. (2.51) by recursion. This signifies that in a very definite sense the fundamental Racah invariants possess structural properties which "explain" the origin of operator patterns.

3. COUPLING OF PROJECTIVE OPERATORS

Almost every equation in the previous discussion of the coupling of Wigner operators implies an analogous equation in terms of the unit $U(n):U(n-1)$ projective operators. The derivations of the relations to follow are completely straightforward, although tedious, to be sure. Let us simply state the basic result:

$$\delta_{(\Lambda')_{n-1}(\Lambda)_{n-1}}\begin{bmatrix} (\Gamma'')_{n-1} \\ [M]_n+[\Delta(\Lambda)]_n \\ (\gamma'')_{n-1} \end{bmatrix} = \sum_{\substack{(\gamma)_{n-1}(\gamma')_{n-1} \\ (\Gamma)_{n-1}(\Gamma')_{n-1}}} \left[\begin{pmatrix} [M]_n+[\Delta(\Lambda)]_n \\ (\gamma'')_{n-1} \end{pmatrix} \begin{pmatrix} (\Lambda)_{n-1} \\ [M']_n \\ (\gamma')_{n-1} \end{pmatrix} \begin{pmatrix} [M]_n \\ (\gamma)_{n-1} \end{pmatrix} \right] \times \left\{ \begin{pmatrix} [M]_n+[\Delta(\Lambda')]_n \\ (\Gamma'')_{n-1} \end{pmatrix} \begin{pmatrix} (\Lambda')_{n-1} \\ [M']_n \\ (\Gamma')_{n-1} \end{pmatrix} \begin{pmatrix} [M]_n \\ (\Gamma)_{n-1} \end{pmatrix} \right\} \times \begin{bmatrix} (\Gamma')_{n-1} \\ [M']_n \\ (\gamma')_{n-1} \end{bmatrix} \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix}, \tag{3.1}$$

where we have introduced a new object—called a *square-bracket invariant* (in analogy to the curly bracket, or Racah, invariant):

$$\left[\begin{pmatrix} [M]_n+[\Delta(\Lambda)]_n \\ (\gamma'')_{n-1} \end{pmatrix} \begin{pmatrix} (\Lambda)_{n-1} \\ [M']_n \\ (\gamma')_{n-1} \end{pmatrix} \begin{pmatrix} [M]_n \\ (\gamma)_{n-1} \end{pmatrix} \right] = \sum_{(\Lambda')_{n-2}} \left\langle \begin{pmatrix} [M]_n+[\Delta(\Lambda)]_n \\ [\gamma]_{n-1}+[\Delta(\Lambda')]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Lambda)_{n-1} \\ [M']_n \\ (\Lambda')_{n-1} \end{bmatrix} \middle| \begin{pmatrix} [M]_n \\ [\gamma]_{n-1} \end{pmatrix} \right\rangle \times \left\{ \begin{pmatrix} [\gamma'']_{n-1} \\ (\gamma'')_{n-2} \end{pmatrix} \begin{pmatrix} (\Lambda')_{n-2} \\ [\gamma']_{n-1} \\ (\gamma')_{n-2} \end{pmatrix} \begin{pmatrix} [\gamma]_{n-1} \\ (\gamma)_{n-2} \end{pmatrix} \right\}, \tag{3.2}$$

in which

$$(\Lambda')_{n-1} = \begin{pmatrix} [\gamma']_{n-1} \\ (\Lambda')_{n-2} \end{pmatrix}. \tag{3.3}$$

The first factor on the right-hand side of definition (3.2) is a $U(n):U(n-1)$ *reduced Wigner coefficient*; the second factor a $U(n-1)$ Racah invariant—its eigenvalue depends only on the labels $[m]_{n-1}$. Thus, the square-bracket invariant, denoted $[\cdots]$, is a $U(n-1)$ invariant. [Note that, for $n=2$, projective operators become Wigner operators, the square-bracket invariant becomes a Wigner *coefficient*, and Eq. (3.1) reduces (properly) to the coupling law for Wigner operators.]

The square-bracket invariants satisfy orthogonality relations of exactly *the same form (2.47) and (2.48) as the Racah invariants*—simply replace the curly brackets by square ones. This result is a direct consequence of the

definition (3.2) and the orthogonality relations of reduced Wigner coefficients and the $U(n-1)$ Racah invariants. There is, however, one very significant structural property which, unlike the Racah invariants, the square-bracket invariants possess: *They retain a remnant of a subgroup reduction condition:* Namely, the square-bracket invariant

$$\left[\begin{pmatrix}[M'']_n\\(\gamma'')_{n-1}\end{pmatrix}\begin{pmatrix}(\Lambda)_{n-1}\\[M']_n\\(\gamma')_{n-1}\end{pmatrix}\begin{pmatrix}[M]_n\\(\gamma)_{n-1}\end{pmatrix}\right] \tag{3.4}$$

is the zero operator unless:

(i) All operator patterns are lexical;

(ii) the following conditions between labels in rows n *and* $n-1$ hold:

$$[M'']_n = [M]_n + [\Delta(\Lambda)]_n,$$

$$[\gamma'']_{n-1} = [\gamma]_{n-1} + \Delta\begin{pmatrix}[\gamma']_{n-1}\\(\Lambda')_{n-2}\end{pmatrix}$$

for some lexical operator pattern $(\Lambda')_{n-2}$;

(iii) the following condition on the deltas of the operator patterns holds:

$$[\Delta(\gamma'')]_{n-1} = [\Delta(\gamma')]_{n-1} + [\Delta(\gamma)]_{n-1}.$$

These relations should be compared with the conditions on the Racah invariant (2.45). The additional constraint (ii), above, is a direct consequence of the fact that the labels in row $n-1$ of a lower operator pattern of a unit $U(n):U(n-1)$ projective operator have subgroup reduction significance.

Let us now return to the basic coupling law (3.1) in order to interpret the implied structural features. The essential fact is that we couple two projective operators

$$\begin{bmatrix}(\Gamma')\\[M']\\(\gamma')\end{bmatrix}\begin{bmatrix}(\Gamma)\\[M]\\(\gamma)\end{bmatrix},$$

to produce a new projective operator

$$\begin{bmatrix}(\Gamma'')\\[M]+[\Delta(\Lambda)]\\(\gamma'')\end{bmatrix}$$

or zero. The upper operator patterns, (Γ') and (Γ), are coupled by a Racah invariant: We denote this coupling by $\{R\}$. The lower operator patterns, (γ') and (γ), are coupled by the square-bracket invariant: we denote this by $[R]$. Thus, we may symbolically interpret the basic coupling law for projective operators by the structurally simple (but highly implicit) equation

$$\begin{bmatrix}\cdot\\[M']\\\cdot\end{bmatrix}\{R\}[R]\begin{bmatrix}\cdot\\[M]\\\cdot\end{bmatrix} = \begin{bmatrix}(\Gamma'')\\[M+\Delta]\\(\gamma'')\end{bmatrix}. \tag{3.5}$$

(Here the dots imply operator patterns summed over; this symbolic equation violates index balance because of the suppression of variables in the two coupling operations.)

Using the orthonormality relations for Racah invariants and square-bracket invariants, we can obtain directly from Eq. (3.1) a variety of relations corresponding to the many equivalent forms for the Racah invariants.

One can hardly fail to notice the striking similarity between Eqs. (3.2) and (2.22). In order to demonstrate this, we first convert Eq. (3.2) from an operator statement to a matrix element relation, by specifying explicitly the appropriate state vector on which the operators act. Consider a maximal basis vector in the carrier space of the $U(n):U(n-1)$ projective operators, i.e., one in which we choose $m_{in-1} = m_{in}$, $i = 1, 2, \cdots, n-1$. On such a basis vector, the eigenvalue of a square-bracket invariant [which depends only on the $U(n-1)$ labels] now depends on the labels $[m_{1n}\, m_{2n} \cdots m_{n-1n}]$; the Racah coefficient depends on $[m_{1n}\, m_{2n} \cdots m_{nn}]$, as usual. These two sets of coefficients satisfy orthogonality relations which are identical in formal structure.

It is natural to ask now if there is any deeper relation between these two very similar sets of coefficients. Does the fact that the square-bracket invariants involve one less label (here m_{nn}) have anything to do with the extra (subgroup-type) constraint?

We *conjecture* that there is a deeper relationship; that, in fact, the following relation holds (the eigenvalue of a Racah or square-bracket invariant is designated by writing the IR labels of an arbitrary state vector on the right-hand side of the invariant):

$$\lim_{m_{nn}\to-\infty}\left\{\begin{pmatrix}[M'']_n\\(\Gamma'')_{n-1}\end{pmatrix}\begin{pmatrix}(\Lambda)_{n-1}\\[M']_n\\(\Gamma')_{n-1}\end{pmatrix}\begin{pmatrix}[M]_n\\(\Gamma)_{n-1}\end{pmatrix}\right\}(m_{1n}\, m_{2n} \cdots m_{nn})$$

$$= \left[\begin{pmatrix}[M'']_n\\(\Gamma'')_{n-1}\end{pmatrix}\begin{pmatrix}(\Lambda)_{n-1}\\[M']_n\\(\Gamma')_{n-1}\end{pmatrix}\begin{pmatrix}[M]_n\\(\Gamma)_{n-1}\end{pmatrix}\right](m_{1n}\, m_{2n} \cdots m_{n-1n}). \tag{3.6}$$

This property can be verified to hold in all instances in which the coefficients are unique; we demonstrate below that it holds for all adjoint coefficients. *It is not yet known to be valid in general.* Our purpose in noting it here is simply to *support* the thesis that operator patterns are related to a definite structure of the calculus of projective operators. Equation (3.6), when combined with Eq. (3.2), takes the form of *a reduction law for operator patterns* in complete analogy to the subgroup reduction law (2.22). Indeed, we can now take successive limits of Eq. (3.6): $m_{n-1n} \to -\infty$, then $m_{n-2n} \to -\infty, \cdots$, and finally, $m_{2n} \to -\infty$. Each time a limit is taken, we gain, in consequence of Eq. (3.2), a subgroup type restriction on the allowed operator patterns, until finally, when the last limit $m_{2n} \to -\infty$ is taken, the Racah coefficient has been reduced to a Wigner coefficient of the same labels.

We repeat that this relationship has not been demonstrated to be valid in general.

To summarize, we have in this section developed the algebra of the unit $U(n):U(n-1)$ projective operators. (For $n = 2$ the algebra is just that of the Wigner operators themselves.) The basic structure of $U(n)$ Wigner operators has itself been built up from the unit $U(n):U(n-1)$, $U(n-1):U(n-2), \cdots$, $U(2):U(1)$ projective operator algebras. In this sense, *it is the algebra of projective operators that is the fundamental structure.* We will return to develop this algebra still further in Sec. 6.

4. GENERAL FORM OF THE ADJOINT WIGNER OPERATORS

The preceding sections have surveyed the general structure of the calculus of Wigner operators and projective operators. These results incorporate a unique content, from which explicit calculations can proceed, only when the structural principle underlying the origin of operator patterns can be stated definitively. We can acquire considerable insight into the significance of operator patterns by examining particular sets of Wigner operators for which we can resolve the multiplicity problem explicitly and canonically. A set of interest for physical applications which can be dealt with exhaustively is the set of all adjoint operators labeled by

$$[1 \quad \dot{0} \quad -1] = [1 \quad 0 \quad 0 \quad \cdots \quad 0 \quad -1].$$

In the next section, we give a direct construction of the $n-1$ Wigner operators which have the Δ pattern $[\dot{0}]$. However, the adjoint Wigner operators can also be obtained by coupling $\langle 1 \quad \dot{0}\rangle$ and $\langle \dot{0} \quad -1\rangle$ in the manner of Eq. (2.51). Comparing the direct construction with the general form of this coupling allows us to identify the Racah invariants of the coupling. These Racah invariants are then used to establish additional structural features of the solution.

It is convenient at this point to write out the coupling formula in detail, in the present context, after introducing some abbreviated notation.

The symbol

$$\begin{pmatrix} [1 \quad \dot{0} \quad -1] \\ (i,j) \end{pmatrix}, \quad i,j = 1, 2, \cdots, n, \tag{4.1}$$

designates a Gel'fand pattern which has weight given by $\Delta_n(i) - \Delta_n(j)$, where $\Delta_n(i)$ denotes the unit row vector of dimension n which has 1 in position i and 0's elsewhere. For $i \neq j$, the pattern (1) is extremal[2] and is thus uniquely determined from its weight; for $i = j$, the weight is $[\dot{0}]$, and there are $n-1$ distinct patterns having this weight. In this case, the pattern (1) (with $j = i = 1, 2, \cdots, n-1$) is *defined* to be the pattern with all 0's in rows 1 through i, the remaining rows being of the type $[1 \quad \dot{0} \quad -1]$. With these definitions, the notation (1) enumerates all $n^2 - 1$ patterns for $[1 \quad \dot{0} \quad -1]$ as we let the (i,j) indices run over the values $i \neq j = 1, 2, \cdots, n$; $i = j = 1, 2, \cdots, n-1$. We use the same notation for operator patterns, but replace the Roman indices $i, j, \cdots$ by Greek indices $\rho, \tau, \cdots$.

We next introduce the following abbreviations for the Wigner coefficients and Racah invariants which are relevant to the coupling of $\langle 1 \quad \dot{0}\rangle$ and $\langle \dot{0} \quad -1\rangle$:

$$\mathcal{O}_{ij} = \left\langle \begin{pmatrix} [1 \quad \dot{0} \quad -1] \\ (i,i) \end{pmatrix} \middle| \begin{pmatrix} 1 \\ [1 \quad \dot{0}] \\ j \end{pmatrix} \middle| \begin{pmatrix} [\dot{0} \quad -1] \\ \bar{j} \end{pmatrix} \right\rangle, \tag{4.2a}$$

$$\mathcal{O}_{n\bar{j}} = \langle(\dot{0})| \begin{pmatrix} n \\ [1 \quad \dot{0}] \\ j \end{pmatrix} \middle| \begin{pmatrix} [\dot{0} \quad -1] \\ \bar{j} \end{pmatrix} \rangle, \tag{4.2b}$$

$$R_{\rho\tau} = \left\{ \begin{pmatrix} [1 \quad \dot{0} \quad -1] \\ (\rho,\rho) \end{pmatrix} \begin{pmatrix} 1 \\ [1 \quad \dot{0}] \\ \tau \end{pmatrix} \begin{pmatrix} [\dot{0} \quad -1] \\ \bar{\tau} \end{pmatrix} \right\}, \tag{4.3a}$$

$$R_{n\tau} = \left\{ (\dot{0}) \begin{pmatrix} n \\ [1 \quad \dot{0}] \\ \tau \end{pmatrix} \begin{pmatrix} [\dot{0} \quad -1] \\ \bar{\tau} \end{pmatrix} \right\}. \tag{4.3b}$$

The following evaluations (from the pattern calculus[2]) are also required:

$$\left\langle \begin{pmatrix} [1 & \dot{0} & -1] \\ & (i,j) & \end{pmatrix} \middle| \left\langle \begin{matrix} & 1 & \\ [1 & & \dot{0}] \\ & i & \end{matrix} \right\rangle \middle| \begin{pmatrix} [\dot{0} & -1] \\ & j & \end{pmatrix} \right\rangle = 1, \quad i \neq j, \tag{4.4a}$$

$$\left\{ \begin{pmatrix} [1 & \dot{0} & -1] \\ & (\rho,\tau) & \end{pmatrix} \begin{pmatrix} & 1 & \\ [1 & & \dot{0}] \\ & \rho & \end{pmatrix} \begin{pmatrix} [\dot{0} & -1] \\ & \bar{\tau} & \end{pmatrix} \right\} = 1, \quad \rho \neq \tau. \tag{4.4b}$$

$$\begin{aligned} \mathcal{O}_{ij} &= 0, && j > i+1 \\ &= (-1)^{i-j}/[i(i+1)]^{\frac{1}{2}}, && j = 1, 2, \cdots, i, \\ &= [i/(i+1)]^{\frac{1}{2}}, && j = i+1, \end{aligned} \tag{4.4c}$$

for $i = 1, 2, \cdots, n-1$,

$$\mathcal{O}_{nj} = (-1)^{n-j}/\sqrt{n}, \tag{4.4d}$$

for $j = 1, 2, \cdots, n$.

Using the above notations and results, we obtain the following couplings of $\langle 1 \quad \dot{0} \rangle$ and $\langle \dot{0} \quad -1 \rangle$ from Eq. (2.49):

$$\left\langle \begin{matrix} & (\rho,\tau) & \\ [1 & \dot{0} & -1] \\ & (i,j) & \end{matrix} \right\rangle = \left\langle \begin{matrix} & \rho & \\ [1 & & \dot{0}] \\ & i & \end{matrix} \right\rangle \left\langle \begin{matrix} & \bar{\tau} & \\ [\dot{0} & & -1] \\ & \bar{\jmath} & \end{matrix} \right\rangle, \quad \rho \neq \tau, \quad i \neq j, \tag{4.5a}$$

$$\left\langle \begin{matrix} & (\rho,\tau) & \\ [1 & \dot{0} & -1] \\ & (i,i) & \end{matrix} \right\rangle = \sum_{j=1}^{n} \mathcal{O}_{ij} \left\langle \begin{matrix} & \rho & \\ [1 & & \dot{0}] \\ & j & \end{matrix} \right\rangle \left\langle \begin{matrix} & \bar{\tau} & \\ [\dot{0} & & -1 \\ & \bar{\jmath} & \end{matrix} \right\rangle, \quad \rho \neq \tau, \tag{4.5b}$$

$$\left\langle \begin{matrix} & (\rho,\rho) & \\ [1 & \dot{0} & -1] \\ & (i,j) & \end{matrix} \right\rangle = \sum_{\tau=1}^{n} R_{\rho\tau} \left\langle \begin{matrix} & \tau & \\ [1 & & \dot{0}] \\ & i & \end{matrix} \right\rangle \left\langle \begin{matrix} & \bar{\tau} & \\ [\dot{0} & & -1] \\ & \bar{\jmath} & \end{matrix} \right\rangle, \quad i \neq j, \tag{4.5c}$$

$$\left\langle \begin{matrix} & (\rho,\rho) & \\ [1 & \dot{0} & -1] \\ & (i,i) & \end{matrix} \right\rangle = \sum_{\tau,j=1}^{n} \mathcal{O}_{ij} R_{\rho\tau} \left\langle \begin{matrix} & \tau & \\ [1 & & \dot{0}] \\ & j & \end{matrix} \right\rangle \left\langle \begin{matrix} & \bar{\tau} & \\ [\dot{0} & & -1] \\ & \bar{\jmath} & \end{matrix} \right\rangle \tag{4.5d}$$

The Racah invariant $R_{n\tau}$ is already uniquely determined from

$$R_{n\tau} = \sum_{j=1}^{n} \mathcal{O}_{nj} \left\langle \begin{matrix} & \tau & \\ [1 & & \dot{0}] \\ & j & \end{matrix} \right\rangle \left\langle \begin{matrix} & \bar{\tau} & \\ [\dot{0} & & -1] \\ & \bar{\jmath} & \end{matrix} \right\rangle, \tag{4.6}$$

which is a special case of Eq. (2.46). This result can be written in another form by using the identity

$$\left\langle \begin{matrix} & \tau & \\ [1 & & \dot{0}] \\ & j & \end{matrix} \right\rangle^{\dagger} = (-1)^{\tau-j} D^{-\frac{1}{2}} \left\langle \begin{matrix} & \bar{\tau} & \\ [\dot{0} & & -1] \\ & \bar{\jmath} & \end{matrix} \right\rangle D^{\frac{1}{2}}, \tag{4.7}$$

where D is the dimension operator. This result can be proved by direct comparison of the known matrix elements of elementary Wigner operators. Equation (4.6) becomes

$$R_{n\tau} = \frac{(-1)^{n-\tau}}{\sqrt{n}} \sum_{j=1}^{n} \left\langle \begin{matrix} & \tau & \\ [1 & & \dot{0}] \\ & j & \end{matrix} \right\rangle D^{\frac{1}{2}} \left\langle \begin{matrix} & \tau & \\ [1 & & \dot{0}] \\ & j & \end{matrix} \right\rangle^{\dagger} D^{-\frac{1}{2}}. \tag{4.8}$$

Operating on the state vector $|(m)\rangle$, we obtain the following result (in consequence of the normalization of the fundamental Wigner coefficients):

$$R_{n\tau} |(m)\rangle = R_{n\tau}([m]) |(m)\rangle, \tag{4.9a}$$

where

$$\begin{aligned} R_{n\tau}([m]) &= \frac{(-1)^{n-\tau}}{\sqrt{n}} \left[\frac{D([m] - \Delta_n(\tau))}{D([m])} \right]^{\frac{1}{2}} \\ &= \frac{(-1)^{n-\tau}}{\sqrt{n}} \left[\prod_{\substack{s=1 \\ s \neq \tau}}^{n} \frac{(p_{sn} - p_{\tau n} + 1)}{(p_{sn} - p_{\tau n})} \right]^{\frac{1}{2}}. \end{aligned} \tag{4.9b}$$

There are additional equations resulting from Eq. (2.49) and corresponding to the coupling of $\langle 1 \quad \dot{0} \rangle$ and $\langle \dot{0} \quad -1 \rangle$ to zero. However, these equations are consequences of the fact that the Racah invariants are required to be orthogonal,

$$\sum_{\tau=1}^{n} R_{\rho\tau} R_{\rho'\tau} = 0, \tag{4.10a}$$

for $\rho \neq \rho' = 1, 2, \cdots, n$. We also require

$$\sum_{\tau=1}^{n} R_{\rho\tau}^2 = 1, \tag{4.10b}$$

whenever $R_{\rho\tau}([m]) \neq 0$ for all $\tau = 1, 2, \cdots, n$. Note, in particular, that the invariants $[R_{\rho 1} R_{\rho 2} \cdots R_{\rho n}]$, $\rho = 1, 2, \cdots, n-1$, comprise a row vector which is perpendicular to the known invariants $[R_{n1} R_{n2} \cdots R_{nn}]$.

Equations (4.5) give the general form of the set of adjoint Wigner operators. Since the Wigner coefficients $\mathcal{O}_{ij}$ and the elementary Wigner operators appearing in these equations are known, we see that the first two equations uniquely determine the adjoint Wigner operators having a Δ pattern of the form $\Delta_n(\rho) - \Delta_n(\tau)$, $\rho \neq \tau$, i.e., a delta which is a permutation of $[1 \quad 0 \quad \cdots \quad 0 \quad -1]$. The last two equations give the

form of the $n-1$ adjoint operators having delta $[\dot{0}]$, and their determination is equivalent to that of the fundamental Racah invariants. This determination is discussed in detail in the next section.

5. CANONICAL ADJOINT WIGNER OPERATORS

We begin with the definition of a "vector operator" with respect to $U(n)$. A vector operator V is defined to be a set of n^2 operators V_{ij} which transform under $\mathcal{O}_U$ in the same manner as the infinitesimal operators E_{ij}, the generators of the representation $\mathcal{O}_U$. Equivalently, the components V_{ij} satisfy the commutation relations

$$[E_{ij}, V_{kl}] = \delta_{jk}V_{il} - \delta_{il}V_{kj}. \tag{5.1}$$

A $U(n)$ vector operator is reducible into an invariant $\sum_k V_{kk}$ and an irreducible operator of n^2-1 components of the form

$$T\begin{pmatrix}[1 & \dot{0} & -1] \\ & (i,j) & \end{pmatrix}. \tag{5.2}$$

Stated differently: If V is a vector operator, then V is reducible into a multiple of $\langle\dot{0}\rangle$ plus a multiple of a $[1\ \ \dot{0}\ \ -1]$ irreducible tensor operator.

The following set of vector operators is of particular utility and interest for our development:

$$\begin{aligned} V_{ij}(0) &= \delta_{ij}, \\ V_{ij}(1) &= E_{ij}, \\ V_{ij}(2) &= \sum_{k=1}^{n} E_{ik}E_{kj}, \\ &\cdots \\ V_{ij}(q) &= \sum_{i_1,\cdots,i_{q-1}=1}^{n} E_{ii_1}E_{i_1i_2}\cdots E_{i_{q-1}j}, \\ &\cdots \end{aligned} \tag{5.3}$$

for $q = 2, 3, \cdots$. The index q refers to the degree of $V(q)$ in the generators. Observe that

$$V_{ij}^{\dagger}(q) = V_{ji}(q). \tag{5.4}$$

The scalar product of two vector operators $V(q)$ and $V(p)$ is defined to be

$$\sum_{i,j=1}^{n} V_{ij}(q)V_{ji}(p) = I_{q+p}, \tag{5.5}$$

where I_k is the Gel'fand form of the invariant operators[24] defined (for any set of generators) by Eq. (B1) of Appendix B for $k = 1, 2, \cdots$. We define $I_0 = n$.

A significant property of the n vector operators $V(q)$, $q = 0, 1, 2, \cdots, n-1$, is that they are linearly independent on *generic* states. Indeed, the Gram determinant is given explicitly by

$$\det\begin{bmatrix} I_0 & I_1 & \cdots & I_{n-1} \\ I_1 & I_2 & \cdots & I_n \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_{n-1} & I_n & \cdots & I_{2n-2} \end{bmatrix} |(m)\rangle$$

$$= \prod_{i<j=1}^{n} [(p_{in} - p_{jn})^2 - 1]\,|(m)\rangle. \tag{5.6}$$

A proof of this result is given in Appendix C.

Each operator $V(q)$, $q = 0, 1, 2, \cdots$, effects the change $\Delta = [\dot{0}]$ on arbitrary IR labels (since generators cause no shift in IR labels). Therefore, each of these vector operators reduces into $\langle\dot{0}\rangle$ and an adjoint tensor operator $T([1\ \ \dot{0}\ \ -1])$ *which belongs to the subspace of adjoint tensor* operators having $\Delta = [\dot{0}]$. Since $V(0)$ clearly reduces into $\langle\dot{0}\rangle$, it follows that the reduction of the remaining $n-1$ operators $V(q)$, $q = 1, 2, \cdots, n-1$, must yield $n-1$ linearly independent irreducible tensor operators having IR labels $[1\ \ \dot{0}\ \ -1]$ and $\Delta = [\dot{0}]$. The inclusion of $V_{ij}(0) = \delta_{ij}$ in the set is important. It assures that each vector $\{V_{ij}\}$ perpendicular to $\{V_{ij}(0)\}$ will have $\sum_i V_{ii} = 0$. Thus, every vector $\{V_{ij}\}$ perpendicular to $\{V_{ij}(0)\}$ is equivalent to a tensor operator $T([1\ \ \dot{0}\ \ -1])$. We can therefore obtain a set of $n-1$ adjoint Wigner operators with $\Delta = [\dot{0}]$ by orthonormalizing and reducing the set of operators (5.3), making sure that all vectors are constructed orthogonal to $\{V_{ij}(0)\}$.

A set of orthonormal vector operators $\{X_{ij}(q)\}$, is obtained by applying the Schmidt orthogonalization procedure to the operators

$$V(0), V(1), \cdots, V(n-1) \tag{5.7}$$

in this order. This ordering by degree is quite natural and, as we prove below, it is, in fact, canonical. We obtain[25]

$$X_{ij}(q) \equiv N_q^{-\frac{1}{2}} \det\begin{bmatrix} I_0 & I_1 & \cdots & I_q \\ I_1 & I_2 & \cdots & I_{q+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_{q-1} & I_q & \cdots & I_{2q-1} \\ V_{ij}(0) & V_{ij}(1) & \cdots & V_{ij}(q) \end{bmatrix} \tag{5.8a}$$

for $q = 0, 1, \cdots, n-1$, where

$$N_q \equiv (\det Y_{q-1})(\det Y_q), \tag{5.8b}$$

$$Y_q \equiv \begin{bmatrix} I_0 & I_1 & \cdots & I_q \\ I_1 & I_2 & \cdots & I_{q+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_q & I_{q+1} & \cdots & I_{2q} \end{bmatrix}, \tag{5.8c}$$

where for $q = 0$ we define $\det Y_{-1} = 1$ so that $X_{ij}(0) = V_{ij}(0)/\sqrt{n}$. The orthogonality relations now take the form[25]

$$\sum_{i,j=1}^{n} X_{ij}(q) X_{ji}(p) = \delta_{qp}, \tag{5.9a}$$

and, in particular (set $p = 0$), we have

$$\sum_{i=1}^{n} X_{ii}(q) = 0, \quad q = 1, 2, \cdots, n-1. \tag{5.9b}$$

The next step is to find those linear combinations of the $X_{ij}(q)$ (q fixed) which transform like the state vector with IR labels $[1 \ \dot{0} \ -1]$. There are several ways of doing this, and we choose a method which leads to the explicit form of the Racah invariants $R_{\rho\tau}$ of the last section. The idea is to write each $X(q)$ as a coupling of the elementary operators $\langle 1 \ \dot{0}\rangle$ and $\langle \dot{0} \ -1\rangle$. The form of Eqs. (4.5) then determines the mapping.

In order to write each $X(q)$ as a coupling of $\langle 1 \ \dot{0}\rangle$ and $\langle \dot{0} \ -1\rangle$, we must first accomplish the same task for $V(q)$. This appears most difficult to do directly from Eqs. (5.3), and it is precisely here that the boson calculus and the factorization lemma come to our aid. We use an explicit realization of the operators $V(q)$ in terms of the boson calculus:

$$\mathcal{U}_{ij}(q) \equiv \sum_{i_1, \cdots, i_{q-1}}^{n} \mathcal{E}_{ii_1} \mathcal{E}_{i_1 i_2} \cdots \mathcal{E}_{i_{q-1} j}, \tag{5.10a}$$

$$\mathcal{U}^{ij}(q) \equiv \sum_{i_1, \cdots, i_{q-1}}^{n} \mathcal{E}^{ii_1} \mathcal{E}^{i_1 i_2} \cdots \mathcal{E}^{i_{q-1} j}. \tag{5.10b}$$

[The $\mathcal{E}_{ij}$ and $\mathcal{E}^{ij}$ operators are realizations of the two sets of generators in the boson calculus; cf. (2.32) and (2.33).]

The identity

$$\mathcal{U}_{ij}(q) = \sum_{k,l=1}^{n} a_i^k (a_j^l)^\dagger \mathcal{U}^{lk}(q-1), \tag{5.11}$$

for $q = 1, 2, \cdots$, can be proved in a manner similar to the proof of Eq. (53) of Ref. 6. [Since the $\mathcal{U}^{lk}(q)$ are invariants with respect to the $U(n)$ transformations generated by the $\mathcal{E}_{ij}$, Eq. (5.11) has the form of a coupling of a $[1 \ \dot{0}]$ boson and a $[1 \ \dot{0}]^\dagger$ boson.]

The next step is to use the factorization lemma in the form (2.42) (and the Hermitian conjugate of this result) to write Eq. (5.11) as follows:

$$\mathcal{U}_{ij}(q) = \sum_{\rho,\tau} \left\langle \begin{matrix} \rho \\ [1 \ \dot{0}] \\ i \end{matrix} \right\rangle_\ell \mathcal{M}^{-1} \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ j \end{matrix} \right\rangle_\ell^\dagger \mathcal{M} \mathcal{J}^{\rho\tau}(q-1), \tag{5.12a}$$

for $q = 1, 2, \cdots$, where

$$\mathcal{J}^{\rho\tau}(q-1) \equiv \sum_{k,l=1}^{n} \left\langle \begin{matrix} \rho \\ [1 \ \dot{0}] \\ k \end{matrix} \right\rangle_u \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ l \end{matrix} \right\rangle_u^\dagger \mathcal{U}^{lk}(q-1). \tag{5.12b}$$

[Index ℓ in Eq. (5.12a) designates "lower"; index u in Eq. (5.12b) designates "upper."] It is easy to prove that the quantities $\mathcal{J}^{\rho\tau}(q-1)$ are also invariants with respect to the $U(n)$ transformations generated by the $\mathcal{E}^{ij}$; hence, they are invariants with respect to $U(n) \star U(n)$. In consequence,

$$\mathcal{J}^{\rho\tau}(q-1) = \delta^{\rho\tau} \mathcal{J}^{\rho\rho}(q-1). \tag{5.13}$$

Now let us carefully consider the result obtained from Eq. (5.12a), upon using property (5.13). The operators appearing in each term of the right-hand side of the resulting equation have matrix elements which depend entirely on the lower Gel'fand patterns of the initial and final boson state vectors. This implies that we can just as well regard Eqs. (5.12) as *abstract operator identities*:

$$V_{ij}(q) = \sum_{\tau=1}^{n} \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ i \end{matrix} \right\rangle \mathcal{M}^{-1} \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ j \end{matrix} \right\rangle^\dagger \mathcal{M} J_\tau(q-1), \tag{5.14a}$$

where

$$J_\tau(q-1) \equiv \sum_{k,l=1}^{n} \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ k \end{matrix} \right\rangle \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ l \end{matrix} \right\rangle^\dagger V_{lk}(q-1). \tag{5.14b}$$

An important special case of Eqs. (5.14) occurs for $q = 1$; in this case $J_\tau(0) = 1$, and we find

$$E_{ij} = \sum_{\tau=1}^{n} \left\langle \begin{matrix} \tau \\ [1 \ \dot{0}] \\ i \end{matrix} \right\rangle \mathcal{M}^{-1} \left\langle \begin{matrix} \tau \\ [1 \ 0] \\ j \end{matrix} \right\rangle^\dagger \mathcal{M}. \tag{5.15}$$

This result is a rather elegant relation which expresses the generators of $U(n)$ directly in terms of the fundamental Wigner operators (in consequence, the explicit

evaluation of the generator matrix elements can be obtained immediately).

The invariants $J_\tau(q)$, $q = 0, 1, \cdots$, given by Eq. (5.14b), have very simple eigenvalues, namely,

$$J_\tau(q)\,|(m)\rangle = (p_{\tau n})^q\,|(m)\rangle. \tag{5.16}$$

(This result is proved in Appendix C. Note that this relation provides an answer to the question: What operators have the labels of a Gel'fand pattern as eigenvalues?)

We can now give Eq. (5.14a) an alternative form by noting the relation between the measure operator $\mathcal{M}$ and the dimension operator D [compare Eqs. (2.4) and (2.38)]:

$$V_{ij}(q) = \sum_\tau \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ i \end{matrix} \right\rangle D \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ j \end{matrix} \right\rangle^\dagger D^{-1} J_\tau(q), \tag{5.17}$$

which turns out to be correct also for $q = 0$ as well as for $q = 1, 2, \cdots$. [Observe that $D^{-1}J_\tau(q)$ can also be written to the left-hand side of the Wigner operators.]

The form of $V(q)$ as a coupling of $\langle 1 \quad \dot{0}\rangle$ and $\langle \dot{0} \quad -1\rangle$ is now obtained by eliminating the Hermitian conjugate operator from Eq. (5.17) by using Eq. (4.7). The final form is the following operator relation:

$$V_{ij}(q) = (-1)^{n-j} n^{\frac{1}{2}} \times \sum_\tau \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ i \end{matrix} \right\rangle \left\langle \begin{matrix} \bar{\tau} \\ [\dot{0} \quad -1] \\ j \end{matrix} \right\rangle J_\tau(q) R_{n\tau}, \tag{5.18}$$

for $q = 0, 1, \cdots$.

Substitution of $V_{ij}(q)$ in the form (5.18) into Eq. (5.8a) yields the coupling formula for the vector operator $X(q)$:

$$(-1)^{n-j-q} X_{ij}(q) = \sum_\tau \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ i \end{matrix} \right\rangle \left\langle \begin{matrix} \bar{\tau} \\ [\dot{0} \quad -1] \\ j \end{matrix} \right\rangle S_{q\tau}, \tag{5.19}$$

where the invariant $S_{q\tau}$ is defined by

$$S_{q\tau} \equiv (-1)^q n^{\frac{1}{2}} N_q^{-\frac{1}{2}} R_{n\tau} \det \begin{bmatrix} I_0 & I_1 & \cdots & I_q \\ I_1 & I_2 & \cdots & I_{q+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_{q-1} & I_q & \cdots & I_{2q-1} \\ J_\tau(0) & J_\tau(1) & \cdots & J_\tau(q) \end{bmatrix}, \tag{5.20}$$

for $q = 0, 1, \cdots, n-1$. (Note the special case $S_{0\tau} \equiv R_{n\tau}$.) Observe that $S_{q\tau}$ can be moved to the left side of the Wigner operators in Eq. (5.19).

We further observe that the invariants $S_{q\tau}$ satisfy the orthonormality relations[25]

$$\sum_{\tau=1}^{n} S_{q\tau} S_{p\tau} = \delta_{qp}, \tag{5.21}$$

for $q, p = 0, 1, \cdots, n-1$.

The simplest proof of this is to notice that the $S_{q\tau}$ are just the result of doing the Schmidt orthogonalization procedure on the operators

$$Z_0, Z_1, \cdots, Z_{n-1}, \tag{5.22a}$$

where Z_q is the row matrix

$$Z_q = [Z_{q1} Z_{q2} \cdots Z_{qn}], \tag{5.22b}$$

in which

$$Z_{q\tau} \equiv J_\tau(q) R_{n\tau}. \tag{5.22c}$$

One needs the result

$$n \sum_{\tau=1}^{n} Z_{q\tau} Z_{p\tau} = n \sum_{\tau=1}^{n} J_\tau(q+p) R_{n\tau}^2 = I_{q+p}, \tag{5.23}$$

which follows from Eq. (B14), to complete the proof.

If one now compares Eq. (5.19) to the right-hand side of Eq. (4.5c), it follows that the $S_{q\tau}$ invariants are indeed none other than Racah invariants. (We must yet prove, however, that the $S_{q\tau}$ are *the* canonical invariants.) Using these Racah invariants in Eqs. (4.5c) *and* (4.5d), we determine directly *a* set of orthonormal Wigner operators having $\Delta = [\dot{0}]$:

$$\left\langle \begin{matrix} q \\ [1 \quad \dot{0} \quad -1] \\ (i,j) \end{matrix} \right\rangle = \sum_{\tau=1}^{n} S_{q\tau} \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ i \end{matrix} \right\rangle \left\langle \begin{matrix} \bar{\tau} \\ [\dot{0} \quad -1] \\ j \end{matrix} \right\rangle, \quad i \neq j, \tag{5.24a}$$

$$\left\langle \begin{matrix} q \\ [1 \quad \dot{0} \quad -1] \\ (i,i) \end{matrix} \right\rangle = \sum_{\tau,j=1}^{n} \mathcal{O}_{ij} S_{q\tau} \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ j \end{matrix} \right\rangle \left\langle \begin{matrix} \bar{\tau} \\ [\dot{0} \quad -1] \\ j \end{matrix} \right\rangle \tag{5.24b}$$

in which $q = 1, 2, \cdots, n-1$ is a mere label, related to degree, but of no operator pattern significance at this stage.

Let us now return to the consideration of Eq. (5.19). Comparing it with Eqs. (5.24), we see, in precise detail, the form of the mapping of a vector operator

(with $\sum_i X_{ii} = 0$) onto an adjoint Wigner operator:

$$(-1)^{n-j-q}X_{ij}(q) = \left\langle \begin{matrix} & q & \\ [1 & \dot{0} & -1] \\ & (i,j) & \end{matrix} \right\rangle, \quad i \neq j, \quad (5.25a)$$

$$(-1)^{n-i-q}H_i(q) = \left\langle \begin{matrix} & q & \\ [1 & \dot{0} & -1] \\ & (i,i) & \end{matrix} \right\rangle,$$
$$i = 1, 2, \cdots, n-1, \quad (5.25b)$$

where

$$H_i(q) \equiv \sum_{j=1}^{n}(-1)^{i-j}\mathcal{O}_{ij}X_{jj}(q)$$
$$= \frac{1}{[i(i+1)]^{\frac{1}{2}}}\sum_{j=1}^{i}X_{jj}(q) - \left[\frac{i}{i+1}\right]^{\frac{1}{2}}X_{i+1\,i+1}(q), \quad (5.25c)$$

for $i = 1, 2, \cdots, n-1$, $q = 1, 2, \cdots, n-1$. The only free choice, in the identifications above, is the over-all phase factor $(-1)^{n-q}$. [This choice occurred in the assignment of the factor $(-1)^q$ to $S_{q\tau}$ in Eq. (5.20), and is based on a general principle to be discussed shortly.]

The orthonormality of the Wigner operators (5.24) is assured because of the orthonormality of the Racah invariants. [It may be worth noting also that it was assured from the very beginning because of the identity[25]

$$\sum_{i,j}\left\langle \begin{matrix} & q & \\ [1 & \dot{0} & -1] \\ & (i,j) & \end{matrix} \right\rangle \left\langle \begin{matrix} & p & \\ [1 & \dot{0} & -1] \\ & (i,j) & \end{matrix} \right\rangle^{\dagger}$$
$$= \sum_{i,j}^{n} \dot{X}_{ij}(q)X_{ji}(p) = \delta_{qp}, \quad q, p = 1, 2, \cdots, n-1,$$

which holds as a direct consequence of $\sum_i X_{ii}(q) = 0$, and again illustrates the convenience of including $V_{ij}(0)$ in the set (5.3).]

Let us summarize. By a rather indirect route, starting from an ad hoc set of linearly independent vector operators, we have constructed an explicit set of Wigner operators which spans the subspace of adjoint tensor operators with $\Delta = [\dot{0}]$. We have obtained these Wigner operators in two forms: Equations (5.24)—which express them as couplings of the known elementary Wigner operators $\langle 1 \ \dot{0}\rangle$ and $\langle \dot{0} \ -1\rangle$ through explicit Racah invariants—and Eqs. (5.25)—which relate them back to the explicit vector operators from which we started. A number of interesting results, e.g., Eqs. (5.15) and (5.16), have emerged as auxiliary relations. Operator patterns have *not yet* been assigned to these Wigner operators or to the Racah invariants, only an index q, and there remains the problem of the origin of the operator patterns and of the structure which, we insist, entitles us to call these operators canonical. This is discussed in the concluding section.

There are several important properties of the adjoint operators and Racah invariants, which can be obtained from the foregoing results.

The first concerns the classification by polynomial degree (in the p_{in}) of the Racah invariants. An alternative (easier but less instructive) construction to determine the adjoint Wigner operators is to define the row vector

$$Z_q([m]) \equiv [p_{1n}^q R_{n1}([m]), p_{2n}^q R_{n2}([m]), \cdots, p_{nn}^q R_{nn}([m])]$$

for $q = 0, 1, \cdots, n-1$. These vectors are linearly independent on generic states [using Appendix B, Eq. (B14)]; they thus constitute a basis for the Racah invariants. If we now ask for an orthonormal set of vectors of the form

$$S_q([m]) = [S_{q1}([m]), S_{q2}([m]), \cdots, S_{qn}([m])],$$

constructed from the vectors $\{Z_q([m])\}$ and having increasing (polynomial) degree in the $\{p_{in}\}$, we obtain precisely the Racah invariants of Eq. (5.20). The origin of these Racah invariants can be traced to a single structural idea—that of degree.

Let us turn to a second property of the adjoint Racah invariants closely related to polynomial degree: the limit properties. The proofs of the following limit properties are given in Appendix D (the arrow signifies the limit $m_{nn} \to -\infty$):

$$S_{0\tau}^{(n)}(m_{1n}\cdots m_{nn})$$
$$\to -[(n-1)/n]^{\frac{1}{2}}S_{0\tau}^{(n-1)}(m_{1n}\cdots m_{n-1n}), \quad (5.26a)$$

for $\tau = 1, 2, \cdots, n-1$,

$$S_{0n}^{(n)}(m_{1n}\cdots m_{nn}) \to 1/\sqrt{n}; \quad (5.26b)$$

$$S_{1\tau}^{(n)}(m_{1n}\cdots m_{nn}) \to S_{0\tau}^{(n-1)}(m_{1n}\cdots m_{n-1n})/\sqrt{n}, \quad (5.27a)$$

for $\tau = 1, 2, \cdots, n-1$,

$$S_{1n}^{(n)}(m_{1n}\cdots m_{nn}) \to [(n-1)/n]^{\frac{1}{2}}; \quad (5.27b)$$

$$S_{q\tau}^{(n)}(m_{1n}\cdots m_{nn}) \to S_{q-1\tau}^{(n-1)}(m_{1n}\cdots m_{n-1n}), \quad (5.28a)$$

for $q = 2, 3, \cdots, n-1$, $\tau = 1, 2 \cdots, n-1$,

$$S_{qn}^{(n)}(m_{1n}\cdots m_{nn}) \to 0, \quad (5.28b)$$

for $q = 2, 3, \cdots, n-1$. [Note that we have used a superscript n on these Racah invariants to indicate explicitly that they are associated with $U(n)$.]

The limit relations given above for the adjoint Racah invariants are all particular instances of the

following statement:

$$\left\{\begin{pmatrix}[M]_n + [\Delta(\Lambda)]_n \\ (\Gamma'')_{n-1}\end{pmatrix}\begin{pmatrix}(\Lambda)_{n-1} \\ [M']_n \\ (\Gamma')_{n-1}\end{pmatrix}\begin{pmatrix}[M]_n \\ (\Gamma)_{n-1}\end{pmatrix}\right\}(m_{1n}\cdots m_{nn})$$

$$\rightarrow\left[\begin{pmatrix}[M]_n + [\Delta(\Lambda)]_n \\ (\Gamma'')_{n-1}\end{pmatrix}\begin{pmatrix}(\Lambda)_{n-1} \\ [M']_n \\ (\Gamma')_{n-1}\end{pmatrix}\begin{pmatrix}[M]_n \\ (\Gamma)_{n-1}\end{pmatrix}\right](m_{1n}\cdots m_{n-1n}). \quad (5.29)$$

As mentioned previously, we have no (complete) proof that this general relation holds. If it is indeed valid for each n, then it implies the result that under the successive limits $m_{in}\rightarrow-\infty$, $i=n, n-1, \cdots, 2$, a Racah invariant limits to a Wigner coefficient. This latter result is, in particular, true for the explicit adjoint Racah invariants developed above. {We observe [cf. Eq. (5.30) below] that the Racah invariants of Eqs. (4.3) and the $S^{(n)}_{q\tau}$ are related by $R^{(n)}_{\rho\tau}=S^{(n)}_{n-\rho\tau}$.}

There is one final point which requires mention—the question of phase. The phases of the Racah invariants (5.20) have been chosen such that the reduction law holds precisely in the form (5.29)—*this uniquely determines all phases.*

We complete this section by noting the explicit forms of the adjoint unit $U(n):U(n-1)$ projective operators. In Sec. 6, we justify the identification of the degree index q with the operator pattern as follows:

$$\begin{pmatrix}[1 & \dot{0} & -1] \\ & q & \end{pmatrix}\rightarrow\begin{pmatrix}[1 & \dot{0} & -1] \\ (n-q, & n-q) & \end{pmatrix}. \quad (5.30)$$

It is convenient to anticipate this result so that we can write out the adjoint projective operators in terms of the notation which employs operator patterns:

$$\begin{bmatrix}(\rho,\tau) \\ [1 \quad \dot{0} \quad -1] \\ (\alpha,\beta)\end{bmatrix}=\begin{bmatrix}\rho \\ [1 \quad \dot{0}] \\ \alpha\end{bmatrix}\begin{bmatrix}\bar{\tau} \\ [\dot{0} \quad -1] \\ \bar{\beta}\end{bmatrix}, \quad (5.31a)$$

for $\rho\neq\tau$, $\alpha\neq\beta$,

$$\begin{bmatrix}(\rho,\tau) \\ [1 \quad \dot{0} \quad -1] \\ (\alpha,\alpha)\end{bmatrix}=\sum_{\beta=1}^{n}R'_{\alpha\beta}\begin{bmatrix}\rho \\ [1 \quad \dot{0}] \\ \beta\end{bmatrix}\begin{bmatrix}\bar{\tau} \\ [\dot{0} \quad -1] \\ \bar{\beta}\end{bmatrix}, \quad (5.31b)$$

for $\rho\neq\tau$,

$$\begin{bmatrix}(\rho,\rho) \\ [1 \quad \dot{0} \quad -1] \\ (\alpha,\beta)\end{bmatrix}=\sum_{\tau=1}^{n}R_{\rho\tau}\begin{bmatrix}\tau \\ [1 \quad \dot{0}] \\ \alpha\end{bmatrix}\begin{bmatrix}\bar{\tau} \\ [\dot{0} \quad -1] \\ \bar{\beta}\end{bmatrix}, \quad (5.31c)$$

for $\alpha\neq\beta$,

$$\begin{bmatrix}(\rho,\rho) \\ [1 \quad \dot{0} \quad -1] \\ (\alpha,\alpha)\end{bmatrix}=\sum_{\beta,\tau=1}^{n}R'_{\alpha\beta}R_{\rho\tau}\begin{bmatrix}\tau \\ [1 \quad \dot{0}] \\ \beta\end{bmatrix}\begin{bmatrix}\bar{\tau} \\ [\dot{0} \quad -1] \\ \bar{\beta}\end{bmatrix}. \quad (5.31d)$$

In these results $R_{\rho\tau}$ and $R'_{\alpha\beta}$ are, respectively, the invariant operators as follows:

$$R_{\rho\tau}=\left\{\begin{pmatrix}[1 & \dot{0} & -1] \\ (\rho, & \rho) & \end{pmatrix}\begin{pmatrix}1 \\ [1 \quad \dot{0}] \\ \tau\end{pmatrix}\begin{pmatrix}[\dot{0} & -1] \\ & \bar{\tau}\end{pmatrix}\right\}, \quad (5.32a)$$

$$R'_{\alpha\beta}=\left[\begin{pmatrix}[1 & \dot{0} & -1] \\ (\alpha, & \alpha) & \end{pmatrix}\begin{pmatrix}1 \\ [1 \quad \dot{0}] \\ \beta\end{pmatrix}\begin{pmatrix}[\dot{0} & -1] \\ & \bar{\beta}\end{pmatrix}\right]. \quad (5.32b)$$

The relations of the square-bracket invariants to $U(n-1)$ Racah invariants are

$$\begin{aligned}R'_{\alpha\beta}&=R^{(n-1)}_{\alpha\beta}, && \text{for } \alpha=1,2,\cdots,n-2,\\ &&&\quad \beta=1,2,\cdots,n-1,\\ R'_{\alpha n}&=0, && \text{for } \alpha=1,2,\cdots,n-2,\\ R'_{n-1\beta}&=R^{(n-1)}_{n-1\beta}/\sqrt{n}, && \text{for } \beta=1,2,\cdots,n-1,\\ R'_{n-1n}&=[(n-1)/n]^{\frac{1}{2}}. && \end{aligned} \quad (5.33)$$

All operators appearing on the right-hand sides of Eqs. (5.31) are known explicitly; *these equations completely define the set of canonical adjoint $U(n):U(n-1)$ projective operators.* The matrix elements of these operators, denoted by

$$\left\langle\begin{pmatrix}[m]_n + \Delta_n(\rho) - \Delta_n(\tau) \\ [m]_{n-1} + \Delta_{n-1}(\alpha) - \Delta_{n-1}(\beta)\end{pmatrix}\middle|\begin{bmatrix}(\rho,\tau) \\ [1 \quad \dot{0} \quad -1] \\ (\alpha,\beta)\end{bmatrix}\middle|\begin{pmatrix}[m]_n \\ [m]_{n-1}\end{pmatrix}\right\rangle, \quad (5.34)$$

in which $\Delta_{n-1}(n) \equiv 0$, comprise *the set of canonical adjoint* $U(n):U(n-1)$ *reduced Wigner coefficients.* These coefficients are calculated straightforwardly by using the pattern calculus rules and the known $U(n)$ and $U(n-1)$ Racah coefficients. The results are given below where the expression on the right-hand side of the arrow is the matrix element (5.34) of the operator appearing on the left-hand side of the arrow. We have also partitioned the list of matrix elements into four classes a, b, c, and d corresponding, respectively, to the four types of operators of Eqs. (5.31a)–(5.31d).

Class a

These are the extremal operators, and their matrix elements are written down directly from the pattern calculus rules:

$$\begin{bmatrix} & (\rho,\tau) & \\ [1 & \dot{0} & -1] \\ & (\alpha,\beta) & \end{bmatrix} \rightarrow (-1)^{\beta-\tau} S(\alpha-\rho) S(\beta-\tau)$$
$$\times \left[\prod_{\substack{s=1 \\ s\neq\alpha,\beta}}^{n-1} \frac{(p_{\rho n}-p_{sn-1})(p_{sn-1}-p_{\tau n}+1)}{(p_{\alpha n-1}-p_{sn-1}+1)(p_{sn-1}-p_{\beta n-1}+1)} \prod_{\substack{s=1 \\ s\neq\rho,\tau}}^{n} \frac{(p_{\alpha n-1}-p_{sn}+1)(p_{sn}-p_{\beta n-1})}{(p_{\rho n}-p_{sn})(p_{sn}-p_{\tau n})} \right.$$
$$\left. \times \frac{(p_{\rho n}-p_{\beta n-1})(p_{\rho n}-p_{\beta n-1}+1)(p_{\alpha n-1}-p_{\tau n}+1)(p_{\alpha n-1}-p_{\tau n}+2)}{(p_{\rho n}-p_{\tau n})(p_{\rho n}-p_{\tau n}+1)(p_{\alpha n-1}-p_{\beta n-1}+1)(p_{\alpha n-1}-p_{\beta n-1}+2)} \right]^{\frac{1}{2}}, \quad (5.35a)$$

for $\rho \neq \tau$ and $\alpha \neq \beta \neq n$,

$$\begin{bmatrix} & (\rho,\tau) & \\ [1 & \dot{0} & -1] \\ & (\alpha,n) & \end{bmatrix} \rightarrow (-1)^{n-\tau} S(\alpha-\rho)$$
$$\times \left[\prod_{\substack{s=1 \\ s\neq\alpha}}^{n-1} \frac{(p_{\rho n}-p_{sn-1})(p_{sn-1}-p_{\tau n}+1)}{(p_{\alpha n-1}-p_{sn-1}+1)} \prod_{\substack{s=1 \\ s\neq\rho,\tau}}^{n} \frac{(p_{\alpha n-1}-p_{sn}+1)}{(p_{\rho n}-p_{sn})(p_{sn}-p_{\tau n})} \right.$$
$$\left. \times \frac{(p_{\alpha n-1}-p_{\tau n}+1)(p_{\alpha n-1}-p_{\tau n}+2)}{(p_{\rho n}-p_{\tau n})(p_{\rho n}-p_{\tau n}+1)} \right]^{\frac{1}{2}}, \quad (5.35b)$$

for $\rho \neq \tau$ and $\alpha \neq n$,

$$\begin{bmatrix} & (\rho,\tau) & \\ [1 & \dot{0} & -1] \\ & (n,\beta) & \end{bmatrix} \rightarrow (-1)^{\beta-\tau} S(\beta-\tau)$$
$$\times \left[\prod_{\substack{s=1 \\ s\neq\beta}}^{n-1} \frac{(p_{\rho n}-p_{sn-1})(p_{sn-1}-p_{\tau n}+1)}{(p_{sn-1}-p_{\beta n-1}+1)} \prod_{\substack{s=1 \\ s\neq\rho,\tau}}^{n} \frac{(p_{sn}-p_{\beta n-1})}{(p_{\rho n}-p_{sn})(p_{sn}-p_{\tau n})} \right.$$
$$\left. \times \frac{(p_{\rho n}-p_{\beta n-1})(p_{\rho n}-p_{\beta n-1}+1)}{(p_{\rho n}-p_{\tau n})(p_{\rho n}-p_{\tau n}+1)} \right]^{\frac{1}{2}}, \quad (5.35c)$$

for $\rho \neq \tau$ and $\beta \neq n$.

Class b

These are the operators which are extremal in their upper patterns and have the lower patterns with $\Delta = [\dot{0}]$:

$$\begin{bmatrix} & (\rho,\tau) & \\ [1 & \dot{0} & -1] \\ & (\alpha,\alpha) & \end{bmatrix} \rightarrow (-1)^{\alpha-\tau-1} [N^{(n-1)}_{n-\alpha-1}([m]_{n-1})]^{-\frac{1}{2}} (\mathrm{PCF})$$
$$\times \det \begin{bmatrix} I_0^{(n-1)}([m]_{n-1}) & \cdots & I^{(n-1)}_{n-\alpha-1}([m]_{n-1}) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ I^{(n-1)}_{n-\alpha-2}([m]_{n-1}) & \cdots & I^{(n-1)}_{2(n-\alpha)-3}([m]_{n-1}) \\ f^{(0)}_{\rho\tau}([m]_n,[m]_{n-1}) & \cdots & f^{(n-\alpha-1)}_{\rho\tau}([m]_n,[m]_{n-1}) \end{bmatrix}, \quad (5.36a)$$

for $\rho \neq \tau$ and $\alpha = 1, 2, \cdots, n-2$, where $N^{(n-1)}_{n-\alpha-1}$ is the invariant normalization operator given by Eq. (5.8b) for $U(n-1)$; (PCF) is given by

$$(\text{PCF}) = \left[\frac{\prod_{s=1}^{n-1} (p_{\rho n} - p_{sn-1})(p_{sn-1} - p_{\tau n} + 1)}{(p_{\rho n} - p_{\tau n})(p_{\rho n} - p_{\tau n} + 1) \prod_{\substack{s=1 \\ s \neq \rho,\tau}}^{n} (p_{\rho n} - p_{sn})(p_{sn} - p_{\tau n})} \right]^{\frac{1}{2}}, \tag{5.36b}$$

and is the pattern calculus factor (PCF) which obtains by applying the pattern calculus rules to the Δ pattern having $\Delta_n = \Delta_n(\rho) - \Delta_n(\tau)$ and $\Delta_{n-1} = [\dot{0}]_{n-1}$; finally, the functions $f^{(q)}_{\rho\tau}$, $q = 0, 1, \cdots$, are given by

$$\begin{aligned} &f^{(q)}_{\rho\tau}([m]_n, [m]_{n-1}) \\ &= \sum_{\beta=1}^{n-1} \left[p^q_{\beta n-1} \prod_{\substack{s=1 \\ s \neq \rho,\tau}}^{n} (p_{sn} - p_{\beta n-1}) \Big/ \prod_{\substack{s=1 \\ s \neq \beta}}^{n-1} (p_{sn-1} - p_{\beta n-1}) \right] \\ &= \sum_{\sigma=0}^{n-2} (-1)^\sigma \varphi^{(n-2)}_\sigma (p_{1n} \cdots \hat{p}_{\rho n} \cdots \hat{p}_{\tau n} \cdots p_{nn}) \\ &\quad \times \beta^{(n-1)}_{q-\sigma}(p_{1n-1} \cdots p_{n-1n-1}), \end{aligned} \tag{5.36c}$$

where the $\varphi^{(n-2)}_\sigma$ are the elementary symmetric functions of order $n-2$ in the $n-2$ variables $p_{1n} \cdots \hat{p}_{\rho n} \cdots \hat{p}_{\tau n} \cdots p_{nn}$, where the notation $\hat{p}_{\rho n}$ and $\hat{p}_{\tau n}$ designates that these variables are omitted from the set of n variables. The $\beta^{(n-1)}_{q-\sigma}$ are the symmetric functions of order $n-1$ discussed in Appendix A.

The reduced matrix element of Eq. (5.31b) for $\alpha = n-1$ is not obtained from Eq. (5.36a). It has the very simple form as follows:

$$\begin{bmatrix} (\rho, \tau) \\ [1 \quad \dot{0} \quad -1] \\ (n-1, n-1) \end{bmatrix} \rightarrow (-1)^{n-\tau} [n/(n-1)]^{\frac{1}{2}} (\text{PCF}), \tag{5.36d}$$

for $\rho \neq \tau$.

Class c

These are the operators which are extremal in their lower patterns and have the upper patterns with $\Delta = [\dot{0}]$:

$$\begin{bmatrix} (\rho, \rho) \\ [1 \quad \dot{0} \quad -1] \\ (\alpha, \beta) \end{bmatrix} \rightarrow (-1)^{\beta-\rho} [N^{(n)}_{n-\rho}([m]_n)]^{-\frac{1}{2}} (\text{PCF})$$

$$\times \det \begin{bmatrix} I^{(n)}_0([m]_n) & \cdots & I^{(n)}_{n-\rho}([m]_n) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ I^{(n)}_{n-\rho-1}([m]_n) & \cdots & I^{(n)}_{2(n-\rho)-1}([m]_n) \\ g^{(0)}_{\alpha\beta}([m]_n, [m]_{n-1}) & \cdots & g^{(n-\rho)}_{\alpha\beta}([m]_n, [m]_{n-1}) \end{bmatrix}, \tag{5.37a}$$

where $N^{(n)}_{n-\rho}$ is the invariant normalization operator given by Eq. (5.8b); (PCF) is the pattern calculus factor appropriate to the Δ pattern for $\Delta_n = [\dot{0}]_n$, $\Delta_{n-1} = \Delta_{n-1}(\alpha) - \Delta_{n-1}(\beta)$ and is given by

$$(\text{PCF}) = \left[\frac{\prod_{s=1}^{n} (p_{sn} - p_{\beta n-1})(p_{\alpha n-1} - p_{sn} + 1)}{(p_{\alpha n-1} - p_{\beta n-1} + 1)(p_{\alpha n-1} - p_{\beta n-1} + 2) \prod_{\substack{s=1 \\ s \neq \alpha,\beta}}^{n-1} (p_{\alpha n-1} - p_{sn-1} + 1)(p_{sn-1} - p_{\beta n-1} + 1)} \right]^{\frac{1}{2}}, \tag{5.37b}$$

$$\begin{aligned} g^{(q)}_{\alpha\beta}([m]_n, [m]_{n-1}) &= \sum_{\tau=1}^{n} \left[p^q_{\tau n} \prod_{\substack{s=1 \\ s \neq \alpha,\beta}}^{n-1} (p_{sn-1} - p_{\tau n} + 1) \Big/ \prod_{\substack{s=1 \\ s \neq \tau}}^{n} (p_{sn} - p_{\tau n}) \right] \\ &= \sum_{\sigma=0}^{n-3} (-1)^\sigma \varphi^{(n-3)}_\sigma (p_{1n-1} + 1 \cdots \widehat{p_{\alpha n-1} + 1} \cdots \widehat{p_{\beta n-1} + 1} \cdots p_{n-1n-1} + 1) \beta^{(n)}_{q-\sigma-2}(p_{1n} \cdots p_{nn}). \end{aligned} \tag{5.37c}$$

Equations (5.37b) and (5.37c) are correct only for $\alpha \neq \beta \neq n$. However, the form (5.37a) is still valid for $\alpha < \beta = n$

and $\beta < \alpha = n$ with the modified factors as follows:

$$(\mathrm{PCF}) = \left[(-)\prod_{s=1}^{n}(p_{\alpha n-1} - p_{sn} + 1) \Big/ \prod_{\substack{s=1\\ s\neq\alpha}}^{n-1}(p_{\alpha n-1} - p_{sn-1} + 1)\right]^{\frac{1}{2}}, \quad (5.37d)$$

$$g^{(q)}_{\alpha n}([m]_n, [m]_{n-1}) = (-)\sum_{\tau=1}^{n}\left[p^q_{\tau n}\prod_{\substack{s=1\\ s\neq\alpha}}^{n-1}(p_{sn-1} - p_{\tau n} + 1) \Big/ \prod_{\substack{s=1\\ s\neq\tau}}^{n}(p_{sn} - p_{\tau n})\right]$$
$$= \sum_{\sigma=0}^{n-2}(-1)^{\sigma} \times \varphi^{(n-2)}_{\sigma}(p_{1n-1} + 1 \cdots \widehat{p_{\alpha n-1} + 1} \cdots p_{n-1n-1} + 1) \times \beta^{(n)}_{q-\sigma-1}(p_{1n} \cdots p_{nn}), \quad (5.37e)$$

for $\alpha < \beta = n$,

$$(\mathrm{PCF}) = \left[(-)\prod_{s=1}^{n}(p_{sn} - p_{\beta n-1}) \Big/ \prod_{\substack{s=1\\ s\neq\beta}}^{n-1}(p_{sn-1} - p_{\beta n-1} + 1)\right]^{\frac{1}{2}}, \quad (5.37f)$$

$$g^{(q)}_{n\beta}([m]_n, [m]_{n-1}) = (-)\sum_{\tau=1}^{n}\left[p^q_{\tau n}\prod_{\substack{s=1\\ s\neq\beta}}^{n-1}(p_{sn-1} - p_{\tau n} + 1) \Big/ \prod_{\substack{s=1\\ s\neq\tau}}^{n}(p_{sn} - p_{\tau n})\right]$$
$$= \sum_{\sigma=0}^{n-2}(-1)^{\sigma} \times \varphi^{(n-2)}_{\sigma}(p_{1n-1} + 1 \cdots \widehat{p_{\beta n-1} + 1} \cdots p_{n-1n-1} + 1) \times \beta^{(n)}_{q-\sigma-1}(p_{1n} \cdots p_{nn}), \quad (5.37g)$$

for $\beta < \alpha = n$.

Observe that $g^{(0)}_{\alpha\beta} = g^{(1)}_{\alpha\beta} = 0$, for all $\alpha \neq \beta = 1, 2, \cdots, n-1$, so that the class of reduced matrix elements (5.37a) for $\rho = n - 1$ (the generator operator pattern) and $\alpha \neq \beta = 1, 2, \cdots, n-1$ vanishes *on all labels.*

Class d

These are the operators which have upper and lower patterns with $\Delta = [\dot{0}]$; their matrix elements are the most complicated:

$$\begin{bmatrix} (\rho,\rho) \\ [1\ \ \dot{0}\ \ -1] \\ (\alpha,\alpha) \end{bmatrix} \to (-1)^{\alpha-\rho}[N^{(n-1)}_{n-\alpha-1}([m]_{n-1})N^{(n)}_{n-\rho}([m]_n)]^{-\frac{1}{2}} \times \det\begin{bmatrix} I^{(n)}_0([m]_n) & \cdots & I^{(n)}_{n-\rho}([m]_n) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ I^{(n)}_{n-\rho-1}([m]_n) & \cdots & I^{(n)}_{2(n-\rho)-1}([m]_n) \\ D^{(0)}_{\alpha}([m]_n, [m]_{n-1}) & \cdots & D^{(n-\rho)}_{\alpha}([m]_n, [m]_{n-1}) \end{bmatrix}, \quad (5.38a)$$

where

$$D^{(q)}_{\alpha}([m]_n, [m]_{n-1}) = \det\begin{bmatrix} I^{(n-1)}_0([m]_{n-1}) & \cdots & I^{(n-1)}_{n-\alpha-1}([m]_{n-1}) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ I^{(n-1)}_{n-\alpha-2}([m]_{n-1}) & \cdots & I^{(n-1)}_{2(n-\alpha)-3}([m]_{n-1}) \\ S^{(q0)}([m]_n, [m]_{n-1}) & \cdots & S^{(q,n-\alpha-1)}([m]_n, [m]_{n-1}) \end{bmatrix}, \quad (5.38b)$$

where

$$S^{(q,r)}([m]_n, [m]_{n-1}) = \sum_{\beta=1}^{n-1}\sum_{\tau=1}^{n}\left[p^q_{\tau n}\prod_{\substack{s=1\\ s\neq\beta}}^{n-1}(p_{sn-1} - p_{\tau n} + 1) \Big/ \prod_{\substack{s=1\\ s\neq\tau}}^{n}(p_{sn} - p_{\tau n})\right] \times \left[p^r_{\beta n-1}\prod_{\substack{s=1\\ s\neq\tau}}^{n}(p_{sn} - p_{\beta n-1}) \Big/ \prod_{\substack{s=1\\ s\neq\beta}}^{n-1}(p_{sn-1} - p_{\beta n-1})\right], \quad (5.38c)$$

for $\alpha = 1, 2, \cdots, n-2$,

$$\begin{bmatrix} (\rho,\rho) \\ [1\ \ \dot{0}\ \ -1] \\ (n-1, n-1) \end{bmatrix} \to (-1)^{n-\rho-1}[(n-1)N^{(n)}_{n-\rho}([m]_n)/n]^{-\frac{1}{2}} \det\begin{bmatrix} I^{(n)}_0([m]_n) & \cdots & I^{(n)}_{n-\rho}([m]_n) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ I^{(n)}_{n-\rho-1}([m]_n) & \cdots & I^{(n)}_{2(n-\rho)-1}([m]_n) \\ g^{(0)}([m]_n, [m]_{n-1}) & \cdots & g^{(n-\rho)}([m]_n, [m]_{n-1}) \end{bmatrix}, \quad (5.38d)$$

where

$$g^{(q)}([m]_n, [m]_{n-1})$$
$$= (-)\sum_{\tau=1}^{n}\left[p_{\tau n}^{q}\prod_{s=1}^{n-1}(p_{sn-1} - p_{\tau n} + 1)\Big/\prod_{\substack{s=1\\ s\neq\tau}}^{n}(p_{sn} - p_{\tau n})\right]$$
$$= (-)\sum_{\sigma=0}^{n-1}(-1)^{\sigma}\varphi_{\sigma}^{(n-1)}(p_{1n-1} + 1 \cdots p_{n-1n-1} + 1)$$
$$\times \beta_{q-\sigma}^{(n)}(p_{1n}\cdots p_{nn}). \tag{5.38e}$$

We still need to evaluate the sum (5.38c), and this can be done using the summation formulas of Appendix A. To obtain the result in the form (5.40) below, it is necessary to use the relations

$$\varphi_{\sigma}^{(n-1)}(x_1\cdots x_{n-1}) = \sum_{\lambda=0}^{\sigma}(-x_n)^{\lambda}\varphi_{\sigma-\lambda}^{(n)}(x_1\cdots x_n), \tag{5.39a}$$

$$\beta_{\sigma}^{(n)}(x_1\cdots x_n) = \sum_{\lambda=0}^{\sigma}x_n^{\lambda}\beta_{\sigma-\lambda}^{(n-1)}(x_1\cdots x_{n-1}). \tag{5.39b}$$

The sum (5.38c) is given explicitly by

$$S^{(q,r)}([m]_n, [m]_{n-1})$$
$$= I_{q+r}^{(n-1)}([m]_{n-1}) - \sum_{\lambda=0}^{n-2}\sum_{\mu=0}^{q-\lambda-2}\sum_{\nu=0}^{\lambda}\sum_{\sigma=0}^{\nu}(-1)^{\lambda-\nu}$$
$$\times \binom{\nu}{\sigma}\beta_{q-\lambda-\mu-2}^{(n)}(x)\varphi_{\lambda-\nu}^{(n-1)}(y+1)$$
$$\times \left(\sum_{\tau=0}^{n}(-1)^{\tau}\varphi_{\tau}^{(n)}(x)\beta_{r+\mu+\sigma-\tau+2}^{(n-1)}(y)\right), \tag{5.40}$$

in which $x_i = p_{in}$ and $y_i = p_{in-1}$. Observe that the sum is zero for $q = 0$ or 1.

The specification of the adjoint $U(n):U(n-1)$ projective operators is complete only when the preceding list of reduced matrix elements is supplemented with a description of the vanishings of the respective matrix elements. It is convenient for the discussion to classify these vanishings into three types [we assume that the initial (state) labels in the reduced matrix element (5.34) *are lexical*]: (1) vanishings which occur because the final labels in the matrix element (5.34) violate lexicality; (2) vanishings which occur when all IR labels *are lexical*, but either one or the other, or both, of the normalization functions $N_{n-\rho}^{(n)}$ or $N_{n-\alpha-1}^{(n-1)}$ vanishes; (3) all other vanishings.

Vanishings of type (1) may also be called "pattern calculus factor vanishings," since they always arise from the vanishing of one or more numerator terms in the pattern calculus factor. These vanishings are easily recognized, and are not difficult to interpret.

Vanishings of type (2), as well as type (1), can always be traced to the following characteristic (for any n) of the direct product: The number of occurrences of the IR, $[m] + [\Delta(\Gamma)]$, in the direct product, $[m] \times [M]$, can be less than the multiplicity of the Δ pattern, $[\Delta(\Gamma)]$. Type (2) vanishings occur only when a Δ pattern has a multiplicity > 1, and the vanishings are more difficult to recognize than are those of type (1). Hence, we choose to discuss them separately.

The zeros of the normalization functions $N_{n-\rho}^{(n)}$ and $N_{n-\alpha-1}^{(n-1)}$ occurring in the explicit expressions for the adjoint reduced matrix elements are established in Appendix E. These results imply that the reduced matrix elements (5.34) vanish if: Class b: The sequence $S_{n-1} = \{m_{1n-1} - m_{2n-1}, \cdots, m_{n-2n-1} - m_{n-1n-1}\}$ contains α or more zeros ($\alpha = 1, 2, \cdots, n-2$); Class c: The sequence $S_n = \{m_{1n} - m_{2n}, \cdots, m_{n-1n} - m_{nn}\}$ contains ρ or more zeros ($\rho = 1, 2, \cdots, n-1$); Class d: Either the sequence S_{n-1} contains α or more zeros or the sequence S_n contains ρ or more zeros, or both ($\alpha = 1, 2, \cdots, n-2$, $\rho = 1, 2, \cdots, n-1$).

Finally, there are the vanishings of type (3). These vanishings occur even when all the detailed conditions imposed by the reduction of the direct product *are satisfied*, i.e., for *initial arbitrary states*. In other words, a particular projective operator for which these vanishings occur *is the zero operator*. In the adjoint system, only the projective operators associated with the $U(n)$ generators possess this property, i.e.,

$$\begin{bmatrix}(n-1, n-1)\\ [1\ \ 0\ \ -1]\\ (\alpha, \beta)\end{bmatrix} = 0, \tag{5.41}$$

for $\alpha \neq \beta = 1, 2, \cdots, n-1$. These zero operators are "intrinsic" to the generators: *A generator cannot effect a shift* $\Delta_{n-1}(\alpha) - \Delta_{n-1}(\beta)$, $\alpha \neq \beta$, of the $U(n-1)$ IR labels $[m]_{n-1}$.

6. THE EXTENDED PROJECTIVE OPERATORS

A $U(n):U(n-1)$ projective operator can be generalized by extending the domain of definition [the sets of $U(n)$ and $U(n-1)$ IR labels of these operators]; namely, we introduce an extra label m_{nn-1} into the set of $U(n-1)$ IR labels. It might appear, at this stage, that such an extension is but a formal construct which recognizes and enhances the similar roles played by upper and lower operator patterns of the projective operator. It is the purpose of this section to demonstrate that, quite to the contrary, the concept of extended projective operators provides an essential structural link between (nonextended) $U(n):U(n-1)$ projective operators and (nonextended) $U(n-1):U(n-2)$ projective operators and, indeed, that extended projective operators have an independent existence. In particular, because these extended operators play a significant role for the understanding

of certain structural properties of the adjoint reduced Wigner coefficients of Sec. 5, we allocate this section to a brief discussion of the ideas.

The idea which underlies the generalization of $U(n):U(n-1)$ projective operators was indicated in the earlier work[2] on the development of the pattern calculus. It was recognized then that the pattern calculus rules could be extended to include n dots in row $n-1$, in which case the shift $\Delta_{nn}(\gamma)$ from the lower pattern is assigned to this dot; the arrow pattern is then constructed just as before. One then assigns the partial hooks $p_{1n} > p_{2n} > \cdots > p_{nn}$, respectively, to the n dots of row n, while the partial hooks $p_{1n-1} > p_{2n-1} > \cdots > p_{n-1n-1} > p_{nn-1}$, respectively, are assigned to the n dots of row $n-1$. *Here p_{nn-1} appears as a new variable.* Finally, one writes out the pattern calculus factor using rules (3)–(5) (cf. Sec. 2D). In this manner, an *extended pattern calculus factor* $(\mathrm{PCF})_{\mathrm{ext}}$ is associated with each $U(n):U(n-1)$ projective operator. It was then observed[2] that one recovers the ordinary pattern calculus factor (PCF) by the simple device of letting p_{nn-1} go to $-\infty$: $(\mathrm{PCF})_{\mathrm{ext}} \to (\mathrm{PCF})$ as $p_{nn-1} \to -\infty$. In particular, when the upper and lower operator patterns are extremal, one obtains the set of extremal $U(n):U(n-1)$ reduced Wigner coefficients as the limit of the corresponding set of extended coefficients.

Extended projective operators are completely defined by the rules of the extended pattern calculus *when the upper and lower operator patterns are extremal.* However, since the associated pattern calculus factor contains a new variable p_{nn-1} and it is not clear that it is meaningful to introduce this new variable into the Hilbert space of state vectors, we avoid the idea of state vectors in interpreting extended operators.

There is another point of view which is vividly suggested by the pattern calculus and which admits of generalization: We introduce a point $([x];[y]) = (x_1, x_2, \cdots, x_n; y_1, y_2, \cdots, y_n)$ of the real, Euclidean space R^{2n}. Next, we define the extended unit projective function of type $[M]_n$, denoted by

$$\begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix}_{\mathrm{ext}}, \tag{6.1}$$

to be a real-valued function which is defined on all *ordered pairs* of points $([x'];[y']) \in R^{2n}$ and $([x];[y]) \in R^{2n}$. We denote the value of this function by the notation

$$\left\langle \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \middle| \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix}_{\mathrm{ext}} \middle| \begin{pmatrix} [x] \\ [y] \end{pmatrix} \right\rangle. \tag{6.2}$$

The value (6.2) of the unit projective function (6.1) is defined to be 0 unless:

(a) The points $([x'], [y'])$ and $([x], [y])$ consist of *ordered integers*

$$x_1 \geq y_1 \geq x_2 \geq y_2 \geq \cdots \geq x_n \geq y_n, \tag{6.3a}$$

$$x'_1 \geq y'_1 \geq x'_2 \geq y'_2 \geq \cdots \geq x'_n \geq y'_n; \tag{6.3b}$$

(b) the point $([x'];[y'])$ is related to the point $([x];[y])$ by

$$[x'] = [x] + [\Delta(\Gamma)], \tag{6.4a}$$

$$[y'] = [y] + [\Delta(\gamma)], \tag{6.4b}$$

where $\Delta(\Gamma)$ and $\Delta(\gamma)$ denote, respectively, the Δ patterns of the upper and lower operator patterns of the function (6.1).

Finally, for (Γ) and (γ) extremal patterns, the value (6.2) of the unit projective function (6.1) is defined to be the result obtained by applying the extended pattern calculus rules and using the identification

$$p_{in} = x_i + n - i, \quad p_{in-1} = y_i + n - 1 - i, \tag{6.5a}$$

for $i = 1, 2, \cdots, n$; or, equivalently,

$$m_{in} = x_i, \quad m_{in-1} = y_i. \tag{6.5b}$$

More generally, we use the term *projective function* to designate any real-valued function P whose domain of definition is the set of all *ordered pairs of points of ordered integers.* The value of such a function is denoted by

$$\left\langle \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \middle| P \middle| \begin{pmatrix} [x] \\ [y] \end{pmatrix} \right\rangle. \tag{6.6}$$

The product of an ordinary point function f [defined on the ordered points (6.3)] with a projective function P is denoted by fP and is defined to be the projective function with values

$$f([x'];[y']) \left\langle \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \middle| P \middle| \begin{pmatrix} [x] \\ [y] \end{pmatrix} \right\rangle. \tag{6.7}$$

Similarly, Pf is the projective function which has the value obtained from (6.7) by replacing $f([x'],[y'])$ with $f([x];[y])$. (Note that $fP \neq Pf$, in general.)

The product of two projective functions, P' and P, is denoted by $P'P$, and is defined to be the projective function with values

$$\left\langle \begin{pmatrix} [x''] \\ [y''] \end{pmatrix} \middle| P'P \middle| \begin{pmatrix} [x] \\ [y] \end{pmatrix} \right\rangle = \sum_{[x'],[y']} \left\langle \begin{pmatrix} [x''] \\ [y''] \end{pmatrix} \middle| P' \middle| \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \right\rangle \left\langle \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \middle| P \middle| \begin{pmatrix} [x] \\ [y] \end{pmatrix} \right\rangle. \tag{6.8}$$

In particular, for the types of projective functions which we consider, the sum in Eq. (6.8) is always finite, so that no problems of convergence arise.

The projective function denoted by $P^\dagger$ is defined to be the projective function with values

$$\left\langle \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \middle| P^\dagger \middle| \begin{pmatrix} [x] \\ [y] \end{pmatrix} \right\rangle = \left\langle \begin{pmatrix} [x] \\ [y] \end{pmatrix} \middle| P \middle| \begin{pmatrix} [x'] \\ [y'] \end{pmatrix} \right\rangle. \quad (6.9)$$

The preceding rules, which serve to define the algebra of projective functions, are clearly designed to duplicate certain aspects of the algebra of the nonextended $U(n):U(n-1)$ projective operators. Indeed, if one deletes variable y_n, then we have simply enumerated various properties of nonextended $U(n):U(n-1)$ projective operators using a different language.

Next, we define the null space of the extended unit projective function (6.1): Let $([x], [y])$ denote a point which satisfies the order relation (6.3a). The *null space* of the extended unit projective function (6.1) is defined to be the set of all points $\{([x]; [y])\}$ for which the value (6.2) is zero. In particular, the null space includes all points $([x]; [y])$ such that the point $([x']; [y'])$ defined by Eqs. (6.4) does not satisfy the order relation (6.3b); however, there are, in general, other points in the null space.

The preceding discussion is an elaboration of the various *definitions* relating to the idea of projective functions and the definitions of the operations of: (i) multiplication by a "scalar," i.e., fP or Pf; (ii) the addition of two projective functions $P' + P$; (iii) the distributive law with respect to scalar multiplication $(f+g)P = fP + gP$; and (iv) the multiplication of two projective functions, $P'P$. [While we did not define operations (ii) and (iii) explicitly, it is clear how this is done.] We now turn to the more interesting problem of constructing *unit projective functions.*

The formal theory we are developing already possesses a great deal of *explicit content*: Namely, we know completely and uniquely the class of unit projective functions which are defined by the rules of the pattern calculus. The problem is to give the more general construction for those cases where the pattern calculus fails to give the complete answer. Furthermore, we are not interested in constructing an arbitrary algebra, but rather one which relates directly to the $U(n):U(n-1)$ projective operators about which we already have a great deal of structural information.

For purposes of discussion, let us assume that we have succeeded in constructing the canonical set of $U(n)$ Wigner operators. Then the canonical $U(n)$ Racah functions [Eq. (2.46)] are also determined. (Even if the explicit construction is unknown, the existence of such Racah functions is firmly established.)

We can therefore define the extended unit projective functions *recursively* by the coupling rule:

$$\begin{bmatrix} \cdot \\ [M] + \Delta_n(\rho) \\ \cdot \end{bmatrix}_{\text{ext}} = \begin{bmatrix} \cdot \\ [1 \quad \dot{0}] \\ \cdot \end{bmatrix}_{\text{ext}} \begin{matrix} \{R_u\} \\ \\ \{R_\ell\} \end{matrix} \begin{bmatrix} \cdot \\ [M] \\ \cdot \end{bmatrix}_{\text{ext}}, \quad (6.10)$$

where $\{R_u\}$ denotes (symbolically) the fundamental $U(n)$ Racah function and couples the upper operator patterns and $\{R_\ell\}$ denotes a similar fundamental $U(n)$ Racah function, but couples the lower operator patterns. More precisely, the result expressed symbolically by Eq. (6.10) is as follows:

$$\begin{aligned} \delta_{\rho\alpha} \begin{bmatrix} (\Gamma') \\ [M] + \Delta_n(\rho) \\ (\gamma') \end{bmatrix}_{\text{ext}} &= \sum_{\substack{\tau,(\Gamma) \\ \beta,(\gamma)}} \left\{ \begin{pmatrix} [M] + \Delta_n(\rho) \\ (\Gamma') \end{pmatrix} \begin{pmatrix} \rho \\ [1 \quad \dot{0}] \\ \tau \end{pmatrix} \begin{pmatrix} [M] \\ (\Gamma) \end{pmatrix} \right\}_u \\ &\times \left\{ \begin{pmatrix} [M] + \Delta_n(\alpha) \\ (\gamma') \end{pmatrix} \begin{pmatrix} \alpha \\ [1 \quad \dot{0}] \\ \beta \end{pmatrix} \begin{pmatrix} [M] \\ (\gamma) \end{pmatrix} \right\}_\ell \\ &\times \begin{bmatrix} \tau \\ [1 \quad \dot{0}] \\ \beta \end{bmatrix}_{\text{ext}} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix}_{\text{ext}} \end{aligned} \quad (6.11)$$

In this definition, the $U(n)$ Racah functions $\{\cdots\}$ play the roles of scalar multipliers introduced earlier. Let us emphasize once more the fact that in this result $\{\cdots\}_u$ and $\{\cdots\}_\ell$ are *each* fundamental $U(n)$ Racah functions: The indices u (for upper) and ℓ (for lower) simply designate that, in evaluating Eq. (6.11) between the points $([x']; [y'])$ and $([x]; [y])$, the Racah function labeled with index u is to be evaluated on $[x']$, while the Racah function labeled with index ℓ is to be evaluated on $[y']$. Thus, for the same operator pattern entries in both $\{\cdots\}_u$ and $\{\cdots\}_\ell$ and for $[y'] = [x']$, we have the result

$$\{\cdots\}_u([x']) = \{\cdots\}_\ell([x']). \quad (6.12)$$

We remark that Eq. (6.11)—together with its analog for coupling $[\dot{0} \quad -1]_{\text{ext}}$—suffices to define all extended unit projective functions, starting from the known results for $[\dot{1}_k \quad \dot{0}_{n-k}]_{\text{ext}}$ and $[\dot{0}_k \quad -\dot{1}_{n-}]_{\text{kext}}$.

At this stage of the development, the introduction of the extended unit projective functions is ad hoc to a certain extent. However, we are justified in following this course if the quantities so introduced can be demonstrated to have a significant structural relation

to the canonical $U(n):U(n-1)$ reduced Wigner coefficients which we seek. It is our intent to demonstrate this relevance explicitly for the adjoint $U(n):U(n-1)$ reduced Wigner coefficients.

Next, we wish to note (without giving the details of the proofs) the following important properties which the extended projective functions, defined by Eq. (6.11), possess;

Orthogonality relations:

$$\sum_{(\gamma)} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix}_{\text{ext}} \begin{bmatrix} (\Gamma') \\ [M] \\ (\gamma) \end{bmatrix}^{\dagger}_{\text{ext}} = \delta_{(\Gamma)(\Gamma')} I_{(\Gamma)}, \quad (6.13a)$$

$$\sum_{(\Gamma)} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix}^{\dagger}_{\text{ext}} \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma') \end{bmatrix}_{\text{ext}} = \delta_{(\gamma)(\gamma')} I'_{(\gamma)}; \quad (6.13b)$$

boundary property for $[y] = [x]$:

$$\left\langle \begin{pmatrix} [x] + [\Delta(\Gamma)] \\ [x] + [\Delta(\gamma)] \end{pmatrix} \middle| \begin{bmatrix} (\Gamma) \\ [M] \\ (\gamma) \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} [x] \\ [x] \end{pmatrix} \right\rangle = \delta_{(\Gamma)(\gamma)} I'_{(\gamma)}([x]). \quad (6.14)$$

In Eq. (6.13a), $I_{(\Gamma)}$ is a scalar function whose values depend only on the variables $[x]$ of the point $([x]; [y])$. It is defined as follows: $I_{(\Gamma)}([x]) = 0$ for each $[x]$ which belongs to *the null space of the $U(n)$ Wigner operator* $\left\langle \begin{matrix} (\Gamma) \\ [M] \\ \cdot \end{matrix} \right|^{\dagger}$; otherwise, it has value 1.

Similarly, $I'_{(\gamma)}$ is a scalar function whose values depend only on the variables $[y]$ of the point $([x]; [y])$. It is defined as follows: $I'_{(\gamma)}([y]) = 0$ for each $[y]$ which belongs to *the null space of the $U(n)$ Wigner operator* $\left\langle \begin{matrix} (\gamma) \\ [M] \\ \cdot \end{matrix} \right|$; otherwise, it has value 1.

The occurrence of the "null-space functions" of $U(n)$ Wigner operators in Eqs. (6.13) and (6.14) assures that the null spaces of extended unit projective operators will relate in a definite manner to the properties of the two $U(n)$ intertwining numbers associated with the triples of IR labels $[x] + [\Delta(\Gamma)]$, $[M]$, $[x]$ and $[y] + [\Delta(\gamma)]$, $[M]$, $[y]$, respectively.

The method of proving Eqs. (6.13) and (6.14) is as follows: One first verifies *directly* that these relations are correct for the $[1 \quad \dot{0}]_{\text{ext}}$ and $[\dot{0} \quad -1]_{\text{ext}}$ projective functions (a nontrivial task!); second, one assumes the validity of Eqs. (6.13) and (6.14) for *all* labels $[M]$ which sum to some fixed integer N; finally, one uses definition (6.11) (and its counterpart for $[\dot{0} \quad -1]_{\text{ext}}$) and the orthogonality properties of $U(n)$ Racah functions to prove that Eqs. (6.13) and (6.14) hold for all labels $[M]$ which sum to $N+1$ $(N-1)$. The general result then follows by induction. In this connection, we wish to note explicitly property (6.14) for the fundamental projective functions (established from the explicit pattern calculus expression):

$$\left\langle \begin{pmatrix} [x] + \Delta_n(\rho) \\ [x] + \Delta_n(\alpha) \end{pmatrix} \middle| \begin{bmatrix} \rho \\ [1 \quad \dot{0}] \\ \alpha \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} [x] \\ [x] \end{pmatrix} \right\rangle = \delta_{\rho\alpha} I'_{\alpha}([x]), \quad (6.15a)$$

where

$$I'_{\alpha}([x]) = 0, \quad \text{if} \quad x_{\alpha-1} = x_{\alpha},$$
$$= 1, \quad \text{otherwise}; \quad (6.15b)$$

$$\left\langle \begin{pmatrix} [x] - \Delta_n(\rho) \\ [x] - \Delta_n(\alpha) \end{pmatrix} \middle| \begin{bmatrix} \bar{\rho} \\ [\dot{0} \quad -1] \\ \bar{\alpha} \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} [x] \\ [x] \end{pmatrix} \right\rangle = \delta_{\bar{\rho}\bar{\alpha}} I'_{\bar{\alpha}}([x]), \quad (6.16a)$$

where

$$I'_{\bar{\alpha}}([x]) = 0, \quad \text{if} \quad x_{\alpha} = x_{\alpha+1},$$
$$= 1, \quad \text{otherwise}. \quad (6.16b)$$

There are two important limit properties relating to the extended projective functions. It is these properties which demonstrate the relevance of the definition of extended unit projective functions to $U(n):U(n-1)$ reduced Wigner coefficients. We state the results and then discuss the method of proof, indicating the limited extent to which we have, in fact, established the general proof:

$$\lim_{y_n \to -\infty} \left\langle \begin{pmatrix} [x]_n + [\Delta(\Gamma)]_n \\ [y]_n + [\Delta(\gamma)]_n \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} [x]_n \\ [y]_n \end{pmatrix} \right\rangle$$
$$= \left\langle \begin{pmatrix} [x]_n + [\Delta(\Gamma)]_n \\ [y]_{n-1} + [\Delta(\gamma)]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \middle| \begin{pmatrix} [x]_n \\ [y]_{n-1} \end{pmatrix} \right\rangle, \quad (6.17a)$$

$$\lim_{x_n \to -\infty} \left\langle \begin{pmatrix} [x]_n + [\Delta(\Gamma)]_n \\ [y]_{n-1} + [\Delta(\gamma)]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \middle| \begin{pmatrix} [x]_n \\ [y]_{n-1} \end{pmatrix} \right\rangle$$
$$= \delta_{[\gamma]_{n-1}[\Gamma]_{n-1}}$$
$$\times \left\langle \begin{pmatrix} [x]_{n-1} + [\Delta(\Gamma)]_{n-1} \\ [y]_{n-1} + [\Delta(\gamma)]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} (\Gamma)_{n-2} \\ [\gamma]_{n-1} \\ (\gamma)_{n-2} \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} [x]_{n-1} \\ [y]_{n-1} \end{pmatrix} \right\rangle. \quad (6.17b)$$

Equation (6.17a) asserts that, in the limit of large negative y_n, the value of an extended unit projective function *is a* $U(n):U(n-1)$ *reduced Wigner coefficient.* This is just the property discussed at the beginning of this section, and known to be valid for the class of extended projective functions having extremal operator patterns. Equation (6.17a) asserts the validity of this property, in general.

Equation (6.17b) is a completely new result. It asserts that, in the limit of large negative x_n $(= p_{nn})$, a $U(n):U(n-1)$ reduced Wigner coefficient limits to zero for $[\Gamma]_{n-1} \neq [\gamma]_{n-1}$, and for $[\Gamma]_{n-1} = [\gamma]_{n-1}$ it limits to the value of definite extended unit projective function defined on R^{2n-2}. *It is this property which will give a precise meaning to operator patterns.*

The proofs of Eqs. (6.17) depend on the validity of the conjectured relation (3.6) as applied to the particular cases $[M'] = [1 \ \dot{0}]$ and $[M'] = [\dot{0} \ -1]$. *If this conjectured relation is correct*, the proofs of Eqs. (6.17) follow from Eq. (6.11) by using an induction argument which parallels the one outlined previously in this section.

Thus, we can claim to have proved Eqs. (6.17) for the following important cases: (a) the class of all unit projective functions having extremal upper and lower operator patterns and (b) *the class of all adjoint* ($[M] = [1 \ \dot{0} \ -1]$) *unit projective functions* [since Eq. (3.6) has been demonstrated to be valid for the adjoint Racah functions]. Although we lack a general proof of Eqs. (6.17a) and (6.17b), the remarkable fact that they are correct for the aforementioned nontrivial cases requires that these relations be noted.

Properties (6.17a) and (6.17b) can be summarized by writing

$$\begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix}_{\text{ext}} \rightarrow \begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \rightarrow \delta_{[\gamma]_{n-1}[\Gamma]_{n-1}} \begin{bmatrix} (\Gamma)_{n-2} \\ [\gamma]_{n-1} \\ (\gamma)_{n-2} \end{bmatrix}_{\text{ext}}, \tag{6.18}$$

where the arrow designates restriction of the domain of definition of the respective projective functions by first letting $y_n \rightarrow -\infty$, and then letting $x_n \rightarrow -\infty$.

Let us also note that the existence of the limit of a (nonextended) projective function at level n *implies* the existence of an extended projective function at level $n-1$: Equation (6.17b) is a quantitative statement of this property.

We conclude this section with some comments relating to $U(2)$ and $U(3)$. For $n = 2$, the $U(2):U(1)$ projective functions are the functions whose values are the ordinary $SU(2)$ Wigner coefficients.[26] But, in this case, the Racah functions, in particular the fundamental (spin $\frac{1}{2}$) ones, are known. We can therefore construct explicitly, using Eq. (6.11), the set of *extended Wigner coefficients,*

$$\left\langle \begin{pmatrix} m'_{12} & & m'_{22} \\ & m'_{11} & \end{pmatrix} \middle| \begin{bmatrix} & \Gamma_{11} & \\ M_{12} & & M_{22} \\ & \gamma_{11} & \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} m_{12} & & m_{22} \\ & m_{11} & \end{pmatrix} \right\rangle. \tag{6.19}$$

Indeed, we have carried out this construction and proved directly the properties expressed by Eqs. (6.13) and (6.14). These extended Wigner coefficients are orthogonal, they satisfy the boundary property (6.14), and they become the ordinary Wigner coefficients in the limit $m_{21} \rightarrow -\infty$. The set of extended $U(2)$ Wigner coefficients, in other words, is a well-defined structure having an independent existence of its own.

One can go still further. We can use Eq. (5.17) (for $q = 1$) to calculate the matrix elements of *the set of "extended generators,"* $\{E_{ij}^{(\text{ext})}, i,j = 1,2,\cdots\}$. However, *the commutation relations of these "extended generators" close only in the limit* $m_{21} \rightarrow -\infty$. This suggests strongly that extended Wigner coefficients are not group-theoretical objects; rather, only their limits possess group properties.

We conjecture [Eq. (6.17b)] that these extended $U(2)$ Wigner coefficients appear in still another context, namely, as the limiting structure of the canonical $U(3):U(2)$ reduced Wigner coefficients:

$$\lim_{m_{33}\rightarrow-\infty} \left\langle \begin{pmatrix} m'_{13} & & m'_{23} & & m'_{33} \\ & m'_{12} & & m'_{22} & \end{pmatrix} \middle| \begin{bmatrix} & & \Gamma_{11} & & \\ & \Gamma_{12} & & \Gamma_{22} & \\ M_{13} & & M_{23} & & M_{33} \\ & \gamma_{12} & & \gamma_{22} & \\ & & \gamma_{11} & & \end{bmatrix} \middle| \begin{pmatrix} m_{13} & & m_{23} & & m_{33} \\ & m_{12} & & m_{22} & \end{pmatrix} \right\rangle$$

$$= \delta_{\Gamma_{12}\gamma_{12}}\delta_{\Gamma_{22}\gamma_{22}} \left\langle \begin{pmatrix} m'_{13} & & m'_{23} \\ & m'_{12} & \end{pmatrix} \middle| \begin{bmatrix} & \Gamma_{11} & \\ \gamma_{12} & & \gamma_{22} \\ & \gamma_{11} & \end{bmatrix}_{\text{ext}} \middle| \begin{pmatrix} m_{13} & & m_{23} \\ & m_{12} & \end{pmatrix} \right\rangle. \tag{6.20}$$

(We repeat that this relation has been verified in many special cases.)

7. A PROPOSITION CONCERNING THE CANONICAL WIGNER OPERATORS

The purpose of this section is to tie together various properties of the explicit adjoint Wigner operators developed in Sec. 5. We are now able to indicate the structural principle which underlies the origin of operator patterns, including those which belong to the same multiplicity set. Furthermore, we wish to demonstrate how this set of operators accords with more general concepts, including null space and conjugation properties and that—far from being arbitrary or ad hoc—this set is, in fact, canonical. That is to say, the set of operators constructed in Sec. 5 will be shown to involve no free choice, aside from the primitive order $1, 2, \cdots, n$ of the Weyl subgroup labeling.

A. An Operational Definition of Operator Patterns

Operator patterns were originally introduced (Ref. 5, Paper IV) in analogy to the state-vector Gel'fand patterns: The labels of a complete set of Wigner operators of prescribed IR labels $[M]$ were shown to be in 1-to-1 correspondence with the Gel'fand patterns of the state vectors; furthermore, one of the significant properties of operator patterns was demonstrated to be the shift property $[m] \rightarrow [m] + [\Delta(\Gamma)]$. The assignments of operator patterns to Wigner operators is then already unique for the class of operator patterns which has multiplicity one (the Δ pattern then determines uniquely the operator pattern). However, when the multiplicity is greater than one, we have a number of distinct operator patterns to assign to an equal number of distinct Wigner operators (the ones having a prescribed Δ pattern for prescribed $[M]$), and we have thus far stated no general property of Wigner operators whereby the mapping: (patterns) $\rightleftarrows$ (operators) is uniquely determined *in all cases.*

The properties of the set of adjoint Wigner operators developed in the preceding sections provide us with the first definitive clue as to the general origin of the mapping of patterns onto operators: *The assignment of operator patterns to Wigner operators is uniquely induced by the limit properties of the Wigner operators.*

Let us illustrate how the limit property could be used to assign operator patterns in the simplest case, $U(2)$. The number of Wigner operators with IR labels $[M_{12}\ M_{22}]$ is $M_{12} - M_{22} + 1$, and a unique operator pattern is assigned to a particular Wigner operator in the set in accordance with the shift $[\Delta_1\ \Delta_2]$ which the particular operator effects on the IR labels $[m_{12}\ m_{22}]$ of a generic state vector. We wish now to demonstrate how the operator label could be assigned by limits. For this purpose, we consider initially that the members of the set of orthonormal Wigner operators are enumerated by an index σ:

$$\left\{T_\sigma\begin{pmatrix} M_{12} & & M_{22} \\ & M_{11} & \end{pmatrix},\ \sigma = 1, 2, \cdots, M_{12} - M_{22} + 1\right\}. \tag{7.1}$$

Since these operators are unique, their matrix elements are fully known [the $U(2)$ Wigner coefficients] on general states. Next, we take the limit $m_{22} \rightarrow -\infty$ in the set of matrix elements of the operators (7.1) corresponding to M_{11} fixed, but having σ ranging over the values $1, 2, \cdots, M_{12} - M_{22} + 1$. We find that the matrix elements of *all but one* of the operators vanish and that all the matrix elements of this one operator limit to unity. We assign this operator the operator pattern M_{11}, and observe that the operator so labeled is precisely the one which effects the shift $\Delta = [M_{11}, M_{12} + M_{22} - M_{11}]$. Repeating this procedure for each $M_{11} = M_{12}, M_{12} - 1, \cdots, M_{22}$, we are able to assign uniquely the operator patterns $\Gamma_{11} = M_{12}, M_{12} - 1, \cdots, M_{22}$ to the Wigner operators (7.1). The final set of fully labeled Wigner operators is then characterized by the limit property

$$\lim_{m_{22}\rightarrow-\infty}\left\langle\begin{pmatrix} m_{12}+\Delta_1 & & m_{22}+\Delta_2 \\ & m_{11}+M_{11} & \end{pmatrix}\right|\left\langle\begin{matrix} & \Gamma_{11} & \\ M_{12} & & M_{22} \\ & M_{11} & \end{matrix}\right\rangle\left|\left\langle\begin{pmatrix} m_{12} & & m_{22} \\ & m_{11} & \end{pmatrix}\right\rangle\right. = \delta_{M_{11}\Gamma_{11}}, \tag{7.2}$$

where $\Delta_1 = \Gamma_{11}$, $\Delta_2 = M_{12} + M_{22} - \Gamma_{11}$. We have thus demonstrated that: *The label* Γ_{11} *induced by limits is precisely the label assigned by the shift property.*

Now let us show how the concept of a limit property can (and hence must) be used to induce *all* the operator pattern labels of the adjoint Wigner operators. This is accomplished by induction on n. Thus, we start with the explicit $U(3):U(2)$ reduced Wigner coefficients in which the lower $U(2)$ operator patterns have been completely assigned, but we use an index $\sigma = 1, 2, \cdots, 8$ to enumerate the eight adjoint Wigner operators $\langle 1\ \ 0\ \ -1\rangle$. Thus, the projective operators are designated by

$$\begin{bmatrix} & \sigma & \\ 1 & 0 & -1 \\ & \alpha\ \ \beta & \\ & \gamma & \end{bmatrix},\ \sigma = 1, 2, \cdots, 8. \tag{7.3}$$

The matrix elements of these operators are just the ones constructed explicitly in Sec. 5 (for $n = 3$), but now identified by an arbitrary index σ in place of upper operator patterns, since it is our aim to illustrate how the limit properties of the matrix elements themselves induce the upper pattern assignments.

We now take the limits, $p_{33} \to -\infty$ followed by $p_{22} \to -\infty$, of the matrix elements of all sixty-four $U(3):U(2)$ projective operators. The results are as follows: For $[\alpha\beta] = [1 \quad -1]$, the matrix elements of all but three of the operators vanish: The matrix elements of each of these three operators has a distinct limit; these limits are, in fact, the matrix elements of the $U(2):U(1)$ projective operators

$$\begin{bmatrix} & \Gamma & \\ 1 & & -1 \\ & \gamma & \end{bmatrix},$$

where Γ takes three values 1, 0, and -1. This limit procedure has therefore assigned the labels $\begin{pmatrix} & \Gamma & \\ 1 & & -1 \end{pmatrix}$ to the respective operators such that

$$\begin{bmatrix} & \Gamma & & \\ 1 & & -1 & \\ & 0 & & -1 \\ 1 & & -1 & \\ & \gamma & & \end{bmatrix} \to \begin{bmatrix} & \Gamma & \\ 1 & & -1 \\ & \gamma & \end{bmatrix}. \tag{7.4}$$

We now go back to the original matrix elements, set $[\alpha\beta] = [1 \quad 0]$, and repeat the limit procedure. We find that the matrix elements of all but two of the operators vanish and, in particular, that the matrix elements of the three already labeled operators also vanish. The two operators which have nonzero matrix elements in the limit are found to have matrix elements which limit, 1-to-1, to the matrix elements of the $U(2):U(1)$ projective operators

$$\begin{bmatrix} & \Gamma & \\ 1 & & 0 \\ & \gamma & \end{bmatrix},$$

where Γ takes on the two values 1 and 0. We assign these two operators the upper pattern in accordance with the limit

$$\begin{bmatrix} & \Gamma & & \\ 1 & & 0 & \\ & 0 & & -1 \\ 1 & & 0 & \\ & \gamma & & \end{bmatrix} \to \begin{bmatrix} & \Gamma & \\ 1 & & 0 \\ & \gamma & \end{bmatrix}. \tag{7.5}$$

Again we repeat the procedure, this time for $[\alpha\beta] = [0 \quad -1]$. The matrix elements of the already labeled operators vanish, but of the three unlabeled operators the matrix elements of two limit, 1-to-1, to the matrix elements of

$$\begin{bmatrix} & \Gamma & \\ 0 & & -1 \\ & \gamma & \end{bmatrix},$$

where Γ takes the two values 0 and -1. Thus, the assignment

$$\begin{bmatrix} & \Gamma & & \\ 1 & & -1 & \\ & 0 & & -1 \\ 0 & & -1 & \\ & \gamma & & \end{bmatrix} \to \begin{bmatrix} & \Gamma & \\ 0 & & -1 \\ & \gamma & \end{bmatrix} \tag{7.6}$$

is induced.

In the last step, we repeat the procedure with $[\alpha\beta] = [0 \quad 0]$. The matrix elements of the seven already labeled operators vanish, but the remaining operator has matrix elements which limit to those of

$$\begin{bmatrix} & 0 & \\ 0 & & 0 \\ & 0 & \end{bmatrix} = 1.$$

It is assigned these labels in accordance with

$$\begin{bmatrix} & 0 & & \\ 0 & & 0 & \\ & 0 & & -1 \\ 0 & & 0 & \\ & 0 & & \end{bmatrix} \to \begin{bmatrix} & 0 & \\ 0 & & 0 \\ & 0 & \end{bmatrix}. \tag{7.7}$$

For the six unique operators (those having $\Delta =$ permutation of $[1 \quad 0 \quad -1]$), the preceding assignments of operator patterns by limits are precisely the same as those determined by the Δ patterns. However, the limit procedure also assigns a unique operator pattern to each of the two operators having $\Delta = [000]$. *The projective operator labeled by the degree index $q = 1$ is the one with property (7.7); the other one, labeled by the degree index $q = 2$, is the one with property (7.4) for $\Gamma = 0$.*

Having assigned all operator patterns for $n = 3$ (in the adjoint system), we now repeat the procedure for the $U(4):U(3)$ projective operators (the limit procedure is now $p_{44} \to -\infty$ followed by $p_{33} \to -\infty$). We continue this process upward to n and arrive at the following general result: The $n(n-1)$ adjoint Wigner operators having Δ pattern equal to a permutation of $[1 \quad 0 \quad -1]$ are assigned operator patterns by the limit procedure in complete agreement with those assigned by the Δ pattern; the $n-1$ adjoint Wigner

operators having $\Delta = [\dot{0}]$ are assigned operator patterns given by

$$\begin{pmatrix} [1 \quad \dot{0} \quad -1] \\ q \end{pmatrix} \to \begin{pmatrix} [1 \quad \dot{0} \quad -1] \\ (n-q, n-q) \end{pmatrix}, \tag{7.8}$$

where q is the degree index introduced in Sec. 5 and the notation on the right-hand side of Eq. (7.8) is that introduced by Eq. (4.1).

One now observes that, in general, the concept of inducing operator patterns by limits depends crucially on properties (6.17a, b). Taking the limit

$$y_{n-1} = m_{n-1\,n-1} \to -\infty$$

of Eq. (6.17b) and using property (6.17a) for $n \to n-1$, we can symbolize the result as follows:

$$\begin{bmatrix} (\Gamma)_{n-1} \\ [M]_n \\ (\gamma)_{n-1} \end{bmatrix} \to \delta_{[\gamma]_{n-1}[\Gamma]_{n-1}} \begin{bmatrix} (\Gamma)_{n-2} \\ [\gamma]_{n-1} \\ (\gamma)_{n-2} \end{bmatrix}, \tag{7.9}$$

in which the arrow designates the restriction of the operator which obtains upon restricting the domain of definition by taking the two limits, first $p_{nn} \to -\infty$, then $p_{n-1\,n-1} \to -\infty$.

If we regard the lower operator pattern in Eq. (7.9) as having already been assigned [by building up from $U(2)$], then Eq. (7.9) is an expression of a very general branching law whereby the upper pattern assignments are induced from the lower ones as follows: Under restriction of the domain of definition by taking limits, a $U(n):U(n-1)$ projective operator either restricts to the zero operator or to a $U(n-1):U(n-2)$ projective operator. This branching uniquely assigns all upper operator patterns from the lower ones; hence, by induction on n, all operator patterns arise in precisely this way. This result has been proven so far only for the class of all unique operators and for the class of all adjoint operators.

B. The Conjugation Properties of the Adjoint Wigner Operators

Having uniquely induced the assignment of operator patterns to the set of adjoint Wigner operators of Sec. 5 through the use of limit properties, we next turn to the question of conjugation properties. We have made no use of conjugation properties in developing the adjoint Wigner operators—the classification by degree uniquely determined the operators in the multiplicity set having $\Delta = [\dot{0}]$. That this classification by degree accords with the classification by sharp conjugation is therefore a property of the set which must be proved.

The $U(n)$ conjugation operator $\mathcal{C}$ is defined in Appendix F. In particular, the following conjugation properties of the adjoint Wigner operators are derived:

$$\mathcal{C}\left\langle \begin{matrix} (\rho,\tau) \\ [1 \quad \dot{0} \quad -1] \\ (i,j) \end{matrix} \right\rangle \mathcal{C}^{-1} = (-1)^{n+1+i-j+\rho-\tau} \left\langle \begin{matrix} (n-\tau+1, n-\rho+1) \\ [1 \quad \dot{0} \quad -1] \\ (j,i) \end{matrix} \right\rangle, \tag{7.10a}$$

for $\rho \neq \tau = 1, 2, \cdots, n$ and all i, j;

$$\mathcal{C}\left\langle \begin{matrix} (\rho,\rho) \\ [1 \quad \dot{0} \quad -1] \\ (i,j) \end{matrix} \right\rangle \mathcal{C}^{-1} = (-1)^{n+i-j+\rho} \left\langle \begin{matrix} (\rho,\rho) \\ [1 \quad \dot{0} \quad -1] \\ (j,i) \end{matrix} \right\rangle, \tag{7.10b}$$

for $\rho = 1, 2, \cdots, n-1$ and all i, j.

We remark that the two $U(3)$ adjoint Wigner operators having $\Delta = [000]$ have sharp conjugation parity; they must therefore be precisely (except possibly for phase[27]) the previously determined (Ref. 5, Paper V) $\langle 2 \quad 1 \quad 0 \rangle$ adjoint operators upon making the following identifications[28]:

$$\left\langle \begin{matrix} & & 1 & & \\ & 1 & & 1 & \\ 2 & & 1 & & 0 \\ & \alpha & & \beta & \\ & & \gamma & & \end{matrix} \right\rangle = \left\langle \begin{matrix} & & 1 & & \\ & 1 & & 1 & \\ 1 & & 1 & & 1 \\ & 1 & & 1 & \\ & & 1 & & \end{matrix} \right\rangle \left\langle \begin{matrix} & & 0 & & \\ & 0 & & 0 & \\ 1 & & 0 & & -1 \\ & \alpha-1 & & \beta-1 & \\ & & \gamma-1 & & \end{matrix} \right\rangle, \tag{7.11a}$$

$$\left\langle \begin{matrix} & & 1 & & \\ & 2 & & 0 & \\ 2 & & 1 & & 0 \\ & \alpha & & \beta & \\ & & \gamma & & \end{matrix} \right\rangle = \left\langle \begin{matrix} & & 1 & & \\ & 1 & & 1 & \\ 1 & & 1 & & 1 \\ & 1 & & 1 & \\ & & 1 & & \end{matrix} \right\rangle \left\langle \begin{matrix} & & 0 & & \\ & 1 & & -1 & \\ 1 & & 0 & & -1 \\ & \alpha-1 & & \beta-1 & \\ & & \gamma-1 & & \end{matrix} \right\rangle. \tag{7.11b}$$

Let us summarize the important conclusions established by the preceding results: The classification of the adjoint Wigner operators (in the multiplicity set having $\Delta = [\dot{0}]$) by degree uniquely determines the operators. In consequence of this classification, the following two properties obtain:

(1) Operator patterns are uniquely induced by the branching law (operator splittings) which results by taking limits;

(2) classification by sharp conjugation parity is achieved automatically.

There is still one set of properties possessed by the adjoint Wigner operators which requires further discussion—the null space aspects of these operators. This is the subject of the concluding section.

C. The Adjoint Splittings Induced by Null Spaces

From the results obtained so far, it would be not unreasonable to assert that the resolution of the adjoint operator multiplicity by the now operationally defined operator patterns is canonical. But this designation can only mean that *no free choices* (aside from the equivalence class of primitive orderings of the Weyl subgroup restrictions: $n, n-1, \cdots, 1$) have been imposed. One might argue that choosing to classify operators by degree is a free choice. It is the purpose of this concluding section to demonstrate from a completely different approach that the degree classification is indeed canonical.

The basic idea which underlies this new approach can be easily understood by example. Consider the two $U(3)$ adjoint operators:

$$\begin{pmatrix} & 0 & \\ 0 & & 0 \\ 1 & 0 & -1 \\ \cdot & & \cdot \end{pmatrix}, \quad \begin{pmatrix} & 0 & \\ 1 & & -1 \\ 1 & 0 & -1 \\ \cdot & & \cdot \end{pmatrix}.$$

When operating on an IR of the form $[p \;\; 0 \;\; 0]$, for example, one knows that the multiplicity, for *any* operator, is at most *one*. Clearly, when we operate on this subspace, one of the two adjoint operators must vanish (the two operators cannot become the same since they are orthogonal); this can only be the nongenerator

$$\begin{pmatrix} & 0 & \\ 1 & & -1 \\ 1 & 0 & -1 \end{pmatrix},$$

aside from the special case $[0 \;\; 0 \;\; 0]$ where *both* operators vanish. From the explicit normalization of the

$$\begin{pmatrix} & 0 & \\ 1 & & -1 \\ 1 & 0 & -1 \end{pmatrix}$$

operator, it is easily seen that this operator *annihilates the space* $[m_{13}\, m_{23}\, m_{33}]$ *characterized by equality of two, or more,* m_{i3}. Let us denote this space that is annihilated, *the null space* $\mathcal{N}$ *of the operator*

$$\begin{pmatrix} & 0 & \\ 1 & & -1 \\ 1 & 0 & -1 \end{pmatrix}.$$

Expressed intuitively (and imprecisely), the idea we seek to exploit is this: An operator is to be characterized *canonically* by its associated null space.

There are immediate difficulties with this idea which we must remove by employing a sharpened language. Let us first define two tensor operators to be *similar* if the two tensor operators: (i) transform according to the same Gel'fand pattern and (ii) possess the same Δ pattern in $U(n)$. It is immediately clear that similarity is an equivalence relation.

The problems which arise in any attempt to characterize tensor operators by their null spaces are of two related types: Firstly, tensor operators admit of two distinct types of scalar multipliers, (a) numerical scalars and (b) numerically-valued (scalar) functions of the $U(n)$ invariant operators; secondly, the limitations on the functional dependence of the scalar multipliers, and, indeed, of the tensor operators themselves, has not been made sufficiently explicit. It follows from Eqs. (5.3)–(5.6) that there exists an orthogonal basis for all adjoint tensor operators which possesses matrix elements that are square roots of rational functions of the Gel'fand labels; hence, it is not an essential limitation to restrict our attention to *that class of tensor operators whose norms are polynomial functions of the invariant operators* $\{I_k\}$. In particular, all null spaces of a given tensor operator of this class must be obtained from the zeros of its norm.

Having made the admissible class of tensor operators explicit, we can now turn to the problem posed by the existence of scalar (polynomial) functions. Clearly, the existence of such multipliers can change the null space of an operator arbitrarily. The problem then is to find a procedure to distinguish these "spurious" or "nonintrinsic" zeros from the "intrinsic" zeros that are to characterize the operator.

Consider the set of all similar tensor operators having polynomial norms, $\{\mathcal{O}_i\}$. Two such operators are defined to be *equivalent*, $\mathcal{O}_1 \sim \mathcal{O}_2$, if there exist polynomial functions of the invariant operators, P_1 and P_2 ($P_i \not\equiv 0$), such that the relation

$$(P_1)^{\frac{1}{2}}\mathcal{O}_1 = (P_2)^{\frac{1}{2}}\mathcal{O}_2 \tag{7.12}$$

is valid on all $U(n)$ representation spaces.

That this is an equivalence relation is again verified directly.

[The existence of one pair of polynomial functions, P_1 and P_2, implies the existence of arbitrarily many since $P_i' = P_i \times$ (polynomial), $i = 1, 2$, would serve just as well. To simplify the situation, these common factors are considered to have been canceled out.]

Equivalent tensor operators may have distinct null spaces. What would be desirable next would be to select from each equivalence class an operator having the "largest" nonnull space. Let us make this construction precise.

Consider an equivalence class of tensor operators; from this class choose two distinct operators. Their null spaces either are identical or they differ. If the former, choose the operator whose norm is of lesser degree (or either operator, if of the same degree). If the null spaces differ, choose the operator having lesser degree (or either, if the degrees are equal): Call this operator $\mathcal{O}_1$, and denote its norm by N_1; call the other operator $\mathcal{O}_2$, and denote its norm by N_2. Then, from Eq. (7.12), we have the polynomial identity

$$P_1 N_1 = P_2 N_2. \tag{7.13}$$

Since P_1 and P_2 had no common factors, we necessarily have then

$$P_1 N_1 = P_2 N_2 = P_1 P_2 K, \tag{7.14}$$

where K is a polynomial in the invariant operators.

This shows, however, that the new operator

$$(P_1)^{-\frac{1}{2}}\mathcal{O}_2 = (P_2)^{-\frac{1}{2}}\mathcal{O}_1$$

has a polynomial norm ($= K$) and is in the same equivalence class as $\mathcal{O}_1$ and $\mathcal{O}_2$. But Eq. (7.14) shows that the norm K vanishes only on the intersection $\mathcal{N}_1 \cap \mathcal{N}_2$. Hence, from any two operators in the equivalence class, we have constructed an operator whose null space is the intersection of the null spaces of the two equivalent operators.

Proceeding in this way through all operators of the given equivalence class, one arrives at a *representative* $\mathcal{C}$ of this class $\mathcal{K}$, having the null space $\bigcap_{\mathcal{O}_i \in \mathcal{K}} \mathcal{N}(\mathcal{O}_i)$.

For the adjoint tensor operators we can assert:

Lemma: The representative (adjoint) tensor operators have null spaces that are simply ordered.

Proof: By construction from the canonical basis, see Appendix E.

Several further properties of the representative operators of a given equivalence class are easily obtainable from the results of Appendix E. In particular, one sees that there exist representatives for each null space $\mathcal{N}_\rho$ of Appendix E. The null spaces do not, however, completely characterize the representatives. In fact, representatives from distinct equivalence classes may have the maximal null space $\mathcal{N}_1$.

In consequence, we define next the concept of *decomposability*. The representative $\mathcal{C}$ of a class $\mathcal{K}$ whose null space $\mathcal{N}(\mathcal{C})$ is maximal is termed *decomposable* if it can be written

$$f_3\mathcal{C} = f_1\mathcal{C}_1 + f_2\mathcal{C}_2, \tag{7.15}$$

where the $(f_i)^2$ are polynomials ($f_i \not\equiv 0$) over the invariant operators such that $f_3 \not\equiv 0$ on $\mathcal{N}_1$; $\mathcal{C}_1$ and $\mathcal{C}_2$ are representatives whose null spaces are *distinct*. Otherwise, the representative $\mathcal{C}$ is *indecomposable*.

Remark: Decomposability relates to a specific set of representatives; the maximal null space similarly relates to the specific set. In applying the concept of decomposability, we will successively decrease the space of admissible operators; see below.

Using now the explicit construction of the canonical adjoint operators and the results of Appendix E, we easily see that indecomposable operators exist and that, moreover, an indecomposable (adjoint) tensor operator is unique to within scalar multipliers that vanish only on the maximal null space. (Hence, upon norming to 1, we could obtain a unique basis operator.)

Having obtained the indecomposable operator belonging to the maximal null space of the adjoint tensor operators, one next considers the orthogonal complement to this operator and then repeats the whole construction to identify that indecomposable operator belonging to the next largest null space. This process identifies, step-by-step, precisely those operators previously designated as canonical.

We summarize this canonical identification of the adjoint unit tensor operators in the following form:

Theorem: The set of indecomposable representative adjoint operators is uniquely determined by the associated simply ordered set of null spaces: $\mathcal{N}_1 \supset \mathcal{N}_2 \supset \cdots \supset \mathcal{N}_{n-1}$, $\mathcal{N}_\rho = \{$all IR spaces with labels $[m]$ in which $\rho + 1$ or more m_{in} are equal$\}$. This construction is canonical and agrees precisely with that induced by (a) degree and (b) conjugation parity.

We remark that, although this construction by null spaces is canonical, it does not, of itself, associate any particular upper pattern labels with a given canonical operator. The direct association of upper pattern labels is a special feature of the use of limits and demonstrates that such concepts are equally important.

APPENDIX A: SUMMATION FORMULAS

In dealing with the explicit matrix elements which arise in the unitary groups, as well as the orthogonal groups,[29,30] the following sums are encountered frequently:

$$\sum_{i=1}^{n}\left[x_i^q \Big/ \prod_{\substack{s=1\\ s\neq i}}^{n}(x_s - x_i)\right] \equiv (-1)^{n-1}\beta_{q-n+1}(x), \quad \text{(A1)}$$

for $q = 0, 1, \cdots$, in which $x_1 \neq x_2 \neq \cdots \neq x_n$ are arbitrary numbers. In this appendix, the general expression for the $\beta(x)$ is obtained in terms of the elementary symmetric functions

$$\varphi_0(x) = 1, \quad \varphi_1(x) = \sum_i x_i, \quad \varphi_2(x) = \sum_{i<j} x_i x_j, \cdots. \quad \text{(A2)}$$

We employ a technique previously used.[29] Define a function f of a complex variable z by

$$f_q(z) = (-1)^n z^q \Big/ \prod_{s=1}^{n}(x_s - z) \quad \text{(A3)}$$

so that

$$\beta_{q-n+1}(x) = \frac{1}{2\pi i}\int_C f_q(z)\,dz, \quad \text{(A4)}$$

where the integration is counterclockwise around a path C which encloses all the simple poles of $f(z)$ (located at the points $x_1 \neq x_2 \neq \cdots \neq x_n$). We now use the fact that

$$\int_C \frac{p_1(z)}{p_2(z)}\,dz = 0 \quad \text{(A5)}$$

for $p_1(z)$ and $p_2(z)$ polynomials in which the degree of p_1 is less than the degree of p_2 by at least 2, where C encloses all the roots of p_2. Thus, we immediately have

$$\beta_{-n+1}(x) = \beta_{-n+2}(x) = \cdots = \beta_{-1}(x) = 0. \quad \text{(A6)}$$

For $q \geq n-1$, we can write

$$f_q(z) = \sum_{p=0}^{q-n+1}\beta_p(x) z^{q-n-p} + \left[g(z) \Big/ z\prod_{s=1}^{n}(x_s - z)\right], \quad \text{(A7)}$$

where $g(z)$ is a polynomial of degree not greater than $n-1$ and the coefficients $\beta_0, \beta_1, \cdots$ [not yet identified as those of Eq. (A1)] satisfy the recursion formulas

$$\begin{aligned} \beta_0 &= 1, \\ \beta_1 &= \varphi_1, \\ \beta_2 &= \beta_1\varphi_1 - \beta_0\varphi_2, \\ &\cdots \\ \beta_p &= -\sum_{\nu=0}^{p-1}(-1)^{p-\nu}\varphi_{p-\nu}\beta_\nu, \end{aligned} \quad \text{(A8)}$$

for $p = 1, 2, \cdots$.

The proof of Eq. (A7) is obtained by multiplying both sides by $z\prod_{s=1}^{n}(x_s - z)$ and comparing like coefficients in the resulting polynomial identity. Integrating Eq. (A7) counterclockwise around a path enclosing the simple poles of $f_q(z)$ yields Eq. (A4), so that the β's of the recursion formula (A8) are the β's of the sum (A1).

Next, we use the recursion formula to prove that the general expression for β_p $(p = 0, 1, \cdots)$ is

$$\beta_p = d_p = \sum_{\alpha_1\cdots\alpha_n}\frac{(-1)^{p-\alpha}\alpha!}{\alpha_1!\,\alpha_2!\cdots\alpha_n!}\varphi_1^{\alpha_1}\varphi_2^{\alpha_2}\cdots\varphi_n^{\alpha_n}, \quad \text{(A9a)}$$

where $\alpha \equiv \alpha_1 + \alpha_2 + \cdots + \alpha_n$ and the sum is over all nonnegative integers $\alpha_1, \alpha_2, \cdots, \alpha_n$ which satisfy

$$\alpha_1 + 2\alpha_2 + 3\alpha_3 + \cdots + n\alpha_n = p. \quad \text{(A9b)}$$

The explicit expression (A9) is designated as d_p by Perron.[31] Thus, we must prove $\beta_p = d_p$. This can be accomplished as follows. The power sums

$$S_p(x) = \sum_i x_i^p, \quad p = 0, 1, 2, \cdots, \quad \text{(A10)}$$

are related to the φ's and the d's by[31]

$$S_p = -\sum_{\nu=0}^{p-1}(p-\nu)(-1)^{p-\nu}\varphi_{p-\nu}d_\nu. \quad \text{(A11a)}$$

They are also related recursively to the φ's by Newton's formula

$$\sum_{\nu=1}^{p}(-1)^\nu\varphi_{p-\nu}S_\nu + p\varphi_p = 0. \quad \text{(A11b)}$$

Now observe from the explicit expression for S_p in terms of the φ's that

$$\sum_{i=1}^{n}\varphi_i\frac{\partial S_p}{\partial\varphi_i} = pd_p. \quad \text{(A12)}$$

Application of the operator

$$\sum_{i=1}^{n}\varphi_i\frac{\partial}{\partial\varphi_i}$$

to Eq. (A11b) and use of result (A12) now yields

$$S_p = \sum_{\nu=1}^{p}(-1)^{p-\nu}\varphi_{p-\nu}\nu d_\nu. \quad \text{(A13)}$$

Comparison of this expression for S_p with Eq. (A11a) shows that the d's satisfy the recursion formula

$$\sum_{\nu=0}^{p}(-1)^{p-\nu}\varphi_{p-\nu}d_\nu = 0, \quad \text{(A14)}$$

for $p = 1, 2, \cdots$. Thus, the functions $\beta_0, \beta_1, \cdots, \beta_p, \cdots$ and $d_0, d_1, \cdots, d_p, \cdots$ satisfy the same recursion relation. Since $\beta_0 = d_0 = 1$, the functions are

the same, i.e.,

$$\beta_p = d_p, \quad p = 0, 1, \cdots. \tag{A15}$$

The following result can also be established for negative integers, but we omit the proof:

$$\beta_{-n-p} = \frac{(-1)^{n+1}}{\varphi_n} \sum_{\alpha_1 \cdots \alpha_n} \frac{(-1)^{p-\alpha} \alpha!\, \varphi_{n-1}^{\alpha_1} \varphi_{n-2}^{\alpha_2} \cdots \varphi_1^{\alpha_{n-1}}}{\alpha_1!\, \alpha_2! \cdots \alpha_n!\, \varphi_n^{\alpha}}, \tag{A16}$$

for $p = 0, 1, 2, \cdots$, where α and the summation have the same significance as in Eq. (A9).

The symmetric functions $\beta_p, p = 0, 1, \cdots$, are the homogeneous symmetric functions denoted by h_p by Littlewood.[32] They can also be expressed in determinantal form:

$$\beta_p = \det \begin{bmatrix} \varphi_1 & 1 & 0 & 0 & \cdots & 0 \\ \varphi_2 & \varphi_1 & 1 & 0 & \cdots & 0 \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \varphi_{p-1} & \varphi_{p-2} & \cdots & & \varphi_1 & 1 \\ \varphi_p & \varphi_{p-1} & \cdots & & \varphi_2 & \varphi_1 \end{bmatrix}. \tag{A17}$$

APPENDIX B: EIGENVALUES OF THE GEL'FAND INVARIANTS

The occurrence of the invariants in the Gel'fand form[33] in the expression (5.20) for Racah invariants means that the eigenvalues of the Racah invariants cannot be written out until those for the Gel'fand invariants are. The eigenvalues of the Gel'fand invariants of $U(n)$ are derived in this appendix. (These results have been noted previously, without proof.[3])

The Gel'fand invariants for $U(n)$ are expressed in terms of the generators by

$$I_k^{(n)} = \sum_{i_1 \cdots i_k}^{n} E_{i_1 i_2} E_{i_2 i_3} \cdots E_{i_k i_1}. \tag{B1}$$

The eigenvalue is denoted by

$$I_k^{(n)}(m) = I_k^{(n)}(m_{1n}, m_{2n}, \cdots, m_{nn}) \tag{B2}$$

for an arbitrary state vector $|(m)\rangle$.

In order to derive the explicit expression for $I_k^{(n)}(m)$, a number of recursion formulas are first derived. The first useful property is

$$I_k^{(n)}(m_{1n} + \lambda, m_{2n} + \lambda, \cdots, m_{nn} + \lambda) = \sum_{s=0}^{k} \binom{k}{s} \lambda^{k-s} I_s^{(n)}(m_{1n}, \cdots, m_{nn}), \tag{B3a}$$

where λ is an arbitrary parameter. This result is a consequence of the identity

$$\sum_{i_1 \cdots i_k}^{n} (E_{i_1 i_2} + \lambda \delta_{i_1 i_2})(E_{i_2 i_3} + \lambda \delta_{i_2 i_3}) \cdots (E_{i_k i_1} + \lambda \delta_{i_k i_1}) = \sum_{s=0}^{k} \binom{k}{s} \lambda^{k-s} I_s^{(n)}, \tag{B3b}$$

where $I_0^{(n)} \equiv n$. To show that Eq. (B3a) obtains from Eq. (B3b), we argue as follows. Clearly, we need only show that the left-hand side of Eq. (B3a) is the eigenvalue of the left-hand side of Eq. (B3b). This is done by operating on a maximal state vector. Since E_{ij}, $i < j$, annihilates a maximal state vector, we can by repeated use of the commutation relations reduce

$$I_k^{(n)} \left| \begin{pmatrix} [m] \\ (\max) \end{pmatrix} \right\rangle = I_k^{(n)}(m) \left| \begin{pmatrix} [m] \\ (\max) \end{pmatrix} \right\rangle$$

to the form

$$F_k^{(n)}(E_{11}, E_{22}, \cdots, E_{nn}) \left| \begin{pmatrix} [m] \\ (\max) \end{pmatrix} \right\rangle = I_k^{(n)}(m) \left| \begin{pmatrix} [m] \\ (\max) \end{pmatrix} \right\rangle.$$

Effecting precisely the same reduction steps on the left-hand side of Eq. (B3b) yields

$$F_k^{(n)}(E_{11} + \lambda, E_{22} + \lambda, \cdots, E_{nn} + \lambda) \left| \begin{pmatrix} [m] \\ (\max) \end{pmatrix} \right\rangle,$$

and, since $E_{ii} \to m_{in}$ on a maximal state, we obtain the desired result, Eq. (B3a).

The result

$$I_k^{(n)}(m_{1n}, \cdots, m_{nn}) = \sum_{s=0}^{k} \binom{k}{s} m_{nn}^{k-s} I_s^{(n)}(m_{1n} - m_{nn}, \cdots, m_{n-1n} - m_{nn}, 0) \tag{B4}$$

now follows from Eq. (B3a) upon setting $\lambda = m_{nn}$ and making the substitution $m_{in} \to m_{in} - m_{nn}$. The usefulness of Eq. (B4) is that it shows us how to calculate the general eigenvalue for $m_{nn} \neq 0$ if it is known for $m_{nn} = 0$.

The next result is more difficult to prove. We first state it and then sketch only the essential steps of the proof. The result relates the eigenvalues of $U(n+1)$ invariants and $U(n)$ invariants:

$$I_k^{(n+1)}(m_{1n+1}, \cdots, m_{nn+1}, 0) = \sum_{s=1}^{k} \binom{k-1}{s-1} I_s^{(n)}(m_{1n+1}, \cdots, m_{nn+1}), \tag{B5a}$$

which can also be written in the form

$$I_k^{(n+1)}(m_{1n+1},\cdots,m_{nn+1},0) = I_k^{(n)}(m_{1n+1}+1,\cdots,m_{nn+1}+1) - I_{k-1}^{(n)}(m_{1n+1}+1,\cdots,m_{nn+1}+1) \quad \text{(B5b)}$$

through the use of the binomial-coefficient identity

$$\binom{k-1}{s-1} = \binom{k}{s} - \binom{k-1}{s}$$

and Eq. (B3a). It is, however, Eq. (B5a) which we prove directly.

A little study of Eqs. (B4) and (B5b) reveals that they can be used to generate the general eigenvalue starting from $I_k^{(1)}(m_{11}) = m_{11}^k$, $k = 0, 1, \cdots$. This is not, however, the technique we use.

Now for the proof of Eq. (B5a). We start with the vector operators to which a superscript n is now attached with, however,

$$V_{ij}^{(n)}(0) = \delta_{ij}, \quad V_{ij}^{(n)}(1) = E_{ij}, \quad \text{(B6a)}$$

for all n.

The identity

$$V_{ij}^{(n+1)}(q) = V_{ij}^{(n)}(q) + \sum_{\nu=1}^{q-1}\left(\sum_{k=1}^{n} V_{ik}^{(n)}(\nu-1)E_{kn+1}\right)V_{n+1j}^{(n+1)}(q-\nu), \quad \text{(B6b)}$$

for $q = 2, 3, \cdots$, results directly from the definitions. We now operate on a maximal state vector of $U(n+1)$. Since E_{kn+1}, for $k = 1, 2, \cdots, n$, annihilates such a state vector, the product $E_{kn+1}V_{n+1j}^{(n+1)}(q-\nu)$ can be replaced by its commutator. Furthermore, the term $V_{n+1n+1}^{(n+1)}(q-\nu)$, which arises from the commutator, annihilates a state vector with $m_{n+1n+1} = 0$. Thus, on such a state vector, the operator (B6b) is equivalent to the following one:

$$V_{ij}^{(n+1)}(q) \to V_{ij}^{(n)}(q) + \sum_{\nu=1}^{q-1}\sum_{k=1}^{n} V_{ik}^{(n)}(\nu-1)V_{kj}^{(n+1)}(q-\nu), \quad \text{(B7)}$$

for $q = 2, 3, \cdots$. We now set $j = i$ and sum from 1 to n, noting that the sum can be extended to $n+1$ on the left-hand side:

$$I_q^{(n+1)} \to I_q^{(n)} + \sum_{\nu=1}^{q-1}\sum_{ik}^{n} V_{ik}^{(n)}(\nu-1)V_{ki}^{(n+1)}(q-\nu). \quad \text{(B8)}$$

The idea is to iterate Eq. (B8) through repeated use of Eq. (B7). To do this, we need the obvious results

$$\sum_{j=1}^{n} V_{ij}^{(n)}(\alpha)V_{jk}^{(n)}(\beta) = V_{ik}^{(n)}(\alpha+\beta) \quad \text{(B9a)}$$

and

$$I_k^{(n)} = \sum_{i=1}^{n} V_{ii}^{(n)}(k). \quad \text{(B9b)}$$

Thus, in the first iteration of Eq. (B8), the term for $\nu = q-1$ is separated off in the sum, and

$$V_{ki}^{(n+1)}(q-\nu),$$

$\nu = 1, 2, \cdots, q-2$, is substituted in from Eq. (B7). After minor manipulations and use of Eqs. (B9), we obtain

$$I_q^{(n+1)} \to I_q^{(n)} + (q-1)I_{q-1}^{(n)} + \sum_{\nu=2}^{q-1}(\nu-1)\sum_{ik}^{n} V_{ik}^{(n)}(\nu-2)V_{ki}^{(n+1)}(q-\nu). \quad \text{(B10)}$$

Continuation of this procedure establishes the proof of

$$I_q^{(n+1)} \to \sum_{\nu=1}^{q}\binom{q-1}{\nu-1}I_\nu^{(n)} \quad \text{(B11)}$$

on maximal $U(n+1)$ states having $m_{n+1n+1} = 0$. Equation (B5a) then follows.

Equations (B4) and (B5b) can be used to generate the desired eigenvalues $I_k^{(n)}(m)$. We follow, however, a different course. We now prove that these eigenvalues are given by the formula

$$D^{(n)}(m)I_k^{(n)}(m) = \sum_{i=1}^{n} p_{in}^k D^{(n)}(m_{1n}\cdots m_{in}-1\cdots m_{nn}), \quad \text{(B12)}$$

where $D^{(n)}(m)$ denotes the dimension of the representation with IR labels $[m]$ given explicitly by Eq. (2.4). We give the proof by showing that the $I_k^{(n)}(m)$ *defined* by Eq. (B12) satisfy Eqs. (B3a) and (B5b). Since Eq. (B12) gives $I_k^{(1)}(m_{11}) = m_{11}^k$, the proof is complete.

Proof: Since the dimension of an IR is invariant to the shift $m_{in} \to m_{in} + \lambda$, property (B3a) is an immediate consequence of definition (B12). Next, we observe the properties

$$D^{(n+1)}(m_{1n+1},\cdots,m_{nn+1},0) = D^{(n)}(m_{1n+1},\cdots,m_{nn+1})\left(\prod_{j=1}^{n} p_{jn+1}\right)\Big/n!, \quad \text{(B13a)}$$

$$D^{(n+1)}(m_{1n+1},\cdots,m_{in+1}-1,\cdots,m_{nn+1},0) = D^{(n)}(m_{1n+1},\cdots,m_{in+1}-1,\cdots,m_{nn+1}) \times\left[\left(\prod_{j=1}^{n} p_{jn+1}\right)(p_{in+1}-1)/n!\,p_{in+1}\right], \quad \text{(B13b)}$$

for $i = 1, 2, \cdots, n$. It is now a simple exercise to validate Eq. (B5b) upon shifting n to $n+1$ in Eq. (B12) and using the above results.

Equation (B12) and Eq. (4.9b) can now be used to write the eigenvalues in the remarkably useful form as follows:

$$I_k^{(n)}(m) = \sum_{\tau=1}^{n}\left(p_{\tau n}^k \prod_{s=1}^{n}(p_{sn} - p_{\tau n} + 1) \Big/ \prod_{\substack{s=1 \\ s\neq\tau}}^{n}(p_{sn} - p_{\tau n})\right)$$

$$= n\sum_{\tau=1}^{n} p_{\tau n}^k [R_{n\tau}^{(n)}(m)]^2. \tag{B14}$$

It is interesting to observe that

$$I_k^{(n)}(m) = \frac{1}{2\pi i}\int_C f_k^{(n)}(z)\,dz, \tag{B15a}$$

where

$$f_k^{(n)}(z) = (-)z^k \prod_{s=1}^{n}\left(\frac{p_{sn} + 1 - z}{p_{sn} - z}\right). \tag{B15b}$$

The summation in Eq. (B14) can be effected in terms of the β's of Appendix A. We proceed as follows:

$$\prod_{s=1}^{n}(p_{sn} - p_{\tau n} + 1) = \sum_{\mu=0}^{n}\varphi_{n-\mu}(p+1)(-p_{\tau n})^{\mu},$$

where $(p+1) = (p_{1n}+1, p_{2n}+1, \cdots, p_{nn}+1)$;

$$I_k^{(n)}(m) = \sum_{\mu=0}^{n}\varphi_{n-\mu}(p+1)(-1)^{n-\mu+1}\beta_{k+\mu-n+1}(p)$$

$$= \sum_{\nu=0}^{k+1}\varphi_{k+1-\nu}(p+1)(-1)^{k-\nu}\beta_\nu(p),$$

where the second sum follows upon noting that $\beta_q(p) = 0$, for $-n+1 \le q \le -1$, *and* that the elementary symmetric functions $\varphi_q(p)$ in n variables are defined to be zero for $q > n$. We next use the property (A8),

$$\sum_{\nu=0}^{k+1}(-1)^{k-\nu}\varphi_{k+1-\nu}(p)\beta_\nu(p) = 0,$$

to obtain

$$I_k^{(n)}(m) = \sum_{\nu=0}^{k}(-1)^{k-\nu}[\varphi_{k+1-\nu}(p+1) - \varphi_{k+1-\nu}(p)]\beta_\nu(p).$$

Using

$$\varphi_\lambda(p+1) - \varphi_\lambda(p) = \sum_{\mu=0}^{\lambda-1}\binom{n-\mu}{n-\lambda}\varphi_\mu(p),$$

we can straightforwardly bring $I_k^{(n)}(m)$ to the form

$$I_k^{(n)}(m) = \sum_{\nu=0}^{k}\sum_{\mu=0}^{\nu}(-1)^{k-\nu+\mu}\binom{n-\mu}{k+1-\nu}\varphi_\mu(p)\beta_{\nu-\mu}(p). \tag{B16}$$

The final explicit form for the eigenvalues is obtained by substituting the expression (A9a) for $\beta_{\nu-\mu}(p)$ into Eq. (B16):

$$I_k^{(n)}(m) = \sum_{\nu=0}^{k}\sum_{\substack{\alpha_1\cdots\alpha_n \\ \alpha_1+2\alpha_2+\cdots n\alpha_n=\nu}} A_{k\nu}(\alpha_1,\cdots,\alpha_n) \times \varphi_1^{\alpha_1}(p)\varphi_2^{\alpha_2}(p)\cdots\varphi_n^{\alpha_n}(p), \tag{B17a}$$

where the coefficients have the following definition (in $A_{k\nu}$, the constraint $\alpha_1 + 2\alpha_2 + \cdots + n\alpha_n = \nu$ is in effect):

$$A_{k\nu}(\alpha_1,\cdots,\alpha_n) = \frac{(-1)^{k-\alpha+1}(\alpha-1)!}{\alpha_1!\,\alpha_2!\cdots\alpha_n!}\sum_{\mu=0}^{n}\binom{n-\mu}{k+1-\nu}\alpha_\mu, \tag{B17b}$$

for $\nu = 1, 2, \cdots$, and in which

$$\alpha = \alpha_1 + \alpha_2 + \cdots + \alpha_n, \quad \alpha_0 \equiv -\alpha, \tag{B17c}$$

$$A_{k0}(0,\cdots,0) = (-1)^k\binom{n}{k+1}. \tag{B17d}$$

We also note that

$$A_{kk}(\alpha_1,\cdots,\alpha_n) = (-1)^{k-\alpha}(\alpha-1)!\,k/\alpha_1!\,\alpha_2!\cdots\alpha_n!\,. \tag{B18a}$$

The term in Eq. (B17a) for $\nu = k$ is therefore just

$$S_k(p) = \sum_{\tau=1}^{n} p_{\tau n}^k. \tag{B18b}$$

We note below the first few eigenvalues expressed in terms of the power sums (B18b):

$$I_0 = n,$$

$$I_1 = S_1 - \binom{n}{2},$$

$$I_2 = S_2 - (n-1)S_1 + \binom{n}{3},$$

$$I_3 = S_3 + \binom{n-1}{2}S_1 - (n - \tfrac{3}{2})S_2 - \tfrac{1}{2}S_1^2 - \binom{n}{4},$$

$$I_4 = S_4 - (n-2)S_3 + \tfrac{1}{2}(n-2)^2 S_2 - \binom{n-1}{3}S_1 - S_1S_2 + \tfrac{1}{2}(n-2)S_1^2 + \binom{n}{5}.$$

Before leaving this subject, let us mention a possible source of confusion concerning the relation of the p_{in} to the invariants $I_k^{(n)}$. As we have seen the $\{I_k^{(n)}\}$ are expressible in terms of the elementary symmetric functions of the $\{p_{in}\}$. As such, any individual p_{in} is not distinguished from any other. How then can one solve the $\{I_k^{(n)}\}$ to determine each p_{in}? The answer lies in the fact that the process of extracting roots destroys the symmetry, and there is no contradiction.

APPENDIX C: PROPERTIES OF THE VECTOR OPERATORS

This appendix contains the proofs of several important properties which relate to the vector operators

$X(q)$. The first of these is Eq. (5.6). This result is easily proved using Eq. (B14). Let V denote the Vandermonde matrix as follows:

$$V = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ p_{1n} & p_{2n} & \cdots & p_{nn} \\ p_{1n}^2 & p_{2n}^2 & \cdots & p_{nn}^2 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ p_{1n}^{n-1} & p_{2n}^{n-1} & \cdots & p_{nn}^{n-1} \end{bmatrix} \tag{C1a}$$

so that the element in row i and column k is

$$V_{ik} = p_{kn}^{i-1}. \tag{C1b}$$

We now verify directly the relation (t denotes "transposition")

$$\begin{bmatrix} I_0^{(n)}(m) & I_1^{(n)}(m) & \cdots & I_{n-1}^{(n)}(m) \\ I_1^{(n)}(m) & I_2^{(n)}(m) & \cdots & I_n^{(n)}(m) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_{n-1}^{(n)}(m) & I_n^{(n)}(m) & \cdots & I_{2n-2}^{(n)}(m) \end{bmatrix} = VDV^t, \tag{C2a}$$

where D is the diagonal matrix with elements

$$D_{kk} = n[R_{nk}^{(n)}(m)]^2. \tag{C2b}$$

Using

$$\det V = \prod_{j<i}^{n}{}_1 (p_{in} - p_{jn}) \tag{C2c}$$

and the explicit expression (4.9b) for $R_{nk}^{(n)}(m)$, we obtain the result

$$\det(VDV^t) = \prod_{i<j}^{n}{}_1 [(p_{in} - p_{jn})^2 - 1]. \tag{C3}$$

The next result in Sec. 5 which needs proof is Eq. (5.16):

$$J_\tau(q)\,|(m)\rangle = p_{\tau n}^q\,|(m)\rangle. \tag{C4}$$

From Eqs. (5.14), we obtain

$$J_\tau(q) = \sum_{\rho=1}^{n}\sum_{k=1}^{n} \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ k \end{matrix} \right\rangle \sum_{l=1}^{n} \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ l \end{matrix} \right\rangle^{\dagger} \left\langle \begin{matrix} \rho \\ [1 \quad \dot{0}] \\ l \end{matrix} \right\rangle \times \mathcal{M}^{-1} \begin{matrix} \rho \\ [1 \quad \dot{0}] \\ k \end{matrix}^{\dagger} \mathcal{M} J_\rho(q-1). \tag{C5}$$

The result

$$\sum_{l=1}^{n} \left\langle \begin{matrix} \tau \\ [1 \quad \dot{0}] \\ l \end{matrix} \right\rangle^{\dagger} \left\langle \begin{matrix} \rho \\ [1 \quad \dot{0}] \\ l \end{matrix} \right\rangle |(m)\rangle = \delta_{\rho\tau}\left[\frac{D([m] + \Delta_n(\rho))}{D([m])}\right] |(m)\rangle \tag{C6}$$

is a direct consequence of Eq. (4.7) and the orthonormality of the $\langle \dot{0} \quad -1 \rangle$ Wigner operators. Taking the diagonal matrix element of Eq. (C5) and using Eq. (C6) {on the shifted $[m] - \Delta_n(\rho)$ IR labels}, we derive the recursion formula

$$\langle (m)|\, J_\tau(q)\,|(m)\rangle = p_{\tau n}\,\langle (m)|\, J_\tau(q-1)\,|(m)\rangle. \tag{C7}$$

Since $\langle (m)|\, J_\tau(0)\,|(m)\rangle = 1$, the desired result, Eq. (C4), is immediate.

We would also like to demonstrate that the Racah invariant functions are invariant under the shift $m_{in} \to m_{in} + \lambda$, $i = 1, \quad 2, \cdots, n$. This invariance is a consequence of the invariance of the operators $X(q)$ to the shift $E_{ij} \to E_{ij} + \lambda\delta_{ij}$ [compare Eqs. (B3a) and (B3b)]. Hence, we now prove the latter. Furthermore, because of the transformation law (B3b) and an identical transformation law for the vector operators $V(q)$, the invariance of $X(q)$ under $E_{ij} \to E_{ij} + \lambda\delta_{ij}$ is a consequence of the following general result (to be proved): Let $x_0, x_1, x_2, \cdots$ denote arbitrary quantities. Then the determinants,

$$\det \begin{bmatrix} x_0 & x_1 & \cdots & x_p \\ x_1 & x_2 & \cdots & x_{p+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ x_p & x_{p+1} & \cdots & x_{2p} \end{bmatrix}, \quad p = 0, 1, \cdots, \tag{C8a}$$

are invariant under the transformation

$$x_q' = \sum_{s=0}^{q} \binom{q}{s} \lambda^{q-s} x_s, \quad q = 0, 1, \cdots. \tag{C8b}$$

Furthermore, if $y_0, y_1, \cdots$ are arbitrary quantities which undergo the same transformation law,

$$y_q' = \sum_{s=0}^{q} \binom{q}{s} \lambda^{q-s} y_s, \quad q = 0, 1, \cdots, \tag{C8c}$$

then the determinants

$$\det \begin{bmatrix} x_0 & x_1 & \cdots & x_p \\ x_1 & x_2 & \cdots & x_{p+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ x_{p-1} & x_p & \cdots & x_{2p-1} \\ y_0 & y_1 & \cdots & y_p \end{bmatrix}, \quad p = 0, 1, \cdots, \tag{C8d}$$

are also invariant.

Proof: Let X_p denote the $(p+1) \times (p+1)$ matrix of the $x_0, x_1, \cdots, x_{2p}$ appearing in Eq. (C8a), and

let X'_p denote the same matrix in terms of the x'_0, $x'_1, \cdots, x'_{2p}$ defined by Eq. (C8b). Furthermore, define a $(p+1) \times (p+1)$ matrix A_p as

$$(A_p)_{ij} = \binom{i-1}{j-1} \lambda^{i-j}, \tag{C9a}$$

where $i, j = 1, 2, \cdots, p+1$ are row and column indices, respectively. Observe that A_p is lower triangular with all its diagonal elements equal to 1, so that $\det A_p = 1$. We assert

$$X'_p = A_p X_p A_p^t. \tag{C9b}$$

This result is proved by direct expansion and use of the binomial-coefficient identity

$$\sum_{\substack{\alpha\beta \\ \alpha+\beta=\gamma}} \binom{r}{\alpha}\binom{s}{\beta} = \binom{r+s}{\gamma}. \tag{C9c}$$

Thus,

$$\det X'_p = \det X_p. \tag{C9d}$$

The proof of the second part, the invariance of Eq. (C8d), proceeds along similar lines, but is somewhat more complicated. Here the relevant matrix relation is

$$\begin{bmatrix} x'_0 & x'_1 & \cdots & x'_p \\ x'_1 & x'_2 & \cdots & x'_{p+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ x'_{p-1} & x'_p & \cdots & x'_{2p-1} \\ y'_0 & y'_1 & \cdots & y'_p \end{bmatrix}$$

$$= \left[\begin{array}{ccc|c} & & & 0 \\ & A_{p-1} & & \cdot \\ & & & \cdot \\ & & & \cdot \\ & & & 0 \\ \hline 0 & \cdots & 0 & 1 \end{array}\right] \begin{bmatrix} x_0 & x_1 & \cdots & x_p \\ x_1 & x_2 & \cdots & x_{p+1} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ x_{p-1} & x_p & \cdots & x_{2p-1} \\ y_0 & y_1 & \cdots & y_p \end{bmatrix}$$

$$\times B_p \left[\begin{array}{ccc|c} & & & 0 \\ & A_{p-1}^t & & \cdot \\ & & & \cdot \\ & & & \cdot \\ & & & 0 \\ \hline 0 & \cdots & 0 & 1 \end{array}\right], \tag{C10a}$$

in which B_p is the matrix

$$B_p = \left[\begin{array}{ccc|c} & & & b_0 \\ & & & b_1 \\ & I & & \cdot \\ & & & \cdot \\ & & & \cdot \\ \hline 0 & \cdots & 0 & b_p \end{array}\right], \tag{C10b}$$

where I is the unit matrix of dimension p and

$$b_q = \binom{p}{q} \lambda^{p-q}, \quad q = 0, 1, \cdots, p. \tag{C10c}$$

We establish Eq. (C10a) by direct block multiplication of the matrices, noting from Eq. (C9b) that

$$X'_{p-1} = A_{p-1} X_{p-1} A_{p-1}^t.$$

The only point which requires additional work is the relation

$$\begin{bmatrix} x'_p \\ x'_{p+1} \\ \cdot \\ \cdot \\ \cdot \\ x'_{2p-1} \end{bmatrix} = A_{p-1} \left\{ X_{p-1} \begin{bmatrix} b_0 \\ b_1 \\ \cdot \\ \cdot \\ \cdot \\ b_{p-1} \end{bmatrix} + \begin{bmatrix} x_p \\ x_{p+1} \\ \cdot \\ \cdot \\ \cdot \\ x_{2p-1} \end{bmatrix} \right\}.$$

Taking the determinant of Eq. (C10a), we establish the proof of the invariance statement relating to Eqs. (C8c) and (C8d).

The final result to be proved in this appendix is: Under the transformation $E_{ij} \to -E_{ji}$, the operator $X(q)$ undergoes the transformation

$$X_{ij}(q) \to (-1)^q X_{ji}(q). \tag{C11}$$

The proof of this result is quite elaborate and occupies the remainder of this appendix. A number of auxiliary results are first required.

First, consider the transformation properties of the $V(q)$ of Eqs. (5.3). The main result is: Under the transformation $E_{ij} \to -E_{ji}$, the operator $V(q)$ undergoes the transformation

$$V_{ij}(q) \to \sum_{\mu=0}^{q} \alpha_{q\mu} V_{ji}(\mu), \tag{C12a}$$

where the $\alpha_{q\mu}$ are functions of the invariants $I_0, I_1, I_2, \cdots$, which are uniquely determined by the recursion relations

$$\alpha_{q+1\mu} = -\alpha_{q\mu-1} + I_0 \alpha_{q\mu}, \tag{C12b}$$

for $\mu = 0, 1, 2, \cdots, q+1$, $q = 0, 1, 2, \cdots$, and with

$$\alpha_{q,-1} \equiv \sum_{\nu=0}^{q} \alpha_{q\nu} I_\nu, \tag{C12c}$$

$$\alpha_{q\nu} \equiv 0, \quad \text{for} \quad \nu > q, \quad \text{all } q. \tag{C12d}$$

The starting point for the iteration is $\alpha_{00} = 1$. Then, from Eq. (C12c), we calculate $\alpha_{0,-1} = I_0$ and, from Eq. (C12b), $\alpha_{10} = 0$ and $\alpha_{11} = -1$. Using these results, we then calculate $\alpha_{1,-1} = -I_1$, $\alpha_{20} = I_1$ $\alpha_{21} = -I_0$, and $\alpha_{22} = +1$. From this procedure, we see that relations (C12b)–(C12d) do uniquely determine the coefficients. The proof of Eqs. (C12) is by induction.

We start with

$$V_{ij}(q+1) = \sum_{k=1}^{n} E_{ik} V_{kj}(q)$$

and assume the validity of Eq. (C12a) for all values up to q. Then, under $E_{ij} \to -E_{ji}$, we have

$$V_{ij}(q+1) \to -\sum_{\mu=0}^{q} \alpha_{q\mu} \sum_{k=1}^{n} E_{ki} V_{jk}(\mu).$$

Using the identity

$$E_{ki} V_{jk}(\mu) = V_{jk}(\mu) E_{ki} + \delta_{ij} V_{kk}(\mu) - V_{ji}(\mu),$$

this result simplifies to

$$V_{ij}(q+1) \to \sum_{\mu=0}^{q+1} (-\alpha_{q\mu-1} + I_0 \alpha_{q\mu}) V_{ji}(\mu),$$

where definitions (C12c) and (C12d) are invoked. The proof of Eqs. (C12) follows.

We next derive a second auxiliary result required in our proof of Eq. (C11). The relation

$$I_q \to \sum_{\mu=0}^{q} \alpha_{q\mu} I_\mu \tag{C13}$$

follows from Eq. (C12a), and is a special case of the more general relation

$$I_{q+p} \to \sum_{\mu=0}^{q} \sum_{\nu=0}^{p} \alpha_{q\mu} \alpha_{p\nu} I_{\mu+\nu}, \tag{C14}$$

which we now prove. Note that setting $p = 0$ in Eq. (C14) yields Eq. (C13). Thus, Eq. (C14) is correct for $p = 0$ and arbitrary q. It can therefore be proved by showing that Eqs. (C14) and (C12) imply that

$$I_{q+(p+1)} \to \sum_{\mu=0}^{q} \sum_{\nu=0}^{p+1} \alpha_{q\mu} \alpha_{p+1\nu} I_{\mu+\nu} \tag{C15}$$

holds for arbitrary q. By the induction hypothesis, Eq. (C14) is assumed to hold for arbitrary q. Thus,

$$I_{(q+1)+p} \to \sum_{\mu=0}^{q+1} \sum_{\nu=0}^{p} \alpha_{q+1\mu} \alpha_{p\nu} I_{\mu+\nu}. \tag{C16}$$

The object is to cast this result in the form (C15) or, equivalently, to show that the difference between Eqs. (C15) and (C16) is zero. The sums in Eqs. (C15) and (C16) can be extended to $q+1$ and $p+1$, respectively. Thus, Eq. (C15) obtains if the following relation holds:

$$\sum_{\mu=0}^{q+1} \sum_{\nu=0}^{p+1} (\alpha_{q\mu} \alpha_{p+1\nu} - \alpha_{q+1\mu} \alpha_{p\nu}) I_{\mu+\nu} = 0. \tag{C17}$$

To show that it does, we use relations (C12) and form

$$\alpha_{q\mu} \alpha_{p+1\nu} - \alpha_{q+1\mu} \alpha_{q\nu} = -(\alpha_{q\mu} \alpha_{p\nu-1} - \alpha_{q\mu-1} \alpha_{p\nu}).$$

Under this substitution, the left-hand side of Eq. (C17) becomes

$$\sum_{\mu=-1}^{q} \sum_{\nu=0}^{p} \alpha_{q\mu} \alpha_{p\nu} I_{\mu+\nu+1} - \sum_{\mu=0}^{q} \sum_{\nu=-1}^{p} \alpha_{q\mu} \alpha_{p\nu} I_{\mu+\nu+1}$$

$$= \alpha_{q,-1} \left(\sum_{\nu=0}^{p} \alpha_{p\nu} I_\nu \right) - \alpha_{p,-1} \left(\sum_{\mu=0}^{q} \alpha_{q\mu} I_\mu \right)$$

$$= \alpha_{q,-1} \alpha_{p,-1} - \alpha_{p,-1} \alpha_{q,-1} = 0.$$

Thus, Eq. (C17) is an identity, and Eq. (C15) holds for arbitrary q and fixed $p+1$, if Eq. (C14) holds for arbitrary q and all nonnegative integers less than or equal to p. Since the result holds for $p = 0$, it holds generally.

Equations (C12) and (C14) are the significant results needed to prove Eq. (C11). Define

$$V'_{ij}(q) = \sum_{\mu=0}^{q} \alpha_{q\mu} V_{ji}(\mu), \tag{C18a}$$

$$I'_{q+p} = \sum_{\mu=0}^{q} \sum_{\nu=0}^{p} \alpha_{q\mu} \alpha_{p\nu} I_{\mu+\nu}, \tag{C18b}$$

$$\alpha_p = \begin{bmatrix} \alpha_{00} & 0 & 0 & \cdots & 0 \\ \alpha_{10} & \alpha_{11} & 0 & \cdots & 0 \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & & & \cdot \\ \alpha_{p0} & \alpha_{p1} & & \cdots & \alpha_{pp} \end{bmatrix}, \tag{C18c}$$

and note that

$$\alpha_{pp} = (-1)^p, \tag{C18d}$$

for $p = 0, 1, \cdots$. Then it is easy to verify

$$Y'_q = \alpha_q Y_q \alpha_q^t, \tag{C19a}$$

where Y_q is the matrix (5.8c). Thus,

$$\det Y'_q = \det Y_q. \tag{C19b}$$

Similarly, using the definition

$$M_{ij}(q) = \begin{bmatrix} I_0 & I_1 & \cdots & I_q \\ I_1 & I_2 & \cdots & I_{q+1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_{q-1} & I_q & \cdots & I_{2q-1} \\ V_{ij}(0) & V_{ij}(1) & \cdots & V_{ij}(q) \end{bmatrix}, \tag{C20a}$$

we obtain the transformation law

$$M'_{ij}(q) = \left[\begin{array}{ccc|c} & & & 0 \\ & \alpha_{q-1} & & \cdot \\ & & & \cdot \\ & & & \cdot \\ & & & 0 \\ \hline 0 & \cdots & 0 & 1 \end{array}\right] \times M_{ji}(q) A_q \left[\begin{array}{ccc|c} & & & 0 \\ & \alpha^t_{q-1} & & \cdot \\ & & & \cdot \\ & & & \cdot \\ & & & 0 \\ \hline 0 & \cdots & 0 & 1 \end{array}\right], \quad \text{(C20b)}$$

where A_q is the $(q+1) \times (q+1)$ matrix

$$A_q = \left[\begin{array}{ccc|c} & & & \alpha_{q0} \\ & I & & \alpha_{q1} \\ & & & \cdot \\ & & & \cdot \\ & & & \cdot \\ \hline 0 & \cdots & 0 & \alpha_{qq} \end{array}\right], \quad \text{(C20c)}$$

in which I is the unit matrix of dimension q.

Equation (C20b) is verified by direct block matrix multiplication. From Eqs. (C20b) and (C20c), we now obtain

$$\det M'_{ij}(q) = (-1)^q \det M_{ji}(q). \quad \text{(C21)}$$

Observing the forms of Eqs. (5.8), we now complete the proof of Eq. (C11): Under $E_{ij} \to -E_{ji}$, the following transformations are effected:

$$Y_q \to Y'_q, \quad Y_{q-1} \to Y'_{q-1}, \quad M_{ij}(q) \to M'_{ij}(q); \quad \text{(C22a)}$$

and, from Eqs. (C19b) and (C21), it follows that

$$X_{ij}(q) \to X'_{ij}(q) = (-1)^q X_{ji}(q). \quad \text{(C22b)}$$

APPENDIX D: LIMITS OF THE RACAH INVARIANTS

Certain limits of the Racah functions as $m_{nn} \to -\infty$ are derived in this appendix. The limit of $S^{(n)}_{0\tau}(m_{1n}, \cdots, m_{nn})$ is easily established, and we omit the derivation. To establish the limits of the other Racah functions, we require some preliminary results. We observe that the determinants of the matrices

$$Y^{(n)}_q(m) = \begin{bmatrix} I^{(n)}_0(m) & I^{(n)}_1(m) & \cdots & I^{(n)}_q(m) \\ I^{(n)}_1(m) & I^{(n)}_2(m) & \cdots & I^{(n)}_{q+1}(m) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I^{(n)}_q(m) & I^{(n)}_{q+1}(m) & \cdots & I^{(n)}_{2q}(m) \end{bmatrix}, \quad \text{(D1a)}$$

$$W^{(n)}_{q\tau}(m) = \begin{bmatrix} I^{(n)}_0(m) & I^{(n)}_1(m) & \cdots & I^{(n)}_q(m) \\ I^{(n)}_1(m) & I^{(n)}_2(m) & \cdots & I^{(n)}_{q+1}(m) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I^{(n)}_{q-1}(m) & I^{(n)}_q(m) & \cdots & I^{(n)}_{2q-1}(m) \\ 1 & p_{\tau n} & \cdots & p^q_{\tau n} \end{bmatrix}, \quad \text{(D1b)}$$

$$W^{(n)}_{0\tau}(m) \equiv 1 \quad \text{(all } n\text{)} \quad \text{(D1c)}$$

are polynomials in m_{nn}. In taking the limit $m_{nn} \to -\infty$, only the term in m_{nn} which is of highest degree is needed from the respective determinants. We state, and later prove, the following results:

$$\det Y^{(n)}_q(m_{1n}, \cdots, m_{nn}) = (m_{nn})^{2q} \det Y^{(n-1)}_{q-1}(m_{1n}, \cdots, m_{n-1n}) + \text{(lower-order terms)}, \quad \text{(D2a)}$$

for $q = 1, 2, \cdots, n-1$,

$$\det W^{(n)}_{q\tau}(m_{1n}, \cdots, m_{nn}) = (-m_{nn})^{2q-1} \det W^{(n-1)}_{q-1\tau}(m_{1n}, \cdots, m_{n-1n}) + \text{(lower-order terms)}, \quad \text{(D2b)}$$

for $q = 1, 2, \cdots, n-1$, $\tau = 1, 2, \cdots, n-1$,

$$\det W^{(n)}_{qn}(m_{1n}, \cdots, m_{nn}) = (m_{nn})^q \det Y^{(n-1)}_{q-1}(m_{1n}, \cdots, m_{n-1n}) + \text{(lower-order terms)}, \quad \text{(D2c)}$$

for $q = 1, 2, \cdots, n-1$.

Let us accept Eqs. (D2) momentarily. Then

$$[N^{(n)}_q(m_{1n}, \cdots, m_{nn})]^{\frac{1}{2}} \equiv [\det Y^{(n)}_{q-1}(m) \det Y^{(n)}_q(m)]^{\frac{1}{2}} = |m_{nn}|^{2q-1} [N^{(n-1)}_{q-1}(m_{1n}, \cdots, m_{n-1n})]^{\frac{1}{2}} + \text{(lower-order terms)}, \quad \text{(D3a)}$$

for $q = 2, 3, \cdots, n-1$,

$$[N^{(n)}_1(m_{1n}, \cdots, m_{nn})]^{\frac{1}{2}} = |m_{nn}| [n(n-1)]^{\frac{1}{2}} + \text{(const)}. \quad \text{(D3b)}$$

Thus,

$$\lim_{m_{nn}\to-\infty} \frac{\det W_{1\tau}^{(n)}(m_{1n},\cdots,m_{nn})}{[N_1^{(n)}(m_{1n},\cdots,m_{nn})]^{\frac{1}{2}}} = 1/[n(n-1)]^{\frac{1}{2}}, \quad \tau = 1,2,\cdots,n-1, \quad = -[(n-1)/n]^{\frac{1}{2}}, \quad \tau = n, \tag{D4a}$$

$$\lim_{m_{nn}\to-\infty} \frac{\det W_{q\tau}^{(n)}(m_{1n},\cdots,m_{nn})}{[N_q^{(n)}(m_{1n},\cdots,m_{nn})]^{\frac{1}{2}}} = \frac{\det W_{q-1\tau}^{(n-1)}(m_{1n},\cdots,m_{n-1n})}{[N_{q-1}^{(n-1)}(m_{1n},\cdots,m_{n-1n})]^{\frac{1}{2}}}, \quad \text{for} \quad q = 2,3,\cdots,n-1, \quad \tau = 1,2,\cdots,n-1, \quad = 0, \quad \text{for} \quad q = 2,3,\cdots,n-1, \quad \tau = n. \tag{D4b}$$

Equations (5.27) and (5.28) are now easy consequences of the above limit relations.

The limits (D4) are established once Eqs. (D2) are proved. This we now do. The derivation of the following recursion relation is an easy task using Eq. (B14):

$$I_{k+1}^{(n)}(m_{1n},\cdots,m_{nn}) - m_{nn}I_k^{(n)}(m_{1n},\cdots,m_{nn}) = I_{k+1}^{(n)}(m_{1n},\cdots,m_{n-1n},0) - m_{nn}I_k^{(n-1)}(m_{1n}+1,\cdots,m_{n-1n}+1). \tag{D5}$$

We now perform the following column operations in $\det Y_q^{(n)}(m)$ without changing its value: To column $q+1$ add $-m_{nn}$ times column q; to column q add $-m_{nn}$ times column $q-1$; $\cdots$; to column 2 add $-m_{nn}$ times column 1. These operations bring the determinant to the following form in consequence of identity (D5):

$$\det \begin{bmatrix} P_0 & P_1(0)-\lambda Q_0 & P_2(0)-\lambda Q_1 & \cdots & P_q(0)-\lambda Q_{q-1} \\ P_1 & P_2(0)-\lambda Q_1 & P_3(0)-\lambda Q_2 & \cdots & P_{q+1}-\lambda Q_q \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ P_q & P_{q+1}(0)-\lambda Q_q & P_{q+2}(0)-\lambda Q_{q+1} & \cdots & P_{2q}(0)-\lambda Q_{2q-1} \end{bmatrix}, \tag{D6a}$$

where we have defined $\lambda \equiv m_{nn}$ and

$$P_k = I_k^{(n)}(m_{1n},\cdots,m_{nn}),$$
$$P_k(0) = I_k^{(n)}(m_{1n},\cdots,m_{n-1n},0), \tag{D6b}$$
$$Q_k = I_k^{(n-1)}(m_{1n}+1,\cdots,m_{n-1n}+1).$$

In its dependence on m_{nn}, P_k is a polynomial of degree k, and, indeed,

$$P_k = \lambda^k + (\text{lower-order terms}).$$

The term of highest degree in λ in the above determinant clearly originates from P_q times its cofactor, and it is

$$\lambda^{2q} \det \begin{bmatrix} Q_0 & Q_1 & \cdots & Q_{q-1} \\ Q_1 & Q_2 & \cdots & Q_q \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ Q_{q-1} & Q_q & \cdots & Q_{2q-2} \end{bmatrix}. \tag{D7}$$

Finally, this determinant of the Q's is invariant to the downward shift $m_{in}+1 \to m_{in}$, $i = 1,2,\cdots,n-1$, of the arguments of the $I_k^{(n-1)}$, and effecting this shift yields the highest-degree term of

$$\det Y_q^{(n)}(m_{1n},\cdots,m_{nn})$$

as

$$m_{nn}^{2q} \det Y_{q-1}^{(n-1)}(m_{1n},\cdots,m_{n-1n}).$$

The second result, Eq. (D2b), is proved in an analogous fashion. Effecting the same column operations as above on the columns of $W_{q\tau}^{(n)}(m_{1n},\cdots,m_{nn})$ yields

$$\det \begin{bmatrix} P_0 & P_1(0)-\lambda Q_0 & \cdots & P_q(0)-\lambda Q_{q-1} \\ P_1 & P_2(0)-\lambda Q_1 & \cdots & P_{q+1}(0)-\lambda Q_q \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ P_{q-1} & P_q(0)-\lambda Q_{q-1} & \cdots & P_{2q-1}(0)-\lambda Q_{2q-2} \\ 1 & p_{\tau n}-\lambda & \cdots & p_{\tau n}^q - \lambda p_{\tau n}^{q-1} \end{bmatrix} \tag{D8}$$

The term of highest degree in λ in this determinant is

$$(-\lambda)^{2q-1} \det \begin{bmatrix} Q_0 & Q_1 & \cdots & Q_{q-1} \\ Q_1 & Q_2 & \cdots & Q_q \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ Q_{q-2} & Q_{q-1} & \cdots & Q_{2q-3} \\ 1 & p_{\tau n} & \cdots & p_{\tau n}^{q-1} \end{bmatrix}, \tag{D9}$$

for $\tau = 1, 2, \cdots, n-1$, and

$$\lambda^q \det \begin{bmatrix} Q_0 & Q_1 & \cdots & Q_{q-1} \\ Q_1 & Q_2 & \cdots & Q_q \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ Q_{q-1} & Q_q & \cdots & Q_{2q-2} \end{bmatrix}, \quad \text{(D10)}$$

for $\tau = n$. Noting the invariance of these determinants to the downward shifts $m_{in} + 1 \to m_{in}$, $i = 1, 2, \cdots, n-1$, we obtain the term of highest degree in m_{nn} of $\det W_{qr}^{(n)}(m_{1n}, \cdots, m_{nn})$,

$$(-m_{nn})^{2q-1} \det W_{q-1\tau}^{(n-1)}(m_{1n}, \cdots, m_{n-1n}), \quad \text{(D11a)}$$

for $\tau = 1, 2, \cdots, n-1$, and

$$(m_{nn})^q \det Y_{q-1}^{(n-1)}(m_{1n}, \cdots, m_{n-1n}), \quad \text{(D11b)}$$

for $\tau = n$.

APPENDIX E: THE ZEROS OF THE NORMALIZATION FUNCTIONS

The zeros of the invariant normalization operators $N_q^{(n)}$ of Eq. (5.8b) are established in this appendix. These zeros are determined by the zeros of the (Gram) determinants of the matrices (D1a) corresponding to $q = 1, 2, \cdots$.

In order to establish the desired results, it is first necessary to obtain two principal new results, which we first state, and then prove:

(i) For all lexical labels

$$m_{1n} \geq \cdots \geq m_{\rho-1n} = m_{\rho n} \geq m_{\rho+1n} \geq \cdots \geq m_{nn},$$

we have that

$$\det Y_q^{(n-1)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho+1n} - 1, \cdots, m_{nn} - 1) = 0$$

implies (E1a)

$$\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = 0,$$

where ρ is any fixed, but arbitrary, integer selected from $2, 3, \cdots, n$.

(ii) For all lexical labels $m_{1n} \geq m_{2n} \geq \cdots \geq m_{\rho n} > m_{\rho+1n} \geq \cdots \geq m_{nn}$, we have that

$$\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = 0$$

implies (E1b)

$$\det Y_q^{(n-1)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho+1n} - 1, \cdots, m_{nn} - 1) = 0,$$

where $\rho = 1, 2, \cdots$, or n.

Observe that there is *one equality* imposed on an adjacent pair of variables in Eq. (E1a) and there is *one strict inequality* imposed on an adjacent pair of variables in Eq. (E1b). The value $\rho = 1$ is not admitted in Eq. (E1a) because there is no variable to the left of m_{1n}; however, for $\rho = n$, the inequality $m_{nn} > m_{n+1n}$ in the variables of Eq. (E1b) simply drops out (these points come out in the proofs below). Finally, for $\rho = 1$, the first variable in Eq. (E1b) is $m_{2n} - 1$; for $\rho = n$ in either equation, the last variable is m_{n-1n}.

The proofs of properties (E1a) and (E1b) are quite detailed. The starting point is the following result relating $U(n-1)$ invariant functions to $U(n)$ invariant functions:

$$\begin{aligned} I_k^{(n-1)}(m_{1n} + 1, \cdots, m_{\rho-1n} + 1, m_{\rho+1n}, \cdots, m_{nn}) &= I_k^{(n)}(m_{1n}, \cdots, m_{\rho-1n}, \rho - n - 1, m_{\rho+1n}, \cdots, m_{nn}) \\ &\quad + I_{k-1}^{(n)}(m_{1n}, \cdots, m_{\rho-1n}, \rho - n - 1, m_{\rho+1n}, \cdots, m_{nn}), \end{aligned} \quad \text{(E2)}$$

for $k = 1, 2, \cdots$ and for $\rho = 1, 2, \cdots, n$. Observe that $m_{\rho n} = \rho - n - 1$ in the right-hand side of Eq. (E2) and that this variable is missing from the left-hand side. Property (E2) is established directly from expression (B14) and, since the proof is straightforward, it is omitted.

Next, we perform the following sequence of operations in the determinant of the matrix (D1a): First, replace each m_{in} by $m_{in} - m_{\rho n} + \rho - n - 1$, $i = 1, 2, \cdots, n$; second, to row $q+1$ add row q, to row q add row $q-1, \cdots$, to row 2 add row 1. In consequence of the invariance of the determinant to these operations and of relation (E2), we obtain the following result:

$$\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = \det \begin{bmatrix} y_0^{(n)}(x) & y_1^{(n)}(x) & \cdots & y_q^{(n)}(x) \\ I_1^{(n-1)}(x) & I_2^{(n-1)}(x) & \cdots & I_{q+1}^{(n-1)}(x) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I_q^{(n-1)}(x) & I_{q+1}^{(n-1)}(x) & \cdots & I_{2q}^{(n-1)}(x) \end{bmatrix}, \quad \text{(E3)}$$

where $(x) = (x_1, x_2, \cdots, x_{n-1})$ with $x_i \equiv m_{in} - m_{\rho n} + \rho - n$, $i = 1, 2, \cdots, \rho - 1$, $x_i \equiv m_{i+1n} - m_{\rho n} + \rho - n - 1$, $i = \rho, \rho + 1, \cdots, n-1$, and where

$$y_k^{(n)}(x) \equiv I_k^{(n)}(x_1 - 1, \cdots, x_{\rho-1} - 1, \rho - n - 1, x_\rho, \cdots, x_{n-1}). \quad \text{(E4)}$$

Equation (E1a) immediately obtains from Eq. (E3) upon demonstrating that the *first row* in the matrix

$Y_q^{(n-1)}(x)$ [cf. Eq. (D1a) for $n \to n-1$] is linearly independent of the remaining rows for arbitrary labels

$$m_{1n} \geq m_{2n} \geq \cdots \geq m_{\rho-1n} = m_{\rho n} \geq m_{\rho+1n} \geq \cdots \geq m_{nn}, \quad \rho = 2, 3, \cdots, n.$$

Once this result is established, we argue as follows: The vanishing of the determinant on the left-hand side of Eq. (E1a) implies the vanishing of the determinant obtained from it by shifting all the labels by $\lambda = -m_{\rho-1n} + \rho - n$, i.e., it implies $\det Y_q^{(n-1)}(x) = 0$, for $m_{\rho n} = m_{\rho-1n}$, or equivalently, for $x_{\rho-1} = \rho - n$. But, from the above result (to be proved), we have that $\det Y_q^{(n-1)}(x) = 0$ (for $x_{\rho-1} = \rho - n$) implies a linear relation among its rows 2 to $q+1$; but these are just the rows which also appear in the determinant on the right-hand side of Eq. (E3) (having first set $m_{\rho n} = m_{\rho-1n}$). Thus, we obtain the result, Eq. (E1a).

Let us therefore turn to the ancillary problem relating to the linear dependence (independence) of the rows of the matrix (D1a) (for arbitrary n, in particular, for $n \to n-1$). It is convenient to write the invariant functions in the form

$$I_{k+l}^{(n)} = n(Z_k, Z_l), \tag{E5}$$

where Z_k, $k = 0, 1, 2, \cdots$, denote the row vectors defined by Eqs. (5.22b) and (5.22c) and the notation (Z_k, Z_l) denotes the scalar product of two row vectors and is defined by the left-hand side of Eq. (5.23). In particular, we have

$$Z_{kr}(m) = p_{\tau n}^{k} R_{n\tau}^{(n)}(m). \tag{E6}$$

A property particular to a Gram matrix is that a linear relation can obtain among its rows if and only if the *same* linear relation obtains among the vectors from which it is constructed, i.e., if, in the matrix (D1a), we have

$$\alpha_0(m)(\text{row } 1) + \alpha_1(m)(\text{row } 2) + \cdots + \alpha_q(m)(\text{row } q+1) = 0, \tag{E7a}$$

then also

$$\alpha_0(m)Z_0(m) + \alpha_1(m)Z_1(m) + \cdots + \alpha_q(m)Z_q(m) = 0, \tag{E7b}$$

and conversely.

Next, we apply the above result (for $n \to n-1$) to the matrix $Y_q^{(n-1)}(x)$ in which variable $x_{\rho-1}$ has the value $x_{\rho-1} = \rho - n$. The partial hook corresponding to this variable is $p_{\rho-1n-1} = x_{\rho-1} + n - \rho = 0$. In particular, it follows from Eq. (E6) for $n \to n-1$ and $\tau = \rho - 1$ that the $(\rho-1)$th component of each of row vectors $Z_k(x_1, \cdots, x_{n-1})$, $k = 1, 2, \cdots, q$, vanishes. But, by direct examination, we establish that the $(\rho-1)$th component, $R_{n-1\rho-1}^{(n-1)}(x)$, of the row vector $Z_0(x_1, \cdots, x_{n-1})$ does not vanish for $x_{\rho-1} = \rho - n$ and for arbitrary lexical choices of the variables in $m_{1n}, \cdots, m_{\rho-2n}, m_{\rho-1n}, m_{\rho-1n}, m_{\rho+1n}, \cdots, m_{nn}$. We therefore conclude that the first row of $Y_q^{(n-1)}(x)$ is independent of the remaining rows for all possible sets of lexical variables $m_{1n}, \cdots, m_{\rho-2n}, m_{\rho-1n}, m_{\rho-1n}, m_{\rho+1n}, \cdots, m_{nn}$. We have thus established the validity of the implication, Eq. (E1a).

The proof of Eq. (E1b) follows similarly. We observe from the manner in which Eq. (E3) was constructed that the elements of the first row can be written as

$$y_l^{(n)} = n(Z_0, Z_l), \quad l = 0, 1, \cdots, q, \tag{E8a}$$

while the elements in row k, $k = 2, 3, \cdots, q+1$, can be expressed as

$$I_{k+l-1}^{(n-1)} = n(Z_{k-2} + Z_{k-1}, Z_l), \quad l = 0, 1, \cdots, q, \tag{E8b}$$

where the invariant functions are evaluated on the labels

$$(x_1 - 1, \cdots, x_{\rho-1} - 1, \rho - n - 1, x_\rho, \cdots, x_{n-1}). \tag{E8c}$$

A linear relation among the rows of the determinant (E3), i.e.,

$$\beta_0(\text{row } 1) + \beta_1(\text{row } 2) + \cdots + \beta_q(\text{row } q+1) = 0 \tag{E9a}$$

implies the linear relation

$$\beta_0 Z_0 + \beta_1(Z_0 + Z_1) + \cdots + \beta_q(Z_{q-1} + Z_q) = 0, \tag{E9b}$$

when evaluated on the labels (E8c). But now observe from Eq. (E6) for $\tau = \rho$ and $p_{\rho n} = m_{\rho n} + n - \rho = -1$ that the ρth component of the vectors $Z_0(m) + Z_1(m)$, $Z_1(m) + Z_2(m), \cdots$ is zero, while the ρth component of $Z_0(m)$ vanishes *if and only if* $m_{\rho+1n} = m_{\rho n}$. Thus, we conclude that β_0 has value zero on the labels (E8c), provided $x_\rho \neq \rho - n - 1$. In other words, the first row of determinant (E3) is independent of the remaining rows for all lexical labels $m_{1n} \geq m_{2n} \geq \cdots \geq m_{\rho n} > m_{\rho+1n} \geq \cdots \geq m_{nn}$. Therefore, the vanishing of determinant (E3), under the restriction $m_{\rho n} > m_{\rho+1n}$, implies a linear relation among the lower q rows and therefore implies

$$\det Y_q^{(n-1)}(x_1, \cdots, x_{n-1}) = 0,$$
$$\det Y_q^{(n-1)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho+1n} - 1, \cdots, m_{nn} - 1) = 0, \tag{E10}$$

and property (E1b) is proved.

Results (E1a) and (E1b) are next utilized in the proof of the following significant result (valid for $q = 1, 2, \cdots, n$).

Lemma: For $m_{1n} \geq m_{2n} \geq \cdots \geq m_{nn}$, we have

$$\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = 0 \qquad \text{(E11a)}$$

if and only if the sequence S_n (of $n-1$ terms)

$$S_n = \{m_{1n} - m_{2n}, m_{2n} - m_{3n}, \cdots, m_{n-1n} - m_{nn}\} \qquad \text{(E11b)}$$

contains $n - q$ or more zeros.

The proof of the lemma is by induction on n. Before noting how one puts in the details of this proof, let us note some particular results:

$$\det Y_1^{(n)}(m) = \sum_{i<j}^{n} {}_1 (p_{in} - p_{jn})^2 - [n^2(n^2-1)/12], \qquad \text{(E12a)}$$

$$\det Y_{n-1}^{(n)}(m) = \prod_{i<j}^{n} {}_1 [(p_{in} - p_{jn})^2 - 1], \qquad \text{(E12b)}$$

$$\det Y_q^{(n)}(m) = 0, \quad q \geq n. \qquad \text{(E12c)}$$

Equation (E12a) is established by direct expansion of the 2×2 determinant; Eq. (E12b) is proved in Appendix C; and Eq. (E12c) follows from the fact that the Gram determinant of more than n vectors in n space is zero. Thus, we verify the lemma directly for $q = 1$ or $q = n - 1$. In particular, for $n = 2$ or 3, Eqs. (E12) give the complete result.

We turn now to the general proof of the lemma. We assume that the lemma is valid for $n - 1$ and show that Eqs. (E1) then imply the validity for n. Since Eqs. (E1) play the key role in this induction, we adapt the notation to facilitate use of these equations.

In the revised notation, the assumption for $n - 1$ takes the form (for $q = 1, 2, \cdots,$ or $n - 1$):

For $m_{1n} \geq \cdots \geq m_{\rho-1n} \geq m_{\rho+1n} \geq \cdots \geq m_{nn}$, $\rho = 1, 2, \cdots,$ or n, we have

$$\det Y_q^{(n-1)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho+1n} - 1, \cdots, m_{nn} - 1) = 0 \qquad \text{(E13a)}$$

if and only if the sequence

$$S'_{n-1} = \{m_{1n} - m_{2n}, \cdots, m_{\rho-2n} - m_{\rho-1n}, m_{\rho-1n} - m_{\rho+1n} + 1, m_{\rho+1n} - m_{\rho+2n}, \cdots, m_{n-1n} - m_{nn}\} \qquad \text{(E13b)}$$

contains $n - q - 1$ or more zeros. (For $\rho = n$, the last term in the sequence is $m_{n-2n} - m_{n-1n}$; for $\rho = 2$, the first term in the sequence is $m_{1n} - m_{3n} + 1$.)

We begin the induction by considering the sequence $S_n = \{m_{1n} - m_{2n}, m_{2n} - m_{3n}, \cdots, m_{n-1n} - m_{nn}\}$. We seek to establish the "if" part of statement (E11): If the sequence S_n contains $n - q$ or more zeros, then $\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = 0$.

The sequence S_n either has no zeros (trivial case, $q = n$) or it has *a first zero reading from the right.* Assume this first zero occurs at position $\rho - 1$, that is, $m_{\rho-1n} - m_{\rho n} = 0$. Then the sequence S'_{n-1} necessarily has $n - q - 1$ or more zeros. But $n - q - 1$ or more zeros in S'_{n-1} implies—by hypothesis at induction level $n - 1$—that

$$\det Y_q^{(n-1)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho+1n} - 1, \cdots, m_{nn} - 1) = 0.$$

By using Eq. (E1a), this then implies that

$$\det Y_q^{(n)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho-1n}, m_{\rho+1n}, \cdots, m_{nn}) = 0.$$

This establishes the induction loop and, since the "if" part of the lemma is true for $n = 3$, it is true in general.

To establish the "only if" part of the lemma, we take as given that $\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = 0$, and we seek to prove that this implies that the sequence S_n has $n - q$ or more zeros.

First, we observe that, for $q = 1, 2, \cdots, n - 1$,

$$\det Y_q^{(n)}(m_{1n}, \cdots, m_{nn}) = 0$$

implies that *at least two adjacent variables are equal.* This result follows directly from Eq. (E12b) and the fact that the nonvanishing of a Gram determinant implies the nonvanishing of all its principal subdeterminants. Second, if all the variables are equal, we choose $\rho = n$ in Eq. (E1b), and the desired result follows immediately from the hypothesis that it is valid at level $n - 1$. (Therefore, in the subsequent argument, we can assume that S_n does not consist of all zeros.)

We now argue as follows: In the sequence S_n, there must exist a first term (*reading from the left*) which is zero *followed by a term which does not vanish.* Assume that this occurs at the $(\rho - 1)$th and ρth terms in the sequence, i.e., that $m_{\rho-1n} - m_{\rho n} = 0$, but $m_{\rho n} - m_{\rho+1n} > 0$ (note that $\neq 0$ implies > 0 by lexicality).

From Eq. (E1b), it now follows that

$$\det Y_q^{(n-1)}(m_{1n}, \cdots, m_{\rho-1n}, m_{\rho+1n} - 1, \cdots, m_{nn} - 1) = 0.$$

By the assumed validity of the lemma—the induction hypothesis at level $n - 1$—this implies that the sequence S'_{n-1} of Eq. (E13b) contains $n - q - 1$ or more

zeros. But all terms in the sequence S'_{n-1}, except the one in position $\rho - 1$, which is not zero, also occur in S_n. Furthermore, S_n contains a zero at position $\rho - 1$, and this zero is *not* in S'_{n-1}. It follows that S_n contains $n - q$ or more zeros. This establishes the induction loop for the "only if" part of the lemma, and the lemma is true in general since it is correct for $n = 3$. [Note that for $q = n$, the result for "only if" also follows from Eq. (E12c).]

Thus, we have established the lemma despite the fact that our two principal results, Eqs. (E1a) and (E1b), apparently distinguish between variables to the left or right of variable $m_{\rho n}$.

The properties of the normalization functions $N_q^{(n)}$ now follow easily from the lemma of Eqs. (E11). Observe that $\det Y_q^{(n)}(m)$ always vanishes whenever $\det Y_{q-1}^{(n)}(m)$ does. We can therefore assert: *For* $m_{1n} \geq m_{2n} \geq \cdots \geq m_{nn}$ *and* $q = 1, 2, \cdots, n-1$, *we have* $N_q^{(n)}(m) = 0$ *if and only if the sequence* S_n *of Eq. (E11b) contains* $n - q$ *or more zeros.*

It is convenient to state the above property in terms of the null space of the function $N_q^{(n)}$. The null space $\mathcal{N}_{n-q}$ of the function $N_q^{(n)}$ is defined to be the set of all IR spaces on which the function $N_q^{(n)}$ has value zero. [The reason for labeling the null spaces in this particular way is simply so that the null space of the Wigner operator with operator pattern (ρ, ρ) becomes $\mathcal{N}_\rho$.] Thus:

$$\mathcal{N}_\rho = \{\text{all IR spaces with labels } [m]_n \text{ in which the sequence } S_n \text{ contains } \rho \text{ or more zeros}\}, \tag{E14}$$

for $\rho = 1, 2, \cdots, n-1$. Clearly, these null spaces possess the inclusion property

$$\mathcal{N}_1 \supset \mathcal{N}_2 \supset \cdots \supset \mathcal{N}_{n-1}. \tag{E15}$$

Then: $N_q^{(n)}([m]) = 0$ *if and only if the labels* $[m]$ *belong to an IR space contained in the null space* $\mathcal{N}_{n-q}$.

Finally, let us note the connection of the zeros of $N_q^{(n)}$ with the reduction of the direct product $[m]_n \times [1\ \dot{0}\ -1]$. We assert the following result (which can be proved directly from the rules for reducing direct products): The number of times which $[m]_n$ appears in the reduction of $[m]_n \times [1\ \dot{0}\ -1]$ is equal to $k - 1$, where $n - k$ is the number of zeros in the sequence S_n of Eq. (E11b), $k = 1, 2, \cdots, n$.

Now let k be fixed. Then since $N_q^{(n)}([m]) \neq 0$ for $q = 1, 2, \cdots, k-1$ and $N_q^{(n)}([m]) = 0$ for $q = k, k+1, \cdots, n-1$, we always obtain precisely $k - 1$ adjoint Wigner operators ($\Delta = [\dot{0}]$) which do *not* annihilate the IR space $|(m)\rangle$ and $n - k$ adjoint Wigner operators which *do* annihilate $|(m)\rangle$. [These two sets of Wigner operators are those with *operator patterns* (ρ, ρ) given by $(n-1, n-1), \cdots, (n-k+1, n-k+1)$ and $(n-k, n-k), \cdots, (1, 1)$, respectively.] Thus, we always obtain precisely the correct number of orthonormalized Wigner coefficients required to effect the reduction of $[m]_n \times [1\ \dot{0}\ -1]$ into its $[m]_n$ constituents.

APPENDIX F: CONJUGATION SYMMETRY

In this appendix, we note the symmetry properties possessed by the fundamental Wigner operators, the adjoint Wigner operators, and the adjoint Racah invariants under the operation of conjugation.

The $SU(n)$ conjugation operator $\mathcal{K}$ was introduced in Ref. 5, Paper III as a mapping on $SU(n)$ state vectors ($m_{nn} = 0$). However, when we consider $m_{nn} \neq 0$ and also admit negative integers into the labels of $U(n)$ state vectors, the operator $\mathcal{K}$ is no longer a convenient operation because it is a "many-to-one" mapping: Each state vector in the set $\{|(m)\rangle : m_{ij} - m_{nn} \text{ is the same}\}$ is mapped by $\mathcal{K}$ to the same $SU(n)$ state vector.

We introduce the $U(n)$ conjugation operator $\mathcal{C}$ to be the mapping (on a generic state vector)

$$\mathcal{C}\,|(m)\rangle = (-1)^{\phi(m)}|(\bar{m})\rangle, \tag{F1a}$$

where

$$\bar{m}_{ij} \equiv -m_{j-i+1\,j}, \tag{F1b}$$

$$\phi(m) \equiv \sum_{j=1}^{n}\sum_{i=1}^{j} m_{ij}. \tag{F1c}$$

The operator A' conjugate to a given operator A is then defined by

$$\langle \mathcal{C}(m')|\, A'\, |\mathcal{C}(m)\rangle = \langle (m')|\, A\, |(m)\rangle, \tag{F2}$$

where the notation $\mathcal{C}(m)$ is an abbreviated designation for $\mathcal{C}\,|(m)\rangle$. Definition (F1) is motivated by the very similar definition of $\mathcal{K}$ and the following important property of the $U(n)$ generators:

$$\langle \mathcal{C}(m')|\, -E_{ji}\, |\mathcal{C}(m)\rangle = \langle (m')|\, E_{ij}\, |(m)\rangle. \tag{F3}$$

The operator $\mathcal{C}$ is 1-to-1 onto, and it therefore possesses a unique inverse. Indeed, one easily verifies that $\mathcal{C}$ is *unitary and Hermitian.* In consequence, property (F3) of the generators is expressed by

$$E'_{ij} = -E_{ji} = \mathcal{C}E_{ij}\mathcal{C}^{-1}, \tag{F4}$$

where the E'_{ij} are the generators of the complex conjugate representations.[3]

The basic relations required for the determination of the conjugation properties of Wigner operators are the following properties of the fundamental reduced

Wigner coefficients:

$$\left\langle \begin{pmatrix} [\bar{m}]_n - \Delta_n(n-\rho+1) \\ [\bar{m}]_{n-1} - \Delta_{n-1}(n-\alpha) \end{pmatrix} \middle| \begin{bmatrix} \overline{n-\rho+1} \\ [\dot{0}\ \ -1] \\ \overline{n-\alpha} \end{bmatrix} \middle| \begin{pmatrix} [\bar{m}]_n \\ [\bar{m}]_{n-1} \end{pmatrix} \right\rangle$$

$$= (-1)^{\alpha-\rho} \left\langle \begin{pmatrix} [m]_n + \Delta_n(\rho) \\ [m]_{n-1} + \Delta_{n-1}(\alpha) \end{pmatrix} \middle| \begin{bmatrix} \rho \\ [1\ \ \dot{0}] \\ \alpha \end{bmatrix} \middle| \begin{pmatrix} [m]_n \\ [m]_{n-1} \end{pmatrix} \right\rangle, \tag{F5a}$$

for $\alpha = 1, 2, \cdots, n-1$,

$$\left\langle \begin{pmatrix} [\bar{m}]_n - \Delta_n(n-\rho+1) \\ [\bar{m}]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} \overline{n-\rho+1} \\ [\dot{0}\ \ -1] \\ \bar{n} \end{bmatrix} \middle| \begin{pmatrix} [\bar{m}]_n \\ [\bar{m}]_{n-1} \end{pmatrix} \right\rangle$$

$$= (-1)^{\rho-1} \left\langle \begin{pmatrix} [m]_n + \Delta_n(\rho) \\ [m]_{n-1} \end{pmatrix} \middle| \begin{bmatrix} \rho \\ [1\ \ \dot{0}] \\ n \end{bmatrix} \middle| \begin{pmatrix} [m]_n \\ [m]_{n-1} \end{pmatrix} \right\rangle. \tag{F5b}$$

These relations are established directly from the explicit expressions for the reduced Wigner coefficients.

The next step is to use relation (F5) in the reduction law which relates $U(n)$ Wigner coefficients to the $U(n):U(n-1)$, $U(n-1):U(n-2), \cdots$ reduced Wigner coefficients. The result which obtains is expressed by

$$\mathcal{C} \left\langle \begin{matrix} \rho \\ [1\ \ \dot{0}] \\ i \end{matrix} \right\rangle \mathcal{C}^{-1} = (-1)^{n+i-\rho} \left\langle \begin{matrix} \overline{n-\rho+1} \\ [\dot{0}\ \ -1] \\ \bar{\imath} \end{matrix} \right\rangle \tag{F6}$$

Particular cases of property (F6) which are required for the determination of the conjugation properties of the adjoint Wigner operators are

$$\left\langle \begin{pmatrix} [1\ \ \dot{0}\ \ -1] \\ (i,j) \end{pmatrix} \middle| \left\langle \begin{matrix} 1 \\ [1\ \ \dot{0}] \\ i \end{matrix} \right\rangle \middle| \begin{pmatrix} [\dot{0}\ \ -1] \\ \bar{\jmath} \end{pmatrix} \right\rangle$$

$$= \left\langle \begin{pmatrix} [1\ \ \dot{0}\ \ -1] \\ (j,i) \end{pmatrix} \middle| \left\langle \begin{matrix} \bar{n} \\ [\dot{0}\ \ -1] \\ \bar{\imath} \end{matrix} \right\rangle \middle| \begin{pmatrix} [1\ \ \dot{0}] \\ j \end{pmatrix} \right\rangle, \tag{F7a}$$

$$\langle (\dot{0}) | \left\langle \begin{matrix} n \\ [1\ \ \dot{0}] \\ j \end{matrix} \right\rangle \middle| \begin{pmatrix} [\dot{0}\ \ -1] \\ \bar{\jmath} \end{pmatrix} \right\rangle$$

$$= (-1)^{n-1} \langle (\dot{0}) | \left\langle \begin{matrix} \bar{1} \\ [\dot{0}\ \ -1] \\ \bar{\jmath} \end{matrix} \right\rangle \middle| \begin{pmatrix} [1\ \ \dot{0}] \\ j \end{pmatrix} \right\rangle. \tag{F7b}$$

Next, we apply the conjugation operation to the Wigner operators of Eqs. (4.5a) and (4.5b). [Note that the two Wigner operators in Eq. (4.5a) commute; note also that, in Eq. (4.5b), we must use relation (F7a) to effect the coupling of the conjugated operators.] The result is

$$\mathcal{C} \left\langle \begin{matrix} (\rho,\tau) \\ [1\ \ \dot{0}\ \ -1] \\ (i,j) \end{matrix} \right\rangle \mathcal{C}^{-1}$$

$$= (-1)^{n+1+i-j+\rho-\tau} \left\langle \begin{matrix} (n-\tau+1, n-\rho+1) \\ [1\ \ \dot{0}\ \ -1] \\ (j,i) \end{matrix} \right\rangle, \tag{F8}$$

for $\rho \neq \tau$ and all i, j.

The conjugation properties of the adjoint Wigner operators having $\Delta = [\dot{0}]$ are determined by property (C22b). In consequence of relation (F4), we can write

$$\mathcal{C} X_{ij}(q) \mathcal{C}^{-1} = (-1)^q X_{ji}(q). \tag{F9}$$

Noting relations (5.25) and the correspondence, (5.30), between the degree index q and operator patterns, we can write Eq. (F9) as follows:

$$\mathcal{C} \left\langle \begin{matrix} (\rho,\rho) \\ [1\ \ \dot{0}\ \ -1] \\ (i,j) \end{matrix} \right\rangle \mathcal{C}^{-1} = (-1)^{n+i-j+\rho} \left\langle \begin{matrix} (\rho,\rho) \\ [1\ \ \dot{0}\ \ -1] \\ (j,i) \end{matrix} \right\rangle. \tag{F10}$$

The last conjugation property we wish to note is that of the Racah invariants of Eqs. (4.3) (determined explicitly in Sec. 5). We use Eq. (2.46) and the explicit conjugation properties, Eqs. (F6) and (F10) to obtain the following results:

$$\mathcal{C} \left\{ (\dot{0}) \begin{pmatrix} n \\ [1\ \ \dot{0}] \\ \tau \end{pmatrix} \begin{pmatrix} [\dot{0}\ \ -1] \\ \bar{\tau} \end{pmatrix} \right\} \mathcal{C}^{-1}$$

$$= \left\{ (\dot{0}) \begin{pmatrix} \bar{1} \\ [\dot{0}\ \ -1] \\ n-\tau+1 \end{pmatrix} \begin{pmatrix} [1\ \ \dot{0}] \\ n-\tau+1 \end{pmatrix} \right\}, \tag{F11a}$$

$$\mathcal{C} \left\{ \begin{pmatrix} [1\ \ \dot{0}\ \ -1] \\ (\rho,\rho) \end{pmatrix} \begin{pmatrix} 1 \\ [1\ \ \dot{0}] \\ \tau \end{pmatrix} \begin{pmatrix} [\dot{0}\ \ -1] \\ \bar{\tau} \end{pmatrix} \right\} \mathcal{C}^{-1}$$

$$= (-1)^{\rho-1} \times \left\{ \begin{pmatrix} [1\ \ \dot{0}\ \ -1] \\ (\rho,\rho) \end{pmatrix} \begin{pmatrix} \bar{n} \\ [\dot{0}\ \ -1] \\ n-\tau+1 \end{pmatrix} \begin{pmatrix} [1\ \ \dot{0}] \\ n-\tau+1 \end{pmatrix} \right\}. \tag{F11b}$$

Remarks:

(i) The fact that the set of adjoint Wigner poerators having $\Delta = [\hat{0}]$ has the sharp conjugation property (F10), can, indeed, be directly attributed to the conjugation property (F11b), of the fundamental Racah invariants;

(ii) The conjugation property of the $U(2)$ Wigner operators can be given completely. It is

$$\mathcal{C}\left\langle \begin{matrix} & \Gamma_{11} & \\ M_{12} & & M_{22} \\ & M_{11} & \end{matrix} \right\rangle \mathcal{C}^{-1} = (-1)^{\phi(M)+M_{12}-\Gamma_{11}} \times \left\langle \begin{matrix} & & \Gamma_{11}-M_{12}-M_{22} \\ -M_{22} & & \\ & -M_{11} & \end{matrix} \right\rangle_{-M_{12}} \tag{F12}$$

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[1] L. C. Biedenharn, A. Giovannini, and J. D. Louck, J. Math. Phys. **8**, 691 (1967).

[2] L. C. Biedenharn and J. D. Louck, Commun. Math. Phys. **8**, 89 (1968).

[3] J. D. Louck, Am. J. Phys. **38**, 3 (1970).

[4] L. C. Biedenharn, J. Math. Phys. **4**, 436 (1963).

[5] G. E. Baird and L. C. Biedenharn, J. Math. Phys. **4**, 1499 (1963) (II); **5**, 1723 (1964) (III); **5**, 1730 (1964) (IV); **6**, 1847 (1965) (V).

[6] J. D. Louck, J. Math. Phys. **6**, 1786 (1965).

[7] L. C. Biedenharn, in *Spectroscopic and Group Theoretical Methods in Physics* (*Racah Memorial Volume*), F. Bloch *et al.*, Eds. (North-Holland, Amsterdam, 1968), p. 59.

[8] H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dover, New York, 1931), pp. 383, 391.

[9] This is to be contrasted with frequent claims of a "generalized Wigner–Eckart theorem"—which are largely vacuous (involving either ad hoc or unspecified labels).

[10] We find it very useful to adopt the generalization (Ref. 3) of $U(n)$ Gel'fand patterns having negative integers, but still obeying "betweenness conditions."

[11] I. M. Gel'fand and M. L. Zetlin, Dokl. Akad. Nauk SSSR, **71**, 825 (1950). See also I. M. Gel'fand, R. A. Minlos, Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Applications* (Pergamon, Oxford, and Macmillan, New York, 1963), p. 358.

[12] E. P. Wigner, Z. Physik **45**, 60 (1927).

[13] The notation $[m]$ always designates a row of IR labels, while (m) always designates a triangular Gel'fand array. Occasionally, it is necessary for clarity to use the more specific notation $[m]_k$ and $(m)_k$ to designate, respectively, that $[m]$ is of length k and that (m) contains k rows. For example, in the symbol (2.3) the specific notation would be $[m]_n$ and $(m)_{n-1}$. We drop such subscripts whenever no confusion can result from doing so.

[14] $\mathcal{O}_U$ is defined on all IR spaces, and Eq. (2.6) is to be considered as a generic equation.

[15] The fact that the coefficient (2.16) is zero whenever $[m'] = [m] + [\Delta(\Gamma)]$ is nonlexical is a special case of the state vector $|(m)\rangle$ belonging to the null space of the Wigner operator, but we choose to note such zeros separately.

[16] We use "unique" rather loosely to mean "unique up to a phase." Phases must be fixed by a convention, and such a convention is introduced later.

[17] "Kinematically independent" means that the two sets of generators commute.

[18] J. J. De Swart, Rev. Mod. Phys. **35**, 916 (1963).

[19] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge U. P., Cambridge, 1935), p. 74.

[20] Papers which relate most directly to our presentation include: J. Schwinger, *Quantum Theory of Angular Momentum*, L. C. Biedenharn and H. van Dam, Eds. (Academic, New York, 1965), p. 229; V. Bargmann, Rev. Mod. Phys. **34**, 829 (1962); T. A. Brody, M. Moshinsky, and I. Renero, J. Math. Phys. **6**, 1540 (1965) (and references therein).

[21] The relation of these polynomials to the IR's of $U(n)$ is discussed in detail in Ref. 3. See also I. M. Gel'fand and M. I. Graev, Izv. Akad. Nauk SSSR Ser. Mat. **29**, 1329 (1965).

[22] In a strict sense, the null-space factor $I_{(\Gamma)}$ should appear on the left-hand side of Eq. (2.46). Omitting this factor has the effect of assigning the value zero to the Racah invariant operator on all state vectors which are annihilated by the right-hand side. We must therefore interpret Eq. (2.46) as the definition of Racah operators.

[23] The results of this section on Racah coefficients may be compared with J.-R. Derome and W. T. Sharp, J. Math. Phys. **6**, 1584 (1965).

[24] A more specific notation for these invariants is $I_k^{(n)}$, where the superscript designates explicitly that these invariants are $U(n)$ invariants. It is often necessary to use the superscript to avoid confusing $U(n)$ invariants with $U(n-1)$ invariants, etc.

[25] For particular IR labels, the normalization functions N_q may have value zero. These vanishings are considered in detail in Appendix E. The more precise statement of orthogonality relations (5.9a) includes a null space factor on the right-hand side.

[26] The relations between the notations of this paper for $U(2)$ Wigner and Racah coefficients and the usual $SU(2)$ notations are given in detail in Ref. 3.

[27] Recall that, in this paper, phases were determined by the limit relation, Eq. (5.29). This assignment can be shown to be equivalent to the following convention on the reduced Wigner coefficients: The sign of a reduced Wigner coefficient is chosen to be positive whenever the upper and lower operator patterns are the same and for the $U(n-1)$ labels maximal, $m_{in-1} = m_{in}$ $(i = 1, 2, \cdots, n-1)$. This convention fixes all phases [and agrees with the $SU(2)$ convention].

[28] The general relation between $U(n)$ Wigner coefficients and $SU(n)$ Wigner coefficients is noted in Ref. 3.

[29] J. D. Louck, Los Alamos Scientific Laboratory Report LA-2451, 1960.

[30] A. Joseph, Rev. Mod. Phys. **40**, 845 (1968).

[31] O. Perron, *Algebra I* (Walter de Gruyter, Berlin, 1951), p. 153.

[32] D. E. Littlewood, *The Theory of Group Characters and Matrix Representations of Groups* (Oxford U. P. London, 1950), 2nd. ed.

[33] I. M. Gel'fand, Mat. Sb. **26**, 103 (1950).

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Derivation of the Wave and Scattering Operators for an Interaction of Rank One

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Expressions for the wave and scattering operators in terms of singular integral operators are rigorously derived for a simple scattering system, for which the interaction Hamiltonian, V is of rank 1. The wave operators, defined by the strong limits, $\lim e^{iHt}e^{-iH_0t}$ as $t \to \mp\infty$, are known to exist for this interaction, and the existence of these limits is assumed throughout the paper. Using complex contour integrals to write down representations for certain operators, we find an identity for the evolution operator in terms of a family of bounded operators, from which singular integral operators are obtained in the limit as $t \to \infty$. The analysis differs from previous applications of time-dependent scattering theory to this system in that at no stage need "smoothness" or Hölder conditions be assumed for the element of $L_2(-\infty, \infty)$ from which V is constructed.

INTRODUCTION

Since the work of Jauch and others,[1-4] the theory of nonrelativistic particle scattering has been set on a firm mathematical footing. There are two approaches, corresponding to the time-dependent and time-independent theories, respectively.

Time-dependent scattering theory involves a study of the strong limits

$$\Omega_{\pm}f = \lim_{t \to \mp\infty} e^{iHt}e^{-iH_0t}f,$$

where H_0 is the free Hamiltonian and H is the total Hamiltonian, both being self-adjoint operators in Hilbert space. For simple scattering systems for which the total Hamiltonian is of the form $H = H_0 + V$, the existence of the wave operators $\Omega_{\pm}$ may be proved for certain classes of interaction V. The wave operators are isometries, and the scattering operator S may be defined in terms of them by $S = \Omega_-^*\Omega_+$, where Ω_-^* denotes the operator adjoint to Ω_-. If the ranges of Ω_+ and of Ω_- are the same, the scattering operator is unitary. Unitarity of S has been proved for a large class of interactions.

The scattering operator, which relates incoming free-particle states at time $t = -\infty$ to outgoing free-particle states at time $t = +\infty$, and the S matrix, defined in terms of the "matrix elements" (g, Sf), are the ultimate goals of scattering theory, and are closely related to the experimental cross sections. It is therefore important to understand how, in time-dependent theory, the wave and scattering operators may be obtained from limits as $t \to \pm\infty$. One of the simplest types of interaction for which the existence and unitarity of S have been proved is an interaction of trace class.[4] An example of such an interaction is a perturbation $V: f(k) \to (\phi, f)\phi(k)$ of rank one, where ϕ is a fixed element of, say, $L_2(-\infty, \infty)$ and the free Hamiltonian H_0 is the multiplication operator $K: f(k) \to kf(k)$. In fact, the existence and unitarity of S for a general perturbation of trace class may be deduced from the corresponding result for perturbations of rank one by using some general properties of wave operators.

This paper is devoted to an investigation of the evaluation of the wave operators in the case of the above interaction of rank one, from strong limits as $t \to \pm\infty$. Most of the techniques we employ are applicable to interactions of greater generality than those of finite rank. However, it seems an advantage to consider a scattering system for which the S matrix may be calculated exactly, i.e., may be expressed in terms of singular integrals of known functions.

In the context of Hilbert space, singular integrals are conveniently expressed in terms of the Hilbert transform. The Hilbert transform is unitarily equivalent (via the Fourier transform) to the operator projecting onto the positive spectrum $(0, \infty)$ of the multiplication operator K. If the projection onto $(0, t)$ is denoted by $\hat{P}_{0t}$, then $\hat{P}_{0\infty}$ is related to $\hat{P}_{0t}$ by a strong limit as $t \to \infty$. In Sec. 1, we define a related operator F_{0t}, from which a singular integral operator $F_{0\infty}$ is obtained by the strong limit as $t \to \infty$. This is the approach we use to express time-dependent limits as singular integrals (we make no use of distributions).

The first step is to express the evolution operator $e^{iHt}e^{-iKt}$ in terms of F_{0t} and $F_{0\infty}$. To do this, we make use of the fact that the resolvent operator $G(\lambda) = (\lambda - H)^{-1}$ may be evaluated exactly for an

interaction of rank one. Our method is essentially to use Cauchy's theorem

$$\int_C \pi(\lambda)G(\lambda)\,d\lambda = 2\pi i\pi(H),$$

where $\pi(\lambda)$ is an analytic function. Since $\|G(\lambda)\|$ is not uniformly bounded for λ on C, using the technique of Lorch,[5] we must introduce into $\pi(\lambda)$ a polynomial which vanishes where the contour intersects the real λ axis. By using the spectral theorem,[5] we obtain an identity for the evolution operator which after some modification becomes Eq. (33).

The time-independent scattering problem would involve a study of the singular integral operator $F_{0\infty}$, which is usually unbounded. Here, it is sufficient to find a dense set of elements which are in the domain of $F_{0\infty}$. Now, given any interaction V, let $\mathcal{S}$ be the set of elements f such that $\|Ve^{iH_0t}f\|$ is absolutely integrable on $(-\infty, \infty)$ with respect to t. Then a sufficient condition for the existence of $\Omega_\pm$ (i.e., for $\Omega_\pm$ to be defined on the whole space) is that V is bounded and that $\mathcal{S}$ is everywhere dense. For the interaction considered here, $\mathcal{S}$ is the set of elements f such that the Fourier transform of $\phi^*(k)f(k)$ is absolutely integrable. It is interesting to note that, in this case, $\mathcal{S}$ is a subset of the domain of $F_{0\infty}$. The $\Omega_\pm$ exist even if $\mathcal{S}$ is not everywhere dense, in which case an alternative specification of the domain of $F_{0\infty}$ must be found. This domain is always everywhere dense, and is investigated in more detail elsewhere.[6]

The wave operators are defined by strong limits, but in practice it is simpler to take the weak limit of Eq. (33a). To do this, we first obtain, in Sec. 3, the weak limit of $\phi^*(k)a_t(k)$, where $a_t(k)$ is defined by Eq. (32). This limit, by use of Cauchy's theorem, may be expressed in terms of singular integrals as in Eq. (44a), and enables us to evaluate the wave operators (56) and (62) and the scattering operator (65).

1. THE SINGULAR OPERATORS

Our Hilbert space is $L_2(-\infty, \infty)$ with inner product

$$(f, g) = \int_{-\infty}^{\infty} f^*(k)g(k)\,dk.$$

Our free Hamiltonian $H_0 = K$ is defined by

$$(Kf)(k) = kf(k), \tag{1}$$

which has maximal domain

$$D_K = \{f(k) \in L_2;\ kf(k) \in L_2\}.$$

The interaction operator $V = |\phi)(\phi|$ is defined on the whole space by

$$Vf = \phi(\phi, f), \tag{2}$$

where ϕ is a fixed element of L_2.

The total Hamiltonian H is given by $H = K + V$, which also has domain D_K; H is self-adjoint with this domain.

We use the notation $\hat{g}$ for the Fourier transform of any element g of $L_1(-\infty, \infty)$, where

$$(\mathcal{F}g)(k) = \hat{g}(k) = \frac{1}{(2\pi)^{\frac{1}{2}}}\int_{-\infty}^{\infty} e^{-ikp}g(p)\,dp, \tag{3a}$$

and we also define

$$(\mathcal{F}^*g)(k) = \frac{1}{(2\pi)^{\frac{1}{2}}}\int_{-\infty}^{\infty} e^{ikp}g(p)\,dp. \tag{3b}$$

The operators Φ and Φ^*: $L_2 \to L_1$ are defined by

$$(\Phi f)(k) = \phi(k)f(k), \tag{4a}$$

$$(\Phi^* f)(k) = \phi^*(k)f(k), \tag{4b}$$

where ϕ^* is the complex conjugate of ϕ. We may also regard Φ and Φ^* as mapping L_∞ to L_2, in which case we retain the notation of Eqs. (4).

The projection $\hat{P}_{ab}$ is defined on L_2 by

$$\begin{aligned}(\hat{P}_{ab}f)(k) &= f(k), \quad k \in (a, b),\\ &= 0, \qquad \text{otherwise.}\end{aligned} \tag{5}$$

In this definition we also allow a and b to take values $\pm\infty$. We define

$$P_{ab} = \mathcal{F}^*\hat{P}_{ab}\mathcal{F}. \tag{6}$$

We now consider the operator F_{ab}. There are two cases of interest.

A. F_{ab} With a, b Finite

If $f \in L_2$, then $\mathcal{F}\Phi^* f \in L_\infty$. Hence, $\hat{P}_{ab}\mathcal{F}\Phi^* f$ is essentially bounded, and also absolutely integrable. Further, $\mathcal{F}^*$ maps L_1 to L_∞, so that $P_{ab}\Phi^* f \in L_\infty$. Hence, $\Phi P_{ab}\Phi^* f \in L_2$. We define the mapping F_{ab}: $L_2 \to L_2$ by

$$F_{ab}f = \Phi P_{ab}\Phi^* f. \tag{7}$$

An equivalent definition is

$$F_{ab}f = \frac{1}{2\pi}\int_a^b e^{iKt}\phi(\phi, e^{-iKt}f)\,dt. \tag{8}$$

Here and subsequently, integrals of the form $\int f_t\,dt$, where $f_t \in L_2$ and is a continuous function of t (in the strong topology defined by the L_2 norm), are to be understood as strong limits of approximating Riemann sums. Whenever integrals of this kind appear, we must verify the strong continuity of f_t, which guarantees the existence of the integral.

F_{ab} is a bounded symmetric linear operator, with

$$\|F_{ab}\| \leq [(b-a)/2\pi]\,\|\phi\|^2, \quad \text{when} \quad b > a.$$

The strong derivative $dF_{ab}f/db$ exists and equals $(2\pi)^{-1}e^{iKb}\phi(\phi, e^{-iKb}f)$, so that $F_{ab}f$ is a strongly continuous function of b and also of a.

From Eq. (8), we readily obtain the identity

$$e^{iKt}F_{ab}e^{-iKt} = F_{a+t,b+t}. \tag{9}$$

If, for any λ such that $\operatorname{Im}\lambda \neq 0$, we differentiate the identity with respect to t at $t = 0$, i.e.,

$$(\lambda - K)^{-1}e^{-i(\lambda-K)t}F_{ab}e^{i(\lambda-K)t}(\lambda - K)^{-1}f = (\lambda - K)^{-1}F_{a+t,b+t}(\lambda - K)^{-1}f,$$

and set $a = 0$, we obtain the commutation relation

$$[(\lambda - K)^{-1}, F_{0b}]f = (2\pi i)^{-1}(\lambda - K)^{-1}e^{iKb}Ve^{-iKb}(\lambda - K)^{-1}f - (2\pi i)^{-1}(\lambda - K)^{-1}V(\lambda - K)^{-1}f, \tag{10}$$

which we shall require later.

B. The Singular Operator $F_{0\infty}$

$F_{0\infty}$ is defined by

$$F_{0\infty}f = \text{s-}\lim_{t\to\infty} F_{0t}f \tag{11}$$

whenever the limit exists.

Similar definitions apply to $F_{b\infty}$, $F_{-\infty a}$, and $F_{-\infty\infty}$. These are all symmetric operators provided their domains are everywhere dense, since F_{ab} is symmetric.

We distinguish two cases:

Case (i): The set S, containing those elements f such that $\|Ve^{-iKt}f\|$ is absolutely integrable on $(-\infty, \infty)$, is everywhere dense.

Then from Eq. (8), with $u < v$, we have

$$\|F_{au}f - F_{av}f\| \leq \frac{1}{2\pi}\int_u^v \|Ve^{-iKt}f\|\,dt, \tag{12}$$

so that, letting $u, v \to \infty$, we see that any element f of the dense set S lies in the domain of $F_{a\infty}$ and, similarly, of $F_{-\infty b}$.

We also have, for such f,

$$F_{0\infty}f = \Phi P_{0\infty}\Phi^* f, \tag{13a}$$

$$F_{-\infty 0}f + F_{0\infty}f = F_{-\infty\infty}f = \Phi\Phi^* f. \tag{13b}$$

Equation (13b) follows from the observation that, if $\mathcal{F}g \in L_1$, then $\mathcal{F}^*\mathcal{F}g = g$.[7]

Case (ii): Suppose S is not necessarily everywhere dense. Let

$$I_\epsilon^{\pm}(k) = \int_{-\infty}^{\infty} \frac{|\phi^2(p)|\,dp}{k - p \pm i\epsilon}, \quad \epsilon > 0. \tag{14}$$

Then the limit

$$I_{\pm}(k) = \lim_{\epsilon\to 0} I_\epsilon^{\pm}(k) \tag{15}$$

exists for almost all k.[8]

The corresponding multiplication operators $I_\pm$ are given by

$$(I_\pm f)(k) = I_\pm(k)f(k) \quad \text{a.e.}, \tag{16}$$

each having domain

$$D_I = \{f(k) \in L_2;\ I_\pm(k)f(k) \in L_2\}.$$

It may be shown[6] that $D_I \subset D_F$, where D_F is the intersection of the domains of $F_{-\infty 0}$ and $F_{0\infty}$.

D_I is everywhere dense, so that, in Case (ii), the set S may be replaced by D_I.

Equations (13) remain valid for $f \in D_I$, except that (a) Φ and Φ^* must be regarded, in Eqs. (4), as mapping part of L_2 into L_2 and (b) in Eq. (6) applied to the definition of $P_{0\infty}$, $\mathcal{F}$ and $\mathcal{F}^*$ are Fourier transforms defined as bounded operators on L_2.

From Eq. (9), it is easily seen that

$$e^{iKt}F_{a\infty}e^{-iKt} = F_{a+t\infty}. \tag{17}$$

Note that, since $F_{s\infty} - F_{t\infty} = F_{sb} - F_{tb}$, $F_{s\infty}f$ is a strongly continuous function of s, for any f in D_F.

2. AN IDENTITY SATISFIED BY THE EVOLUTION OPERATOR

In order to obtain the wave operator, we first prove an identity for the evolution operator $e^{iHt}e^{-iKt}$. This identity is stated in Eq. (33).

The resolvent operator is given for $\operatorname{Im}\lambda \neq 0$ by

$$G(\lambda) = (\lambda - H)^{-1} = (\lambda - K)^{-1} + (\lambda - K)^{-1}g(\lambda)(\lambda - K)^{-1}, \tag{18}$$

where

$$g(\lambda) = [1 - I(\lambda)]^{-1}\,|\phi)\,(\phi| \tag{19}$$

and

$$I(\lambda) = \int_{-\infty}^{\infty} \frac{|\phi^2(p)|\,dp}{(\lambda - p)}. \tag{20}$$

We apply Cauchy's theorem to various contour integrals. The precise shape of the contour does not matter, but we choose the rectangular contour C of Fig. 1, which cuts the real λ axis at two points ξ and μ.

Now,

$$\|(\lambda - H)^{-1}\| \leq (|\operatorname{Im}\lambda|)^{-1},$$

so that, if we take

$$P(\lambda) = (\lambda - \xi)^n(\mu - \lambda)^n, \tag{21}$$

then, if $n > 1$, $\|P(\lambda)(\lambda - H)^{-1}\|$ is bounded on C and tends to zero as $\lambda \to \xi$ and $\lambda \to \mu$.

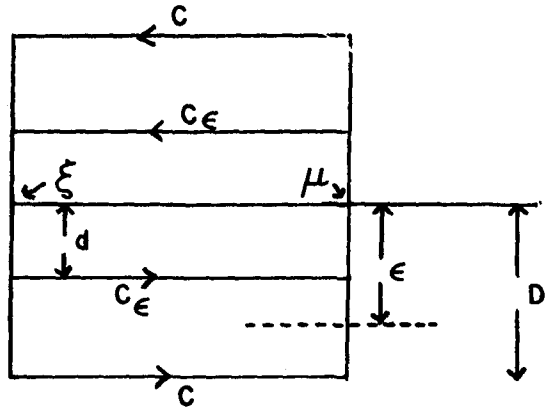

FIG. 1. Applications of Cauchy's theorem to various contour integrals.

Therefore, $P(\lambda)(\lambda - H)^{-1}f$ is a strongly continuous function of λ on C, and the contour integral

$$\int_C d\lambda\, P(\lambda)(\lambda - H)^{-1}f$$

is well defined if the integrand is regarded as vanishing when $\lambda = \xi$ or $\lambda = \mu$. The contour integral is defined in terms of Riemann integrals in the obvious way.

We have the two well-known identities

$$g(\lambda) = V + VG(\lambda)V, \tag{22a}$$

$$g(\lambda)(\lambda - K)^{-1} = VG(\lambda). \tag{22b}$$

Using Eqs. (22a) and (19), we find that $P(\lambda)/[1 - I(\lambda)]$ is a continuous function of λ on C, and we define

$$\Delta(t) = \int_C \frac{e^{i\lambda t}P(\lambda)}{1 - I(\lambda)}\, d\lambda. \tag{23}$$

For all real t, $\Delta(t)$ is a C^∞ function.

To obtain the identity for the evolution operator, we evaluate, in two ways, the integral

$$Tf = \iint\limits_{0\le t_1\le t_2\le t} \Delta(t_2 - t_1)e^{iKt_1}\phi(\phi, e^{-iKt_2}f)\, dt_1\, dt_2. \tag{24}$$

Using Eq. (23), we may express Tf as a multiple integral with respect to λ, t_1, and t_2. The integrand is strongly continuous in the three variables, so that the order of integration does not matter. Integrating first with respect to t_1, we find

$$\begin{aligned} Tf &= \iiint\limits_{\substack{0\le t_1\le t_2\le t\\ \lambda\in C}} \frac{P(\lambda)}{1 - I(\lambda)}\, e^{-i(\lambda - K)t_1} \\ &\quad \times \phi(\phi, e^{i(\lambda - K)t_2}f)\, dt_1\, dt_2\, d\lambda \\ &= \iint\limits_{\substack{0\le t_2\le t\\ \lambda\in C}} \frac{iP(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}(e^{-i(\lambda - K)t_2} - 1) \\ &\quad \times \phi(\phi, e^{i(\lambda - K)t_2}f)\, dt_2\, d\lambda, \end{aligned} \tag{25}$$

where we have used the result that, if the strong derivative df_t/dt exists and is strongly continuous in t, then

$$\int_0^{t_2} \frac{df_{t_1}}{dt_1}\, dt_1 = f_{t_2} - f_0.$$

Taking $n > 2$ in Eq. (21), we can express the integrand of Eq. (25) as a sum of two terms, each strongly continuous in λ and t_2 (and, by convention, vanishing at $\lambda = \xi, \mu$). Integrating one of these terms with respect to t_2 now yields

$$\begin{aligned} Tf = \iint\limits_{\substack{0\le t_2\le t\\ \lambda\in C}} &\frac{iP(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}e^{iKt_2}\phi(\phi, e^{-iKt_2}f)\, dt_2\, d\lambda \\ &- \int_C d\lambda \frac{P(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1} \\ &\times \phi(\phi, (\lambda - K)^{-1}[e^{i(\lambda - K)t} - 1]f). \end{aligned} \tag{26a}$$

Using Eq. (18), we may write the second term in Eq. (26a) as

$$-i\int_C d\lambda\, P(\lambda)[(\lambda - H)^{-1} - (\lambda - K)^{-1}][e^{i(\lambda - K)t} - 1]f. \tag{26b}$$

This integral may be evaluated by means of the spectral theorem. We substitute the spectral representation for $(\lambda - H)^{-1}$. Since the integrand in (26b) is a continuous function of λ on C, due to the factor $P(\lambda)$, we may invert the order of integration in the double integral to obtain

$$-2\pi i\, P(H)P_{\xi\mu}(H)(e^{iHt}e^{-iKt} - 1)f,$$

where $P_{\xi\mu}(H)$ is the operator projecting onto that subset of the spectrum of H lying in the interval (ξ, μ).

Using Eq. (8), we may also evaluate the remaining integral in Eq. (26a) to give, finally,

$$\begin{aligned} Tf = 2\pi i\int_C d\lambda \frac{P(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}F_{0t}f \\ - 2\pi i\, P(H)P_{\xi\mu}(H)(e^{iHt}e^{-iKt} - 1)f. \end{aligned} \tag{27}$$

To make an alternative evaluation of Tf, we make, in Eq. (24), the change of variables

$$t_1 = u, \quad t_2 - t_1 = v,$$

so that

$$Tf = \iint\limits_{\substack{u+v\le t.\\ u,v\ge 0}} \Delta(v)e^{iKu}\phi(\phi, e^{-iKu}e^{-iKv}f)\, du\, dv. \tag{28}$$

Again using Eq. (8), we may carry out the u integration to give

$$Tf = 2\pi\int_0^t \Delta(v)F_{0t-v}e^{-iKv}f\, dv. \tag{29}$$

Now, for the first time, we choose f to be in the intersection D_F of the domains of $F_{0\infty}$, $F_{-\infty 0}$. We then see that $\Delta(v)F_{t-v\infty}e^{-iKv}f$ is a strongly continuous function of v, since, from Eq. (17), this is just $\Delta(v)e^{-iKv}F_{t\infty}f$, and $\Delta(v)$ is continuous. Thus we may subtract this term from the integrand in Eq. (29) which gives

$$\begin{aligned} Tf &= 2\pi\int_0^t \Delta(v)F_{0\infty}e^{-iKv}f\,dv \\ &\quad - 2\pi\int_0^t \Delta(v)F_{t-v\infty}e^{-iKv}f\,dv \\ &= 2\pi\int_0^t \Delta(v)F_{0\infty}e^{-iKv}f\,dv \\ &\quad - 2\pi\int_0^t \Delta(v)e^{-iKv}F_{t\infty}f\,dv. \end{aligned} \tag{30}$$

Now

$$\begin{aligned} &\|F_{0s}e^{-iKv}f - F_{0\infty}e^{-iKv}f\| \\ &\qquad = \|F_{s\infty}e^{-iKv}f\| \\ &\qquad = \|F_{v+s\infty}f\| \to 0, \quad \text{as} \quad s \to \infty. \end{aligned}$$

Further, the convergence of $F_{0s}e^{-iKv}f$ to $F_{0\infty}e^{-iKv}f$ is uniform for $v \in [0, t]$, so that

$$\begin{aligned} &\int_0^t \Delta(v)F_{0\infty}e^{-iKv}f\,dv \\ &\quad = \text{s-lim}_{s\to\infty}\int_0^t \Delta(v)F_{0s}e^{-iKv}f\,dv \\ &\quad = \text{s-lim}_{s\to\infty} F_{0s}\int_0^t \Delta(v)e^{-iKv}f\,dv \text{ (since } F_{0s} \text{ is bounded)} \\ &\quad = F_{0\infty}\int_0^t \Delta(v)e^{-iKv}f\,dv. \end{aligned}$$

Hence, $F_{0\infty}$ in Eq. (30) may be taken outside the integral sign, even when $F_{0\infty}$ is unbounded. To simplify Eq. (30) further, we define the bounded linear operator A_t by

$$A_t f = \int_0^t \Delta(s)e^{-iKs}f\,ds. \tag{31a}$$

Since A_t is a multiplication operator, we may write

$$(A_t f)(k) = a_t(k)f(k), \tag{31b}$$

where

$$a_t(k) = \int_0^t \Delta(s)e^{-iks}\,ds. \tag{32}$$

The adjoint operator A_t^* is the operator of multiplication by $a_t^*(k)$. Applying Eq. (31a) to Eq. (30) and comparing with the previous expression for Tf of Eq. (27), we have the identity

$$\begin{aligned} &P(H)P_{\xi\mu}(H)(e^{iHt}e^{-iKt} - 1)f \\ &\qquad = iF_{0\infty}A_t f - iA_t F_{t\infty}f \\ &\qquad\quad + \int_C d\lambda\,\frac{P(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}F_{0t}f. \end{aligned} \tag{33a}$$

Although we have taken $t > 0$, this identity remains valid for $t \leq 0$, as may be verified by slightly modifying the above proof. But, for $t < 0$, it is more convenient to make the substitutions $F_{0\infty} = F_{-\infty\infty} - F_{-\infty 0}$ and $F_{t\infty} = F_{-\infty\infty} - F_{-\infty t}$. In that case, setting $F_{-\infty\infty}f = \Phi\Phi^* f$, we see that Eq. (33a) becomes

$$\begin{aligned} &P(H)P_{\xi\mu}(H)(e^{iHt}e^{-iKt} - 1)f \\ &\qquad = iF_{0\,-\infty}A_t f - iA_t F_{t\,-\infty}f \\ &\qquad\quad + \int_C d\lambda\,\frac{P(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}F_{0t}f. \end{aligned} \tag{33b}$$

We use Eqs. (33) to obtain the wave operators.

3. THE WEAK LIMIT OF $\phi^*(k)a_t(k)$

The existence of the wave operator Ω_- implies the strong convergence of the lhs of Eq. (33) as $t \to \infty$. So we may determine the wave operator from strong limit of the rhs. In fact, we choose to evaluate the weak limit. This we do because, although the sum of the terms on the rhs converges strongly, the individual terms need only converge weakly.

To facilitate the evaluation, we first prove the weak convergence of $\phi^*(k)a_t(k)$, and then evaluate this limit as a singular integral.

Now, from Eqs. (23) and (32), we obtain

$$a_t(k) = \int_C \frac{-iP(\lambda)}{(\lambda - k)(1 - I(\lambda))}(e^{i(\lambda-k)t} - 1)\,d\lambda. \tag{34}$$

Hence, for any element g,

$$\begin{aligned} &\phi(\phi, A_t g) \\ &\quad = -i\int_C d\lambda\,\frac{P(\lambda)}{1 - I(\lambda)}\,\phi(\phi, (\lambda - K)^{-1}(e^{i(\lambda-K)t} - 1)g), \end{aligned} \tag{35}$$

where the integrand is a continuous function of λ. Using Eqs. (19) and (22b), we now have

$$\begin{aligned} &\phi(\phi, A_t g) \\ &\quad = -i\phi\int_C d\lambda\,P(\lambda)(\phi, (\lambda - H)^{-1}(e^{i(\lambda-K)t} - 1)g). \end{aligned} \tag{36}$$

The contour integral may be evaluated by the method of Sec. 2 to give

$$(\phi, A_t g) = 2\pi(\phi, P(H)P_{\xi\mu}(H)(e^{iHt}e^{-iKt} - 1)g). \tag{37}$$

Since g is a general element of the Hilbert space, we may use Eq. (37) to obtain an explicit formula for $A_t^*\phi$, and deduce that $\|A_t^*\phi\|$ is bounded uniformly in t. Hence, $\|\phi^*(k)a_t(k)\|_2$ is bounded, and the existence of the wave operator enables us to take the limit of Eq. (37) as $t \to \infty$ and to show that $\phi^*(k)a_t(k)$ converges weakly to some element of L_2.

Now, to *evaluate* the weak limit of $f_t(k) = \phi^*(k)a_t(k)$ we have, from Eq. (32),

$$(g,f_t) = \int_0^t ds\,\Delta(s)\left(\int_{-\infty}^{\infty} e^{-iks}\phi^*(k)g^*(k)\,dk\right), \quad (38)$$

the double integral being absolutely convergent for any $g \in L_2$.

If we define

$$\int_0^{\to\infty} \psi(s)\,ds = \lim_{t\to\infty}\int_0^t \psi(s)\,ds,$$

where $\psi(s)$ is any continuous and bounded function such that $\int_0^{\to\infty}\psi(s)\,ds$ exists, it may be proved that

$$\int_0^{\to\infty} \psi(s)\,ds = \lim_{\epsilon\to 0+}\int_0^{\infty} e^{-\epsilon s}\psi(s)\,ds.$$

[This result may be obtained from the second mean value theorem for integrals. Note that $e^{-\epsilon s}\psi(s) \in L_1(0,\infty)$, whereas we do not require $\psi(s) \in L_1(0,\infty)$.]

Now, in Eq. (38), the integrand is a bounded and continuous function of s, since, as we show in Appendix A, $\Delta(s)$ is bounded for $s \in (-\infty,\infty)$. If f_∞ is the weak limit of f_t, then from Eq. (38) we have

$$\begin{aligned}(g,f_\infty) &= \int_0^{\to\infty} ds\,\Delta(s)\left(\int_{-\infty}^{\infty} e^{-iks}\phi^*(k)g^*(k)\,dk\right)\\ &= \lim_{\epsilon\to 0+}\int_0^{\infty} ds e^{-\epsilon s}\Delta(s)\left(\int_{-\infty}^{\infty} e^{-iks}\phi^*(k)g^*(k)\,dk\right).\end{aligned} \quad (39)$$

The double integral is now absolutely convergent, and we may invert the order of integration. We integrate first with respect to s. Now, in the definition of $\Delta(s)$ in Eq. (23), the precise integration contour does not matter. We may replace C by a contour C_ϵ (see Fig. 1), which is chosen in such a way that, on C_ϵ, $\operatorname{Im}\lambda > -\epsilon$. (I.e., referring to Fig. 1, we require $d < \epsilon$.) In that case, integrations with respect to s and λ may be inverted, to give

$$\int_0^{\infty} ds e^{-i(k-i\epsilon)s}\Delta(s) = i\int_{C_\epsilon}\frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k+i\epsilon)}. \quad (40)$$

The requirement that $d < \epsilon$ guarantees that the pole $\lambda = k - i\epsilon$ of the integrand in Eq. (40) lies *outside* the contour of integration.

If ϵ is sufficiently small that $\epsilon \lesssim \frac{1}{2}D$, say, we can use Cauchy's theorem to obtain in Eq. (40) an integral round the original fixed contour C (see Fig. 1).

We have, then, provided $k \neq \xi, \mu$,

$$\begin{aligned} i\int_{C_\epsilon}&\frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k+i\epsilon)}\\ &= i\int_C \frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k+i\epsilon)} + \frac{2\pi P(k-i\epsilon)}{1-I(k-i\epsilon)}P_{\xi\mu}(k), \end{aligned} \quad (41)$$

where

$$\begin{aligned} P_{\xi\mu}(k) &= 1, \quad k\in(\xi,\mu),\\ &= 0, \quad \text{otherwise}. \end{aligned}$$

Substituting Eq. (40) into Eq. (39) and using Eq. (41), we have

$$\begin{aligned}(g,f_\infty) = \lim_{\epsilon\to 0+}&\int_{-\infty}^{\infty} dk\,\phi^*(k)g^*(k)\\ &\times\left(i\int_C\frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k+i\epsilon)} + \frac{2\pi P(k-i\epsilon)}{1-I(k-i\epsilon)}P_{\xi\mu}(k)\right). \end{aligned} \quad (42a)$$

Now,

$$\int_C\frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k+i\epsilon)}$$

defines a function of k and ϵ which is bounded uniformly for $k \in (\xi,\mu)$, and $0 \leq \epsilon \leq \frac{1}{2}D$. To verify this, we can use Cauchy's theorem to distort the integration contour to that of Fig. 2. Taking $n > 2$ in Eq. (21), we have, for example,

$$\begin{aligned}\left|\int_\mu^{B'}\frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k+i\epsilon)}\right| &\leq \text{const}\int_\mu^{B'}\frac{|\lambda-\mu||d\lambda|}{|\lambda-k+i\epsilon|}\\ &\leq \text{const}\int_\mu^{B'}|d\lambda|\\ &\leq \text{const},\end{aligned}$$

where we have used the fact that $|(\lambda-\mu)/[1-I(\lambda)]|$ is bounded for λ on the contour from μ to B' and

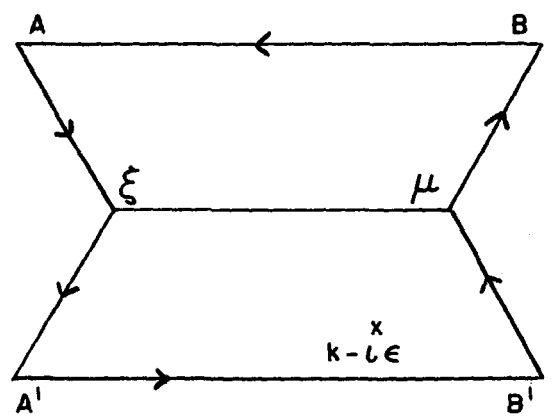

FIG. 2. Use of Cauchy's theorem to distort the integration contour.

that $(1/\sqrt{2})\,|\lambda-\mu| < |\lambda - k + i\epsilon|$. A similar argument shows that the integral round the entire closed contour defines a uniformly bounded function for $k > \mu$ or $k < \xi$, with $0 \le \epsilon \le \frac{1}{2}D$. Hence, we may use the Lebesgue-dominated convergence theorem[9] to take the limit under the integral sign of Eq. (42a), the integrand being dominated by const $|\phi(k)g(k)|$.

We then have

$$(g,f_\infty) = i\int_{-\infty}^{\infty} dk\ \phi^*(k)g^*(k) \times \left(\int_C \frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k)}\right) + \lim_{\epsilon\to 0+} 2\pi\int_{-\infty}^{\infty} dk\,\frac{\phi^*(k)g^*(k)}{1-I(k-i\epsilon)}\,P_{\xi\mu}(k). \quad (42b)$$

But g is a general element of L_2, so that we have

$$f_\infty(k) - i\phi^*(k)\int_C \frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k)} = \text{w-lim}_{\epsilon\to 0+} \frac{2\pi\phi^*(k)P(k-i\epsilon)}{1-I(k-i\epsilon)}\,P_{\xi\mu}(k), \quad \text{a.e.} \quad (43)$$

This limit not only converges weakly to an element of L_2, but we also have pointwise convergence a.e. (see Appendix B). The weak limit and the pointwise limit must be the same a.e., so that we have

$$\text{w-lim}_{t\to\infty}\,\phi^*(k)a_t(k) = i\phi^*(k)\int_C \frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k)} + \frac{2\pi\phi^*(k)P(k)P_{\xi\mu}(k)}{1-I_-(k)}, \quad (44a)$$

where $I_-(k)$ is defined by Eq. (15).

A similar calculation shows that

$$\text{w-lim}_{t\to-\infty}\,\phi^*(k)a_t(k) = i\phi^*(k)\int_C \frac{P(\lambda)\,d\lambda}{[1-I(\lambda)](\lambda-k)} + \frac{2\pi\phi^*(k)P(k)P_{\xi\mu}(k)}{1-I_+(k)}. \quad (44b)$$

We may use Eqs. (44) to take the weak limits of Eqs. (33).

4. THE WAVE OPERATOR AS A WEAK LIMIT

Since we are taking f to be in D_F, the final term on the rhs of Eq. (33a) actually converges strongly to a limit, which may be written down immediately, since the contour integral defines a *bounded* operator. However, it is convenient to use the commutation relations for F_{0t} to bring $F_{0\infty}$ *outside* the integral sign. Using Eq. (10), with $b = t$, we have

$$\begin{aligned}
&\int_C \frac{d\lambda\,P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}F_{0t}f \\
&\quad - F_{0t}\int_C \frac{d\lambda\,P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}f \\
&= \frac{1}{2\pi i}\int_C \frac{d\lambda\,P(\lambda)}{1-I(\lambda)}e^{iKt}(\lambda-K)^{-1}V(\lambda-K)^{-1}e^{-iKt}f \\
&\quad - \frac{1}{2\pi i}\int_C \frac{d\lambda\,P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}V(\lambda-K)^{-1}f \\
&= \frac{1}{2\pi i}\int_C d\lambda\,P(\lambda)e^{iKt}[(\lambda-H)^{-1}-(\lambda-K)^{-1}]e^{-iKt}f \\
&\quad - \frac{1}{2\pi i}\int_C d\lambda\,P(\lambda)[(\lambda-H)^{-1}-(\lambda-K)^{-1}]f,
\end{aligned} \quad (45)$$

where we have used Eq. (18).

The rhs may be evaluated by the techniques of Sec. 2, to give

$$\begin{aligned}
&\int_C d\lambda\,\frac{P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}F_{0t}f \\
&\quad = F_{0t}\int_C d\lambda\,\frac{P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}f \\
&\qquad + e^{iKt}P(H)P_{\xi\mu}(H)\,e^{-iKt}f - P(H)P_{\xi\mu}(H)f.
\end{aligned} \quad (46a)$$

Now,

$$\begin{aligned}
&\lim_{t\to\infty}\|e^{iKt}P(H)P_{\xi\mu}(H)e^{-iKt}f - P(K)P_{\xi\mu}(K)f\| \\
&\quad = \lim_{t\to\infty}\|P(H)P_{\xi\mu}(H)e^{iHt}e^{-iKt}f \\
&\qquad - e^{iHt}e^{-iKt}P(K)P_{\xi\mu}(K)f\| \\
&\quad = \|P(H)P_{\xi\mu}(H)\Omega_-f - \Omega_-P(K)P_{\xi\mu}(K)f\| = 0,
\end{aligned}$$

using the intertwining property[1] of the wave operator Ω_-.

Letting $t \to \infty$ in Eq. (46a), we now have

$$\begin{aligned}
&\int_C d\lambda\,\frac{P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}F_{0\infty}f \\
&\quad = F_{0\infty}\int_C d\lambda\,\frac{P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}f \\
&\qquad - P(H)P_{\xi\mu}(H)f + P(K)P_{\xi\mu}(K)f,
\end{aligned} \quad (46b)$$

and we also obtain the same equation with $F_{0\infty}$ replaced by $F_{0-\infty}$.

Applying Eq. (46b) to Eq. (33a), we obtain

$$\begin{aligned}
&(\Omega_- - 1)P(K)P_{\xi\mu}(K)f - F_{0\infty}\int_C \frac{d\lambda\,P(\lambda)}{1-I(\lambda)}(\lambda-K)^{-1}f \\
&\quad = i\lim_{t\to\infty}[F_{0\infty}A_tf - A_tF_{t\infty}f],
\end{aligned} \quad (47a)$$

and from Eq. (33b) we obtain

$$(\Omega_+ - 1)P(K)P_{\xi\mu}(K)f - F_{0-\infty}\int_C d\lambda \frac{P(\lambda)}{1-I(\lambda)}(\lambda - K)^{-1}f = i\lim_{t\to-\infty}[F_{0-\infty}A_t f - A_t F_{t-\infty}f]. \quad (47b)$$

As in Sec. 1, we distinguish 2 cases.

Case (i): Let f belong to the set $\mathcal{S}$, defined in the discussion following Eq. (11) [i.e., suppose the Fourier transform $\hat{\Phi^*f}$ of $\phi^*(k)f(k)$ is an element of L_1].

Then

$$(A_t F_{t\infty}f)(k) = \frac{1}{(2\pi)^{\frac{1}{2}}}a_t(k)\phi(k)\int_t^\infty ds\, e^{iks}(\hat{\Phi^*f})(s).$$

Hence,

$$|(A_t F_{t\infty}f)(k)| \le \frac{1}{(2\pi)^{\frac{1}{2}}}|a_t(k)\phi(k)|\int_t^\infty ds\,|(\hat{\Phi^*f})(s)|. \quad (48)$$

Now we have seen that $\|a_t(k)\phi^*(k)\|_2$ is bounded uniformly in t, so that Eq. (48) implies

$$\text{s-lim}_{t\to\infty} A_t F_{t\infty}f = 0. \quad (49)$$

Hence, we see from Eq. (47a) that, in this case, $\lim F_{0\infty}A_t f$ as $t\to\infty$ exists as a strong limit.

Now let g be a second element of $\mathcal{S}$. Then

$$i(g, F_{0\infty}A_t f) = i(F_{0\infty}g, A_t f) = i\int_{-\infty}^\infty dk\, a_t(k)f(k)\phi^*(k)[(P_{0\infty}\Phi^* g)(k)]^*, \quad (50)$$

where we have used Eq. (13a).

Now $(P_{0\infty}\Phi^*g)(k)$ is bounded for any fixed element $g\in\mathcal{S}$, so that $f(k)[(P_{0\infty}\Phi^*g)(k)]^* \in L_2$. Hence, to evaluate $i\lim(g, F_{0\infty}A_t f)$, as $t\to\infty$, we may use the weak limit of $\phi^*(k)a_t(k)$ obtained in Sec. 3.

If we use Eq. (44a) and make the further assumption that f is in the domain of $(1-I_-)^{-1}$, where I_- is defined by Eq. (16), we obtain

$$\lim_{t\to\infty} i(g, F_{0\infty}A_t f) = (F_{0\infty}g, h), \quad (51)$$

where

$$h(k) = -\int_C \frac{P(\lambda)\,d\lambda}{(1-I(\lambda))(\lambda - k)}f(k) + \frac{2\pi i P(k)P_{\xi\mu}(k)}{1-I_-(k)}f(k); \quad (52)$$

i.e., using the inner product of Eq. (47a) with g, together with Eq. (49), we have

$$(g, (\Omega_- - 1)P(K)P_{\xi\mu}(K)f) = (F_{0\infty}g, 2\pi i P(K)P_{\xi\mu}(K)(1-I_-)^{-1}f) \quad (53a)$$

$$= (g, 2\pi i F_{0\infty}(1-I_-)^{-1}P(K)P_{\xi\mu}(K)f), \quad (53b)$$

since any element of the range of $(1-I_-)^{-1}$ is in the domain D_I of I_- and hence, as we observed in Sec. 1, is also in D_F.

Since for case (i) we assume that the set $\mathcal{S}$ to which f and g belong is everywhere dense, Eq. (53b) is sufficient to determine Ω_-. But our further assumption that f belong to the domain $D_{(1-I_-)^{-1}}$ means that, in fact, Eq. (53) apparently determines Ω_- only on the closure of $\mathcal{S}\cap D_{(1-I_-)^{-1}}$.

Case (ii): Now let us assume instead that $f, g \in D \equiv D_I \cap D_{(1-I_-)^{-1}} \cap L_\infty$. In that case, Eq. (49) may no longer hold.

Now, $\Phi^*f \in L_2$, for all $f\in L_\infty$. As a linear operator mapping L_2 into L_2, $P_{t\infty}$ is defined by Eq. (6), where $\mathcal{F}$ and $\mathcal{F}^*$ are Fourier transforms defined on L_2, and $P_{t\infty}$ is a projection operator defined by Eq. (5). We may deduce, since $\mathcal{F}$ and $\mathcal{F}^*$ are bounded, that

$$\text{s-lim}_{t\to\infty} P_{t\infty}\Phi^*f = 0.$$

Further,

$$\|\phi^*(k)a_t(k)g(k)\|_2 \le \text{const}\,\|\phi^*(k)a_t(k)\|_2$$

and, hence, is bounded uniformly in t.

Thus, instead of Eq. (49) we now have

$$\lim_{t\to\infty}(g, A_t F_{t\infty}f) = \lim_{t\to\infty}(\Phi^*A_t^*g, P_{t\infty}\Phi^*f) = 0. \quad (54)$$

We also have $i(g, F_{0\infty}A_t f) = i(P_{0\infty}\Phi^*g, \Phi^*A_t f)$, so that, having $f\in L_\infty$, we may use the weak limit of $\phi^*(k)a_t(k)$, as in case (i), to deduce Eq. (53).

Now it is readily verified that *any* element of D which is of bounded support is of the form $P(K)P_{\xi\mu}(K)f$, for some f.

Hence, we may replace Eq. (53) by

$$(g, (\Omega_- - 1)u') = (F_{0\infty}g, 2\pi i(1-I_-)^{-1}u'), \quad (55)$$

where u', $g\in D$ and u' is of bounded support.

It may further be verified that *any* element u of $D_{(1-I_-)^{-1}}$ is a strong limit of elements $u_n'\in D$, where the u_n' are of bounded support. Moreover, the sequence u_n' can be chosen such that $u_n'\to u$, $(1-I_-)^{-1}u_n' \to (1-I_-)^{-1}u$, both being strong limits. Since Ω_- is bounded, it follows that we can take limits in this way to obtain Eq. (55) with u' replaced by u. Since $D_I \subset D_F$ and the g's belong to a dense set, we have then

$$\Omega_- u = u + 2\pi i F_{0\infty}(1-I_-)^{-1}u, \quad (56a)$$

provided only that $u\in D_{(1-I_-)^{-1}}$.

A similar calculation shows that

$$\Omega_+ u = u + 2\pi i F_{0-\infty}(1-I_+)^{-1}u. \quad (56b)$$

Equations (56) are valid only for a dense set of elements in L_2. We may extend the wave operators onto the whole of L_2 by continuity, and, in this way, we may express $\Omega_\pm u$ as a strong limit. The most convenient way to do this is first to obtain $\Omega_\pm u$ for all u of bounded support $[a, b]$, so that for a general element of L_2 the wave operator is defined by the strong limits as $b \to \infty$, $a \to -\infty$. The extension of the wave operators to elements of bounded support is given by Eq. (61), which we now set out to prove.

Using Eq. (17), we deduce from Eq. (56) that, for all $u \in D_{(1-I_-)^{-1}}$,

$$\Omega_- u - e^{iKt}\Omega_- e^{-iKt}u = 2\pi i F_{0t}(1 - I_-)^{-1}u. \quad (57)$$

We saw in Eq. (44) that

$$\phi^*(k)P(k)P_{\xi\mu}(k)/[1 - I_-(k)] \in L_2,$$

and it readily follows that

$$\phi^*(k)/[1 - I_-(k)] \equiv \psi(k) \in L_2(a, b)$$

for any finite a, b. If in Eq. (57) the support of $u(k)$ is contained in $[a, b]$, then according to Eq. (7) we may write

$$F_{0t}(1 - I_-)^{-1}u = \Phi P_{0t}\Psi u, \quad (58)$$

where Ψ is the multiplication operator corresponding to $\psi(k)$ which maps u into an element of L_1. Therefore, $\Phi P_{0t}\Psi$ has an integral representation similar to that of Eq. (8) for F_{ab}, and is a bounded operator defined for all $u \in L_2$ having bounded support. Thus Eq. (57), initially proved only for $u \in D_{(1-I_-)^{-1}}$, may now be extended to give

$$\Omega_- u - e^{iKt}\Omega_- e^{-iKt}u = 2\pi i \Phi P_{0t}\Psi u, \quad (59)$$

provided supp $u(k) \subset [a, b]$.

Using the intertwining property of Ω_-, we find that, as $t \to \infty$, the lhs of Eq. (59) converges strongly to $\Omega_- u - u$. The weak limit of the rhs may be evaluated by the same technique that we used to find the weak limit of $\phi^*(k)a_t(k)$. We find

$$\lim_{t\to\infty}(g, 2\pi i\Phi P_{0t}\Psi u) = \lim_{\epsilon\to 0+} i\int_0^\infty ds\, e^{-\epsilon s}(g, e^{iKs}\phi)\left(\int_a^b e^{-ips}\psi(p)u(p)\,dp\right), \quad (60)$$

which leads to the result

$$(\Omega_- u - u)(k) = -\phi(k)\lim_{\epsilon\to 0+}\int_a^b \frac{\psi(p)u(p)\,dp}{(k - p + i\epsilon)} \text{ a.e.} \quad (61)$$

The wave operator may be evaluated for a general element u by taking the strong limits as $a \to -\infty$, $b \to +\infty$. In practice, however, it is convenient to express $\Omega_- u$ in terms of pointwise integrals and limits.

From the existence of the strong limits, we may deduce, for example, that

$$\phi(k)\int_{b+1}^N \frac{\psi(p)u(p)}{(p - k)}\,dp,$$

regarded as an element of $L_2(a, b)$, must converge strongly to a limit as $N \to \infty$. But the phase of $u(p)$ may be chosen such that $\psi(p)u(p)$ is real and positive. Hence,

$$\int_{b+1}^\infty \frac{\psi(p)u(p)}{(p - k)}\,dp$$

converges absolutely for $k \in [a, b]$. The strong limit (s-lim) as $N \to \infty$ must equal the pointwise limit, so that

$$\text{s-lim}_{N\to\infty}\,\phi(k)\int_{b+1}^N \frac{\psi(p)u(p)\,dp}{(p - k)} = \phi(k)\int_{b+1}^\infty \frac{\psi(p)u(p)\,dp}{(p - k)} = -\phi(k)\lim_{\epsilon\to 0+}\int_{b+1}^\infty \frac{\psi(p)u(p)\,dp}{(k - p + i\epsilon)},$$

where the limits are taken in $L_2(a, b)$.

Arguments such as these enable us to deduce from Eq. (61) that

$$(\Omega_- u - u)(k) = -\phi(k)\lim_{\epsilon\to 0+}\int_{-\infty}^\infty \frac{\psi(p)u(p)\,dp}{(k - p + i\epsilon)}, \quad (62)$$

where $\psi(p) = \phi^*(p)/[1 - I_-(p)]$, and $I_-(p)$ is defined a.e. by Eq. (15). Equation (62) is valid for any $u \in L_2(-\infty, \infty)$.

5. THE SCATTERING OPERATOR

From Eq. (56b), we have, for $u \in D_{(1-I_+)^{+1}}$,

$$\begin{aligned}\Omega_+ u &= u - 2\pi i F_{-\infty 0}(1 - I_+)^{-1}u \\ &= u - 2\pi i\Phi\Phi^*(1 - I_+)^{-1}u \\ &\quad + 2\pi i F_{0\infty}(1 - I_+)^{-1}u, \end{aligned} \quad (63)$$

where we have used Eq. (13b). Therefore,

$$\Omega_+ u = [1 - 2\pi i\Phi\Phi^*(1 - I_+)^{-1}]u + 2\pi i F_{0\infty}(1 - I_-)^{-1}[(1 - I_-)(1 - I_+)^{-1}u]. \quad (64)$$

We now define the multiplication operator S by

$$(Sf)(k) = S(k)f(k), \quad (65)$$

where

$$S(k) = [1 - I_-(k)]/[1 - I_+(k)] \text{ a.e.} \quad (66a)$$

From Eq. (B1) of Appendix B, we have also

$$S(k) = 1 - 2\pi i\,|\phi(k)|^2/[1 - I_+(k)], \quad (66b)$$

so that Eq. (64), from Eq. (56), becomes

$$\Omega_+ u = \Omega_- S u. \tag{67}$$

Since Ω_- is isometric, we have $\Omega_-^* \Omega_- = 1$, so that

$$\Omega_-^* \Omega_+ u = S u. \tag{68}$$

Equation (68) is just the definition of the scattering operator S. We see that S is unitary, and Eqs. (65) and (66a) define S on the entire Hilbert space, since the elements u, for which Eq. (67) was originally proved, are everywhere dense.

APPENDIX A

Here, we prove that the function $\Delta(t)$, defined for real t by Eq. (23), is bounded uniformly in t.

Now, from Eqs. (21) and (22) we find that

$$[1 - I(\lambda)]^{-1} = 1 + (\phi, G(\lambda)\phi), \tag{A1}$$

where $G(\lambda) = (\lambda - H)^{-1}$.

Hence, from Eq. (23) we have

$$\begin{aligned}\Delta(t) &= \int_C e^{i\lambda t} P(\lambda)\, d\lambda + \int_C (\phi, e^{i\lambda t} P(\lambda) G(\lambda)\phi)\, d\lambda \\ &= \int_C (\phi, e^{i\lambda t} P(\lambda) G(\lambda)\phi)\, d\lambda,\end{aligned} \tag{A2}$$

since $P(\lambda)$ is analytic.

The contour integral may readily be evaluated by the technique of Sec. 2, and we find

$$\Delta(t) = 2\pi i(\phi, P(H) P_{\xi\mu}(H) e^{iHt}\phi). \tag{A3}$$

Since $P(H)P_{\xi\mu}(H)$ is a bounded operator, we see that $\Delta(t)$ is indeed uniformly bounded in t.

APPENDIX B

We here summarize the results which we need regarding boundary values of analytic functions.

Since $\phi^2(p) \in L_1(-\infty, \infty)$, the limits

$$I_\pm(k) = \lim_{\epsilon \to 0+} \int_{-\infty}^{\infty} \frac{|\phi^2(p)|\, dp}{k - p \pm i\epsilon}$$

exist for almost all k.[8] Here, the $I_\pm(k)$ are boundary values of the analytic function

$$I(\lambda) = \int_{-\infty}^{\infty} \frac{|\phi^2(p)|\, dp}{(\lambda - p)}$$

as λ approaches the real axis along a normal to the real axis. Therefore, the $I_\pm(k)$ may also be regarded as sectorial limits of $I(\lambda)$ (see Ref. 10, p. 105). The sectorial-limit theorem applies to functions analytic in a half-plane which are *bounded*. However, in the upper half-plane, say, $\text{Im}\,[I(\lambda)] \leq 0$, so that the theorem may be applied to $e^{-i\alpha I(\lambda)}$, for any $\alpha > 0$, to show that $I(\lambda)$ has sectorial limit for almost all k.

The set of real values k such that $I_\pm(k) = 1$ is of measure zero. [This follows from a result of Luzin and Privalov, quoted in Ref. 11, p. 371.]

Hence, $[1 - I_\pm(k)]^{-1}$ is almost everywhere defined. This is necessary for the definition on a dense domain of the operators $(1 - I_\pm)^{-1}$, where the operators $I_\pm$ are defined by Eq. (16).

Often, in the present paper, we meet sequences of functions $f_n(k)$ which converge not only pointwise a.e. but also weakly, regarding the f_n as elements of a Hilbert space. Under these conditions, the weak and pointwise limits may be shown to coincide almost everywhere.

In Ref. 8, it is shown that

$$I_-(k) - I_+(k) = 2\pi i\, |\phi^2(k)| \quad \text{a.e.} \tag{B1}$$

[1] J. M. Jauch, Helv. Phys. Acta **31**, 127 (1958).
[2] S. T. Kuroda, Nuovo Cimento **12**, 431 (1959).
[3] K. O. Friedrichs, *Perturbation of Spectra in Hilbert Space* (American Mathematical Society, Providence, R.I., 1965).
[4] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1966).
[5] E. R. Lorch, *Spectral Theory* (Oxford U.P., New York, 1962).
[6] D. B. Pearson, J. Math. Phys. **11**, 2425 (1970).
[7] R. Goldberg, *Fourier Transforms* (Cambridge U.P., Cambridge, 1961).
[8] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford U.P., London, 1937).
[9] R. G. Bartle, *The Elements of Integration* (Wiley, New York, 1966).
[10] M. Heins, *Selected Topics in the Classical Theory of Functions of a Complex Variable* (Holt, Rinehart, and Winston, New York, 1962).
[11] A. I. Markushevich, *Theory of Functions of a Complex Variable*, translation by R. A. Silverman (Prentice-Hall, Englewood Cliffs, N.J., 1965), Vol. I.

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Singular Integral Operator Encountered in Scattering Theory

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The domain of an unbounded singular integral operator occurring in scattering theory is investigated and is proved to be everywhere dense. An application is made to a simple scattering system, for which the interaction Hamiltonian is of rank one, and the existence of the wave operator is proved by a "time-dependent" method which does not assume "smoothness" of the element of $L_2(-\infty, \infty)$ from which the interaction is constructed.

INTRODUCTION

Since the pioneering work of Friedrichs and others[1,2] in the theory of time-independent scattering, the importance has been recognized of the study of the solutions F of the commutation relation $[H_0, F] = (i/2\pi)V$, where H_0 is the free Hamiltonian and V is the interaction Hamiltonian.

For the special case of an interaction of rank one, a link was established in Ref. 3 with the time-dependent theory. A family of operators F_{0t} was defined, from which a solution $F_{0\infty}$ of the above commutation relation may be obtained from the strong limit as $t \to \infty$, and the wave operators and scattering operator were obtained by a time-dependent method.

The main purpose of the present paper is to show that the domain of the singular integral operator is everywhere dense in L_2. Although a simple specification of the domain of $F_{0\infty}$ is not generally possible, we prove in Sec. 1 that a dense subset of the domain may be identified with the domain of a given multiplication operator in L_2.

$F_{0\infty}$ is a semibounded operator, and it is possible to prove that the closure $\bar{F}_{0\infty}$ is self-adjoint. However, we are not directly interested in the (maximal) domain of $\bar{F}_{0\infty}$, since there may be elements g in this domain for which the connection $F_{0t}g$ and $F_{0\infty}g$ is not preserved.

As an illustration of the application of our results, we give a new time-dependent proof of the existence of the wave operators $\Omega_{\pm}$ for the above interaction of rank one. Previous proofs have entailed first proving the existence of $\Omega_{\pm}$ for "smooth" interactions $V = |\phi\rangle\langle\phi|$, where $\phi(k)$ is assumed to satisfy Hölder conditions or other smoothness criteria. For these interactions, $F_{0\infty}$ is defined on the whole of L_2. However, the proof we give in Sec. 2 makes no assumptions about $\phi(k)$ except that ϕ is an element of L_2; in that case, $F_{0\infty}$ may well be unbounded.

1. CONSTRUCTION OF A SET OF ELEMENTS BELONGING TO THE DOMAIN OF THE SINGULAR OPERATOR

We state, for completeness, a number of definitions from Ref. 3.

The linear operator F_{0t} is defined on the space $L_2 \equiv L_2(-\infty, \infty)$ by

$$F_{0t}f = \frac{1}{2\pi}\int_0^t ds\, e^{iKs}\phi(\phi, e^{-iKs}f), \tag{1}$$

where ϕ is a fixed element of L_2 and K is defined by

$$(Kf)(k) = kf(k). \tag{2}$$

The domain D_K of K is given by

$$D_K = \{f(k) \in L_2;\ kf(k) \in L_2\}.$$

More generally, we define F_{ab} by

$$F_{ab}f = \frac{1}{2\pi}\int_a^b ds\, e^{iKs}\phi(\phi, e^{-iKs}f). \tag{3}$$

The multiplication operator Φ is defined by

$$(\Phi f)(k) = \phi(k)f(k) \tag{4}$$

having domain

$$D_\Phi = \{f(k) \in L_2;\ \phi(k)f(k) \in L_2\}.$$

This differs slightly from the definition of the operator Φ in Ref. 3; we now require the range of Φ to be contained in L_2.

The adjoint Φ^* of Φ is the operator of multiplication by the complex conjugate ϕ^* of ϕ. Both Φ and Φ^* are closed operators; note also that $D_\Phi = D_{\Phi^*}$.

If $\mathcal{F}: L_2 \to L_2$ is the Fourier transform, we define the projection operator P_{ab} by

$$P_{ab} = \mathcal{F}^{-1}\hat{P}_{ab}\mathcal{F}, \tag{5}$$

where, for any $f \in L_2$,

$$\begin{aligned}(\hat{P}_{ab}f)(k) &= f(k),\ k \in (a, b),\\ &= 0, \text{ otherwise},\end{aligned} \tag{5'}$$

P_{ab} is defined on L_2, and we allow $a = -\infty$ or $b = +\infty$ in Eq. (5').

The singular integral operator $F_{0\infty}$ in which we are interested is defined by

$$F_{0\infty}f = \operatorname*{s-lim}_{t\to\infty} F_{0t}f \tag{6}$$

for all f such that the strong limit exists. Inspection of Eq. (3) shows that F_{ab} is an extension of the operator $\Phi P_{ab}\Phi^*$. Although F_{ab} is a bounded operator defined on L_2, the domain of $\Phi P_{ab}\Phi^*$ is only D_Φ. $D_\Phi = L_2$ only if $\phi \in L_\infty$. Nevertheless, $\Phi P_{ab}\Phi^*$ is densely defined and symmetric. $P_{0\infty}$ is a Hilbert transform, and we may write

$$(P_{0\infty}f)(k) = \text{l.i.m.}_{\epsilon\to 0+} \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{f(p)\,dp}{p-k-i\epsilon}, \tag{7}$$

the limit being in-the-mean in L_2; i.e., if we define a linear operator T_ϵ by

$$(T_\epsilon f)(k) = \int_{-\infty}^{\infty} \frac{f(p)\,dp}{p-k-i\epsilon}, \tag{8}$$

then

$$P_{0\infty}f = \text{s-lim}_{\epsilon\to 0+} \frac{1}{2\pi i} T_\epsilon f. \tag{8'}$$

It may be verified, for $\epsilon > 0$, that

$$\|T_\epsilon f\| \leq 2\pi \|P_{0\infty}f\|. \tag{9}$$

The singular operators $F_{-\infty 0}$ and $F_{-\infty\infty}$ are defined by equations similar to Eq. (6); for example, $F_{-\infty 0}f$ is obtained from $F_{s0}f$ by taking the strong limit as $s \to -\infty$.

Finally, we define, for real nonzero ϵ,

$$I_\epsilon^{\pm}(k) = \int_{-\infty}^{\infty} \frac{|\phi^2(p)|\,dp}{k-p\pm i\epsilon} \tag{10}$$

and

$$I^{\pm}(k) = \lim_{\epsilon\to 0+} I_\epsilon^{\pm}(k) \quad \text{a.e.} \tag{10'}$$

We now proceed to construct a set of elements which are in the domain of $F_{0\infty}$. To this end, we suppose first that we have a family $Z_\epsilon(k)$ of measurable functions parametrized by a real positive number ϵ; then we define in terms of Z_ϵ three further families of measurable functions by

$$\begin{aligned} u_\epsilon(k) &= \phi^*(k)Z_\epsilon(k), \\ v_\epsilon(k) &= \phi^*(k)Z_\epsilon(k)/[1-I_\epsilon^-(k)], \\ w_\epsilon(k) &= Z_\epsilon(k)/[1-I_\epsilon^-(k)]. \end{aligned} \tag{11}$$

We assert the following:

Lemma 1: Suppose that

(i) u_ϵ, v_ϵ, and w_ϵ are all elements of L_2,

(ii) the L_2 norm of u_ϵ is bounded uniformly in ϵ, for $\epsilon > 0$,

(iii)

$$\text{l.i.m.}_{\epsilon\to 0+} v_\epsilon(k) = v(k), \tag{12}$$

where v is some element of L_2, and

(iv)

$$\text{l.i.m.}_{\epsilon\to 0+} w_\epsilon(k) = w(k), \tag{12'}$$

where w is some element of L_2.

Then the function ψ_ϵ defined by

$$\psi_\epsilon(k) = \phi(k)\int_{-\infty}^{\infty} dp\, \frac{\phi^*(p)Z_\epsilon(p)}{[1-I_\epsilon^-(p)](k-p+i\epsilon)} \tag{13}$$

is an element of L_2 and converges weakly to a limit as $\epsilon \to 0+$.

Proof: We have

$$|\psi_\epsilon(k)| = |\phi(k)|\left|\int_{-\infty}^{\infty} \frac{dp\, w_\epsilon(p)\phi^*(p)}{(k-p+i\epsilon)}\right|$$

$$\leq \frac{1}{\epsilon}|\phi(k)|\,\|w_\epsilon\|\,\|\phi\|,$$

so that certainly $\psi_\epsilon \in L_2$. Also,

$$\|\psi_\epsilon\|^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \times \frac{dk\,dp\,dp'\,|\phi^2(k)|\,u_\epsilon(p)u_\epsilon^*(p')}{[1-I_\epsilon^-(p)][1-I_\epsilon^+(p')](k-p+i\epsilon)(k-p'-i\epsilon)}.$$

The triple integral is absolutely convergent. Carrying out the integration first with respect to k and substituting

$$\int_{-\infty}^{\infty} \frac{dk\,|\phi^2(k)|}{(k-p+i\epsilon)(k-p'-i\epsilon)} = \frac{1}{(p-p'-2i\epsilon)}[I_\epsilon^+(p') - I_\epsilon^-(p)],$$

we find

$$\begin{aligned} \|\psi_\epsilon\|^2 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dp\,dp' u_\epsilon(p)u_\epsilon^*(p')}{(p-p'-2i\epsilon)} \\ &\quad \times \left(\frac{1}{1-I_\epsilon^+(p')} - \frac{1}{1-I_\epsilon^-(p)}\right) \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dp\,dp' \left(\frac{u_\epsilon(p)v_\epsilon^*(p') - v_\epsilon(p)u_\epsilon^*(p')}{p-p'-2i\epsilon}\right), \end{aligned} \tag{14}$$

where we have used Eq. (11). With the notation of Eq. (8), we now have

$$\|\psi_\epsilon\|^2 = (v_\epsilon, T_{2\epsilon}u_\epsilon) + (T_{2\epsilon}u_\epsilon, v_\epsilon). \tag{15}$$

From Eq. (12) we see that (for ϵ sufficiently small) $\|v_\epsilon\|$ is bounded, and from hypothesis (ii) $\|u_\epsilon\|$ is bounded. Hence, using (9), we may deduce from Eq. (15) that $\|\psi_\epsilon\|$ is bounded uniformly [for ϵ in some interval $(0, a)$].

To evaluate the weak limit of ψ_ϵ, consider any

element y in the domain D_Φ of Φ^*. Then we have

$$(y, \psi_\epsilon) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk\, dp \left(\frac{\phi^*(k)y(k)}{k - p - i\epsilon}\right)^* v_\epsilon(p) = (T_\epsilon \Phi^* y, v_\epsilon), \tag{16}$$

using Eq. (8). Hence, from Eqs. (8′) and (12), we have

$$\lim_{\epsilon \to 0+} (y, \psi_\epsilon) = -2\pi i (P_{0\infty}\Phi^* y, v). \tag{17}$$

Since the elements y in D_Φ are dense in L_2 and since $\|\psi_\epsilon\|$ is uniformly bounded, we may deduce from Eq. (17) that ψ_ϵ converges weakly to a limit; this completes the proof of the lemma. Moreover, $\lim (y, \psi_\epsilon)$, as $\epsilon \to 0+$, defines on D_Φ a bounded antilinear functional. By the Riesz representation theorem, there exists an element x of L_2 such that

$$-2\pi i (P_{0\infty}\Phi^* y, v) = -2\pi i (\Phi^* y, P_{0\infty} v) = -2\pi i (y, x). \tag{18}$$

Equation (18) is valid for all $y \in D_{\Phi^*}$; from the definition of the adjoint of an operator, by noting that $(\Phi^*)^* = \Phi$, Eq. (18) tells us that $P_{0\infty}v \in D_\Phi$ and that

$$\Phi P_{0\infty} v = x.$$

Hence

$$\text{w-lim}_{\epsilon \to 0+} \psi_\epsilon = -2\pi i x = -2\pi i \Phi P_{0\infty} v. \tag{19}$$

Since Φ^* is closed, we deduce from Eqs. (12), together with Eq. (11), that $v = \Phi^* w$, so that Eq. (19) becomes

$$\text{w-lim}_{\epsilon \to 0+} \psi_\epsilon = -2\pi i \Phi P_{0\infty}\Phi^* w. \tag{19′}$$

Theorem 1: With the same assumptions as the lemma, it follows that w is in the domain of $F_{0\infty}$.

Proof: From Eq. (19) we have

$$\|-2\pi i x\| \leq \limsup_{0<\epsilon<a} \|\psi_\epsilon\|.$$

We have already deduced from Eq. (15) that $\|\psi_\epsilon\|$ is bounded; in fact, using Eq. (9), we have

$$\limsup_{0<\epsilon<a} \|\psi_\epsilon\|^2 \leq \text{const} \limsup_{0<\epsilon<a} \|P_{0\infty} v_\epsilon\| = \text{const}\, \|P_{0\infty} v\|,$$

so that

$$\|x\| = \|\Phi P_{0\infty}\Phi^* w\| \leq \text{const}\, \|P_{0\infty} v\|^{\frac{1}{2}}. \tag{20}$$

Now the above analysis may be carried out with $Z_\epsilon(k)$ replaced by $e^{-ikt}Z_\epsilon(k)$. In that case, we may replace v and w by e^{-ikt} and $e^{-ikt}w$ respectively. Using the fact that $e^{iKt}P_{0\infty}e^{-iKt} = P_{t\infty}$ and the unitarity of e^{-iKt}, we see that (20) becomes

$$\|\Phi P_{t\infty}\Phi^* w\| \leq \text{const}\, \|P_{t\infty} v\|^{\frac{1}{2}}. \tag{20′}$$

Substituting

$$\Phi P_{t\infty}\Phi^* w = \Phi P_{0\infty}\Phi^* w - \Phi P_{0t}\Phi^* w = \Phi P_{0\infty}\Phi^* w - F_{0t} w$$

and using the fact that, for any element v,

$$\text{s-lim}_{t \to \infty} P_{t\infty} v = 0,$$

we may deduce from (20′) that

$$\text{s-lim}_{t \to \infty} F_{0t} w = \Phi P_{0\infty}\Phi^* w; \tag{21}$$

i.e., comparison with Eq. (6) shows that we have proved the conclusion of the theorem, that w is in the domain of $F_{0\infty}$, and that

$$F_{0\infty} w = \Phi P_{0\infty}\Phi^* w. \tag{22}$$

Using Eq. (15) to obtain a bound for $\|\psi_\epsilon\|$, we now have

$$\|x\| = \|F_{0\infty} w\| \leq (2\pi)^{-1}\left[\limsup_{0<\epsilon<a} \{(v_\epsilon, T_{2\epsilon}u_\epsilon) + (T_{2\epsilon}u_\epsilon, v_\epsilon)\}\right]^{\frac{1}{2}}. \tag{23}$$

If we make the further assumption that

$$\text{s-lim}_{\epsilon \to 0+} u_\epsilon = u, \tag{24}$$

where u is some element of L_2, Eq. (23) becomes

$$\|F_{0\infty} w\| \leq (2\pi)^{-1}[(v, 2\pi i P_{0\infty} u) + (2\pi i P_{0\infty} u, v)]^{\frac{1}{2}}. \tag{25}$$

2. PROOF THAT THE DOMAIN OF $F_{0\infty}$ IS DENSE IN L_2

We now show that elements w in the domain of $F_{0\infty}$, obtained by the construction of the previous section, are dense in L_2.

We first define, for any positive ϵ and N, the two sets of real numbers

$$S_\epsilon = \{k;\ N^{-1} \leq |1 - I_\alpha^-(k)| \leq N \text{ for any } \alpha \text{ in } (0, \epsilon]\} \tag{26}$$

and

$$S(N) = \bigcup_{\epsilon > 0} S_\epsilon, \tag{26′}$$

where $I_\alpha^-(k)$ is defined by Eq. (10). Since $I_\alpha^-(k)$, for $\alpha > 0$, is a continuous function of α and k, it may be shown that both S_ϵ and $S(N)$ are measurable sets. We denote by I_- the operator of multiplication by $I^-(k)$, where $I^-(k)$ is defined by Eq. (10′). I_- has maximal domain

$$D_I = \{f(k) \in L_2;\ I^-(k)f(k) \in L_2\}.$$

Since the set $\{k; I^-(k) = 1\}$ has measure zero, the inverse $(1 - I_-)^{-1}$ exists, but is not necessarily defined on the whole of L_2.

We now prove the following:

Theorem 2: Given any element g of L_2, let g_N denote the projection of g onto $S(N)$; i.e.,

$$g_N(k) = g(k), \quad \text{if} \quad k \in S(N),$$
$$= 0, \quad \text{otherwise.} \tag{27}$$

Then g_N lies in the domain of $F_{0\infty}$. Further the restriction, for fixed N, of $F_{0\infty}$ to elements g_N is bounded. If both N and g are varied, then the elements g_N are dense in L_2 (so that the domain of $F_{0\infty}$ is dense in L_2).

Proof: With the notation of Sec. 1, let

$$Z_\epsilon(k) = g(k)[1 - I_\epsilon^-(k)], \quad \text{if} \quad k \in S_\epsilon,$$
$$= 0, \quad \text{otherwise.} \tag{28}$$

Then from Eq. (11) we have

$$v_\epsilon(k) = \phi^*(k)g(k), \quad \text{if} \quad k \in S_\epsilon,$$
$$= 0, \quad \text{otherwise,} \tag{29}$$

and

$$w_\epsilon(k) = g(k), \quad \text{if} \quad k \in S_\epsilon,$$
$$= 0, \quad \text{otherwise.} \tag{29'}$$

We have the *pointwise* limits a.e.:

$$\lim_{\epsilon \to 0+} v_\epsilon(k) = \phi^*(k)g(k), \quad \text{if} \quad k \in S(N),$$
$$= 0, \quad \text{otherwise,} \tag{30}$$

and

$$\lim_{\epsilon \to 0+} w_\epsilon(k) = g(k), \quad \text{if} \quad k \in S(N),$$
$$= 0, \quad \text{otherwise.} \tag{30'}$$

But it follows from Eqs. (10) that

$$|\phi^2(k)| = \pi^{-1} \operatorname{Im} I^-(k)$$

a.e., so that, using Eq. (26), we see that, for fixed N, $|\phi^2(k)|$ is bounded a.e. for $k \in S_\epsilon$. Hence $|v_\epsilon(k)| \leq$ const $|g(k)|$, where the constant is independent of ϵ. Since $g \in L_2$, we may use the Lebesgue-dominated convergence theorem to deduce that Eq. (30) is valid for the *strong* limit in L_2, and similarly for Eq. (30'). Thus Eqs. (12) are valid, and comparison with Eq. (27) shows that $w = g_N$ and $v = \Phi^* g_N$.

A further application of the Lebesgue-dominated convergence theorem enables us to show from Eqs. (11) and (28) that

$$u = \text{s-}\lim_{\epsilon \to 0+} u_\epsilon = \Phi^*(1 - I_-)g_N. \tag{31}$$

The assumptions of Lemma 1 and of Theorem 1 are satisfied, and it follows immediately that g_N is in the domain of $F_{0\infty}$.

Now, for $k \in S(N)$, $|\phi^*(k)[1 - I^-(k)]|$ is bounded for fixed N, so that from Eq. (31) we have $\|u\| \leq$ const $\|g_N\|$. Similarly, we have $\|v\| \leq$ const $\|g_N\|$, so that from (25) we find that

$$\|F_{0\infty} g_N\| \leq c(N) \|g_N\|. \tag{32}$$

This proves the second statement of Theorem 2. It remains only to prove that the elements g_N, given by Eq. (27), are dense in L_2 as g and N are varied.

Now, for almost all k, $I^-(k) \neq 1$. Hence almost all k belong to $S(N)$ for some N. So the measure of $R \setminus S(N)$ tends to zero as $N \to \infty$, from which we conclude that

$$\lim_{N \to \infty} \|g - g_N\| = 0 \quad \text{for any } g \in L_2.$$

This concludes the proof of Theorem 2.

We refer to the set of elements g_N given by Eq. (27) for any g and N as the *restricted domain* of $F_{0\infty}$. It may similarly be proved that these elements are also in the domain of $F_{-\infty 0}$. The set of elements on which we know $F_{0\infty}$ to be defined may be enlarged by means of the following:

Theorem 3: Let D_F be the intersection of the domains of $F_{0\infty}$ and $F_{-\infty 0}$, and let D_I be the domain of the multiplication operator I_-, where $I^-(k)$ is given by Eq. (10'). Then $D_I \subset D_F$.

Proof: Substituting $w = g_N$ and $v = \Phi^* g_N$ and using Eq. (31), we may write the inequality (25) as

$$\|2\pi i F_{0\infty} g_N\|^2 \leq (2\pi i(1 - I_-)g_N, F_{0\infty} g_N) + (F_{0\infty} g_N, 2\pi i(1 - I_-)g_N). \tag{33}$$

This inequality may be simplified by replacing g_N by $(1 - I_-)^{-1} g_N$, this element also being in the restricted domain.

We then have

$$\|\omega_- g_N\|^2 = (\omega_- g_N, \omega_- g_N) \leq \|g_N\|^2, \tag{34}$$

where

$$\omega_- g_N \equiv g_N + 2\pi i F_{0\infty}(1 - I_-)^{-1} g_N. \tag{35}$$

ω_- is actually the wave operator for the interaction considered in the following section; (34) tells us that ω_- is a bounded operator with $\|\omega_-\| \leq 1$. (Actually ω_- is an isometry, so that $\|\omega_-\| = 1$.)

We extend ω_- by continuity onto the entire space L_2. Now any element in D_I is of the form $(1 - I_-)^{-1} f$ for some f. We define on D_I an operator $G_{0\infty}$ by

$$2\pi i G_{0\infty}(1 - I_-)^{-1} f = (\omega_- - 1)f, \tag{36}$$

for any f belonging to

$$D_{(1-I_-)^{-1}}.$$

From Eq. (35) we see that $F_{0\infty}$ and $G_{0\infty}$ have the same restrictions to the restricted domain. Defining $G_{t\infty} = e^{iKt}G_{0\infty}e^{-iKt}$ and $G_{0t} = G_{0\infty} - G_{t\infty}$, we have, from Eq. (36),

$$2\pi i G_{0t}(1 - I_-)^{-1}f = (\omega_- - 1)f - e^{iKt}(\omega_- - 1)e^{-iKt}f. \tag{37}$$

If f_N is in the restricted domain, then

$$G_{0t}(1 - I_-)^{-1}f_N = F_{0t}(1 - I_-)^{-1}f_N \tag{38}$$

since the construction of G_{0t} in terms of $G_{0\infty}$ agrees with the construction of F_{0t} in terms of $F_{0\infty}$.

Now, given any

$$f \in D_{(1-I_-)^{-1}},$$

we can find a sequence f_N in the restricted domain such that

$$\text{s-lim}_{N\to\infty} f_N = f, \quad \text{s-lim}_{N\to\infty}(1 - I_-)^{-1}f_N = (1 - I_-)^{-1}f.$$

Hence, from Eq. (38) we have

$$\begin{aligned}\text{s-lim}_{N\to\infty} G_{0t}(1 - I_-)^{-1}f_N &= G_{0t}(1 - I_-)^{-1}f \\ &= F_{0t}(1 - I_-)^{-1}f,\end{aligned}$$

since F_{0t} is bounded and since from Eq. (37) $G_{0t}(1 - I_-)^{-1}$ is also bounded.

It follows that F_{0t} is an extension of G_{0t}. It remains only to prove that $F_{0\infty}$ is an extension of $G_{0\infty}$. Now

$$\begin{aligned}\lim_{t\to\infty} \|e^{iKt}(\omega_- - 1)e^{-iKt}f_N\| \\ = \lim_{t\to\infty} \|2\pi i F_{t\infty}(1 - I_-)^{-1}f_N\| = 0.\end{aligned}$$

But, given any $\epsilon > 0$, we may find an N sufficiently large that $\|f - f_N\| < \epsilon$, and in that case

$$\begin{aligned}\|e^{iKt}(\omega_- - 1)e^{-iKt}f - e^{iKt}(\omega_- - 1)e^{-iKt}f_N\| \\ \leq 2\|f - f_N\| < 2\epsilon.\end{aligned}$$

It follows that

$$\lim_{t\to\infty} \|e^{iKt}(\omega_- - 1)e^{-iKt}f\| = 0.$$

Using Eq. (37), with G_{0t} now replaced by F_{0t}, we have

$$\text{s-lim}_{t\to\infty} F_{0t}(1 - I_-)^{-1}f = \frac{1}{2\pi i}(\omega_- - 1)f. \tag{39}$$

Hence any element $(1 - I_-)^{-1}f$ in D_I belongs also to the domain of $F_{0\infty}$, and from Eq. (36) we see that $F_{0\infty}$ is an extension of $G_{0\infty}$. This completes the proof of Theorem 3; similar arguments show that the domain of $F_{-\infty 0}$ also contains D_I.

3. PROOF OF THE EXISTENCE OF THE WAVE OPERATORS FOR AN INTERACTION OF RANK ONE

The free Hamiltonian is the operator K defined by Eq. (2). The interaction Hamiltonian $V = |\phi\rangle\langle\phi|$ is defined by

$$Vf = \phi(\phi, f), \tag{40}$$

where ϕ is a fixed element of L_2. The total Hamiltonian H is given by $H = K + V$, having domain D_K.

We shall prove the existence of the wave operators $\Omega_\pm$; i.e., we shall prove that

$$\Omega_\pm f = \text{s-lim}_{t\to\mp\infty} e^{iHt}e^{-iKt}f$$

exists for any f in L_2.

We first restate a number of results and definitions from Ref. 3. The results may be obtained without first assuming the existence of $\Omega_\pm$; proofs may be found in Ref. 3.

With

$$P(\lambda) = (\lambda - \xi)^n(\mu - \lambda)^n, \tag{41}$$

where $n > 2$ and ξ and μ are real numbers, we define a multiplication operator A_t by

$$A_t f = -i\int_C \frac{d\lambda\, P(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}(e^{i(\lambda-K)t} - 1)f, \tag{42}$$

where

$$I(\lambda) = \int_{-\infty}^{\infty} \frac{|\phi^2(p)|\, dp}{(\lambda - p)} \tag{43}$$

and C is a closed contour intersecting the real axis at $\lambda = \xi, \mu$.

We then have the following identity for the evolution operator $e^{iHt}e^{-iKt}$:

$$\begin{aligned}P(H)P_{\xi\mu}(H)(e^{iHt}e^{-iKt} - 1)f \\ = iF_{0\infty}A_t f - iA_t F_{t\infty}f \\ + \int_C d\lambda \frac{P(\lambda)}{1 - I(\lambda)}(\lambda - K)^{-1}F_{0t}f,\end{aligned} \tag{44}$$

where $P_{\xi\mu}(H)$ is the operator projecting onto the subset (ξ, μ) of the spectrum of H.

Equation (44) holds for any f in the intersection D_F of the domains of $F_{0\infty}$ and $F_{-\infty 0}$.

We also require, for $\text{Im}\,\lambda \neq 0$, the commutation relation

$$\begin{aligned}[(\lambda - K)^{-1}, F_{0t}]f \\ = (2\pi i)^{-1}(\lambda - K)^{-1}e^{iKt}\phi(\phi, e^{-iKt}(\lambda - K)^{-1}f) \\ - (2\pi i)^{-1}(\lambda - K)^{-1}\phi(\phi, (\lambda - K)^{-1}f).\end{aligned} \tag{45}$$

The resolvent operators $(\lambda - H)^{-1}$ and $(\lambda - K)^{-1}$ are related by

$$(\lambda - H)^{-1} - (\lambda - K)^{-1} = (\lambda - K)^{-1} \frac{|\phi\rangle\langle\phi|}{1 - I(\lambda)} (\lambda - K)^{-1}. \quad (46)$$

In order to prove the existence of $\Omega_{\pm}$, we shall use Eq. (44) to show that

$$\lim_{s,t\to\pm\infty} \| e^{iHt} e^{-iKt} f - e^{iHs} e^{-iKs} f \| = 0.$$

We first prove two lemmas.

Lemma 2: Suppose g_N is any element belonging to the restricted domain of $F_{0\infty}$ (and of $F_{-\infty 0}$), and suppose that, for t real, $\|A_t g_N\|$ is a bounded function of t (for fixed g_N). Then

$$\lim_{s,t\to\infty} (e^{-iKt} g_N, P(H) P_{\xi\mu}(H) \times (e^{iH(s-t)} e^{-iK(s-t)} - 1) e^{-iKt} g_N) = 0. \quad (47)$$

The inner product also tends to zero as $s, t \to -\infty$.

Proof: From Eq. (44), the inner product on the lhs is

$$\begin{aligned} &i(e^{-iKt} g_N, F_{0\infty} A_{s-t} e^{-iKt} g_N) \\ &\quad - i(e^{-iKt} g_N, A_{s-t} F_{s-t,\infty} e^{-iKt} g_N) \\ &\quad + \left(e^{-iKt} g_N, \int_C d\lambda \frac{P(\lambda)}{1 - I(\lambda)} (\lambda - K)^{-1} F_{0,s-t} e^{-iKt} g_N\right) \\ &= i(g_N, F_{t\infty} A_{s-t} g_N) - i(g_N, A_{s-t} F_{s\infty} g_N) \\ &\quad + \left(g_N, \int_C \frac{d\lambda\, P(\lambda)}{1 - I(\lambda)} (\lambda - K)^{-1} F_{ts} g_N\right). \end{aligned} \quad (48)$$

Now

$$\int_C \frac{d\lambda\, P(\lambda)}{1 - I(\lambda)} (\lambda - k)^{-1}, \quad \text{for real } k,$$

is a bounded function, so that the contour integral in Eq. (48) defines a bounded linear operator. Further, $\|A_{s-t} g_N\|$ is bounded and, since

$$\text{s-lim}_{t\to\infty} F_{t\infty} g_N = \text{s-lim}_{s,t\to\infty} F_{ts} g_N = 0,$$

we may take the limit as $s, t \to \infty$ to obtain Eq. (47). To prove similarly that the limit also vanishes as $s, t \to -\infty$, we note that

$$\text{s-lim}_{t\to-\infty} F_{t\infty} g_N = \Phi\Phi^* g_N,$$

and that the operators $\Phi\Phi^*$ and A_{s-t} commute.

Lemma 3: If g_N belongs to the restricted domain of $F_{0\infty}$, then

$$\text{s-lim}_{t\to\pm\infty} e^{iKt} P(H) P_{\xi\mu}(H) e^{-iKt} g_N = P(K) P_{\xi\mu}(K) g_N, \quad (49)$$

where $P_{\xi\mu}(K)$ is the operator projecting onto the subset (ξ, μ) of the spectrum of K.

Proof: By the Riemann–Lebesgue lemma, applied to elements of L_1, taking the limit as $t \to \infty$ of Eq. (45) gives the following commutation relation, applied to any element h_N of the restricted domain:

$$[(\lambda - K)^{-1}, F_{0\infty}] h_N = -(2\pi i)^{-1} (\lambda - K)^{-1} \phi(\phi, (\lambda - K)^{-1} h_N). \quad (50)$$

Multiplying each side of Eq. (50) by $P(\lambda)/[1 - I(\lambda)]$ and carrying out a contour integration, we have

$$\begin{aligned} &\int_C \frac{d\lambda\, P(\lambda)}{1 - I(\lambda)} (\lambda - K)^{-1} F_{0\infty} h_N \\ &\quad = F_{0\infty} \int_C \frac{d\lambda\, P(\lambda)}{1 - I(\lambda)} (\lambda - K)^{-1} h_N \\ &\quad\quad - P(H) P_{\xi\mu}(H) h_N + P(K) P_{\xi\mu}(K) h_N, \end{aligned} \quad (51)$$

where we have used Cauchy's theorem, together with Eq. (46). We have taken $F_{0\infty}$ outside the integral sign on the rhs of Eq. (51). This is valid since, by Theorem 2, the restriction of $F_{0\infty}$ to the set of elements h_N for fixed N is bounded. Substituting $h_N = e^{-iKt} g_N$ and operating by e^{iKt} on each side of Eq. (51), we obtain Eq. (49) by taking the limits as $t \to \pm\infty$.

We found it necessary for the proof of Lemma 2 to assume that $\|A_t g_N\|$ is bounded. Since the operator A_t defined by Eq. (42) depends on the value of the constant n in Eq. (41), we now find it convenient to express the dependence by use of a superscript, so that we have a family of operators $A_t^{(n)}$ as t and n are varied. The polynomial given by Eq. (41) we now denote by $P^{(n)}(\lambda)$. It is necessary to have $n > 2$, to guarantee that our contour integrals converge.

We may now find, by using the two lemmas, a set of elements in the domain of the wave operators:

Theorem 4: Let f_N be an element in the restricted domain of $F_{0\infty}$, such that

(i) $f_N(k)$ is of bounded support, and
(ii) $\|A_t^{(2n)} f_N\|$ is bounded uniformly in t (for fixed n and f_N).

Then f_N is in the domain of the wave operators $\Omega_{\pm}$.

Proof: Let g_N belong to the restricted domain of $F_{0\infty}$, and suppose that $\|A_t^{(2n)} g_N\|$ is bounded uniformly

in t. Then, using Eq. (47) with $P(\lambda) = P^{(2n)}(\lambda)$, we have

$$\lim_{s,t\to\infty} [(P^{(n)}(H)P_{\xi\mu}(H)e^{-iKt}g_N, e^{iH(s-t)}P^{(n)}(H)P_{\xi\mu}(H)e^{-iKs}g_N) - (P^{(n)}(H)P_{\xi\mu}(H)e^{-iKt}g_N, P^{(n)}(H)e^{-iKt}g_N)] = 0. \tag{52}$$

Using Eq. (49), we deduce that

$$\lim_{s,t\to\infty} [(P^{(n)}(K)P_{\xi\mu}(K)e^{-iKt}g_N, e^{iH(s-t)}P^{(n)}(K)P_{\xi\mu}(K)e^{-iK(s-t)}e^{-iKt}g_N) - (e^{-iKt}P^{(n)}(K)P_{\xi\mu}(K)g_N, e^{-iKt}P^{(n)}(K)P_{\xi\mu}(K)g_N)] = 0. \tag{52'}$$

Now the element f_N in the statement of Theorem 4 is certainly of the form $P^{(n)}(K)P_{\xi\mu}(K)g_N$ for some g_N in the restricted domain and for some ξ, μ, where $\|A_t^{(2n)}g_N\|$ is bounded uniformly in t.

Substituting $P^{(n)}(K)P_{\xi\mu}(K)g_N = f_N$ into Eq. (52'), we have

$$\lim_{s,t\to\infty} (e^{-iKt}f_N, (e^{iH(s-t)}e^{-iK(s-t)} - 1)e^{-iKt}f_N) = 0. \tag{53}$$

Now, for any element x,

$$\|(e^{iH\alpha}e^{-iK\alpha} - 1)x\|^2 = (e^{iH\alpha}e^{-iK\alpha}x, (e^{iH\alpha}e^{-iK\alpha} - 1)x) - (x, (e^{iH\alpha}e^{-iK\alpha} - 1)x) = -2R[(x, (e^{iH\alpha}e^{-iK\alpha} - 1)x)].$$

Hence, taking $x = e^{-iKt}f_N$ and $\alpha = s - t$, we may deduce from Eq. (53) that

$$\lim_{s,t\to\infty} \|(e^{iH(s-t)}e^{-iK(s-t)} - 1)e^{-iKt}f_N\| = 0$$

or

$$\lim_{s,t\to\infty} \|(e^{iHs}e^{-iKs} - e^{iHt}e^{-iKt})f_N\| = 0.$$

From the completeness of the space it follows that

$$\Omega_- f_N = \text{s-lim}_{t\to\infty} e^{iHt}e^{-iKt}f_N$$

exists. We may similarly prove that $\Omega_+ f_N$ exists.

Theorem 5: The wave operators $\Omega_\pm$ are defined on the whole space.

Proof: Since the domain of the wave operators is always closed, we know that $\Omega_\pm$ is defined on the closure of the set of elements f_N satisfying the conditions of Theorem 4.

Now, certainly $\|A_t^{(2n)}\phi\|$ is bounded uniformly in t. (This is proved in Ref. 3.) It is therefore sufficient, for the conclusion of Theorem 4, to assume that the element f_N of the restricted domain satisfies

(i) $f_N(k)$ is of bounded support, as before, and
(ii) $|f_N(k)| \leq \text{const}\,|\phi(k)|$ a.e.

The closure of the set of elements f_N satisfying (i) and (ii) consists of those elements f such that $f(k) = 0$ a.e., for all k such that $\phi(k) = 0$.

The subspace orthogonal to this latter set of elements consists of those elements f satisfying, a.e., $f(k) = 0$ for all k such that $\phi(k) \neq 0$. But for those elements, $F_{ab}f = F_{0\infty}f = 0$, and it may be shown from Eq. (44) that in that case $e^{iHt}e^{-iKt}f = f$, so that $\Omega_\pm f = f$. So $\Omega_\pm$ are defined both on a subspace of L_2 and on the corresponding orthogonal subspace, so that the wave operators are indeed defined on the whole space.

A derivation of the wave operators is given in Ref. 3.

[1] K. O. Friedrichs, *Perturbation of Spectra in Hilbert Space* (American Mathematical Society, Providence, R.I., 1965).
[2] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1966).
[3] M. A. Grubb and D. B. Pearson, J. Math. Phys. **11**, 2415 (1970).

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Rotation in Closed Perfect-Fluid Cosmologies*

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A Lagrangian is presented which describes the evolution of anisotropy in rotating closed (Bianchi type IX) cosmologies. It is assumed that the matter is a perfect fluid with an adiabatic equation of state $p = P(\rho)$ such that $0 < dp/d\rho < 1 - \gamma$, $\gamma > 0$. The matter terms enter the Lagrangian as a potential which for large anisotropy is essentially identical to one found previously for dust. Because the dust potential has been thoroughly investigated by Ryan, we confine our discussion of the dynamics to a few brief remarks. The matter terms are crucial for the rotation since the constraint equations require matter for the presence of rotation. The chief effect of the rotation is the appearance of centrifugal terms in the Lagrangian which exclude certain parameter values to the system. An appendix gives a proof that $R = 0$ is a true infinite-density singularity.

1. INTRODUCTION

The metric for a homogeneous cosmology is often written[1]

$$ds^2 = -dt^2 + R^2 e^{2\beta}_{ij}\omega^i\omega^j. \tag{1.1}$$

The variables R and β_{ij} are functions only of the cosmic time t, while the ω^i are functions only of the coordinates in the $t = \text{const}$ surfaces. The matrix β_{ij} is symmetric and traceless. It gives the anisotropy of the spatial surfaces, while R gives their volume.

The symmetry group of the constant-t surface enters when we require that ω^i be invariant under action of a group; this implies[2] that

$$d\omega^i = \tfrac{1}{2}C^i_{jk}\omega^j\omega^k \tag{1.2}$$

for the curl of the basis vectors ω^i. (For notation, see Flanders[3] or Misner.[4]) In Eq. (1.2), the C^i_{jk} are the structure constants of the group. We will consider a Bianchi type IX universe which has[5] $C^i_{jk} = \epsilon_{ijk}$, the totally antisymmetric symbol. When $\beta_{ij} \equiv 0$, Eq. (1.1) describes a *closed* Robertson–Walker line element.

We shall consider a perfect-fluid stress tensor

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu + pg_{\mu\nu} \tag{1.3}$$

as a source for these cosmologies, with an adiabatic equation of state, $p = P[\rho]$. (To avoid confusion between the value of a quantity and its functional form, we will write capital letters for the function, and use the square bracket exclusively to indicate functional dependence.)

There are important simplifications when the kinematic rotation[6] vanishes. Because of the special form of the expression for the rotation in these homogeneous cosmologies, the spatial components of the velocity u_i must then also vanish.[7,8] Hence, the matter currents T_{0i} vanish.

Now the $0i$ component of the Einstein tensor is

$$G_{0i} = \tfrac{1}{2}e^{\beta}_{il}\epsilon_{ljk}(e^{2\beta}\sigma - \sigma e^{2\beta})_{jk} \tag{1.4}$$

where $\sigma_{ij} = \frac{1}{2}\{(e^\beta)^\cdot e^{-\beta} + e^{-\beta}(e^\beta)^\cdot\}_{ij}$ is the traceless second fundamental form of the space slices. Equation (1.4) shows that $G_{0i} = 0$ means that (e^β) and $(e^\beta)^\cdot$ commute. That is, the principal axes of the metric do not rotate when the matter rotation vanishes, and conversely.

The $T_{00} = G_{00}$ Einstein equation reads

$$3(\dot{R}/R)^2 = (\rho + p)u_0^2 - p + \tfrac{1}{2}\sigma_{ij}\sigma_{ij} + \tfrac{3}{4}R^{-2}V_g(\beta) - \tfrac{3}{4}R^{-2}. \tag{1.5}$$

Here,

$$V_g(\beta) = \tfrac{1}{3}\,\mathrm{Tr}\,(e^{4\beta} - 2e^{-2\beta} + 1)$$

is a potential due to the distortion of the space surface from an exactly spherical shape ($\beta = 0$).[9] It arises from the scalar curvature of the 3-surfaces and is a function only of the eigenvalues of β.

With the definitions[9]

$$\beta_+ = -\tfrac{1}{2}\beta_3, \quad \beta_- = (2\sqrt{3})^{-1}(\beta_1 - \beta_2), \tag{1.6}$$

this potential is

$$V_g(\beta_+, \beta_-) = \tfrac{2}{3}e^{4\beta_+}[\cosh(4\sqrt{3})\beta_- - 1] + 1 - \tfrac{4}{3}e^{-2\beta_+}\cosh(2\sqrt{3})\beta_- + \tfrac{1}{3}e^{-8\beta_+}. \tag{1.7}$$

The equipotentials are circular near $|\beta| = 0$ (we define $|\beta|^2 = \beta_+^2 + \beta_-^2$), where the potential is approximately simple harmonic:

$$V_g = 8\,|\beta|^2 + O(|\beta|^3). \tag{1.8}$$

For large values of $|\beta|$ the potential takes on the shape of an equilateral triangle. The sides are extremely straight, and the only deviation from this exact triangular shape comes in the corners, where there are channels which reach out to infinity. Exactly in the corner direction the potential is bounded: $V_g < 1$.

One of the straight walls of the potential crosses the negative β_+ axis, and one finds

$$V_g = \tfrac{1}{3}e^{-8\beta_+} \tag{1.9}$$

for the asymptotic behavior in the triangular sector that includes the negative β_+ axis. Because of the triangular symmetry of the potential, Eq. (1.9) gives the behavior in the other sectors as well.

The positive β_+ axis lies along one of the corner channels. The asymptotic behavior for small β_- and large β_+ is

$$V_g = 16e^{4\beta_+}\beta_-^2 + 1, \tag{1.10}$$

so the equipotentials narrow exponentially. For most purposes the equipotential can be considered exactly triangular. Details of the properties of V_g are discussed further by Misner,[9,10] by MSW, and by Ryan.[8]

In discussing the motion of the matrix β_{ij}, it is useful to introduce a new time coordinate,[10]

$$\Omega = \ln (R_m/R), \tag{1.11}$$

where R_m is the maximum radius of the universe. (To within an additive constant, $\Omega = -\alpha$, where α is the "volume" variable used by MSW.) Since closed models always recollapse (MSW), t is a 2-valued function of Ω. Except near the maximum of expansion, however, Ω is a very good coordinate. One of its advantages is that the "coordinate" $\beta_+\beta_-$ of the state of the universe then moves with speed $(d/d\Omega)$

$$\left|\frac{d\beta}{d\Omega}\right| < 1. \tag{1.12}$$

The upper limit is approximately reached when the system is far from the potential "walls." (That is, far from the turning points due to V_g and to the matter potential contained in the matter Lagrangian $\mathfrak{L}_m$ which we introduce in Sec. 3 below.)

The Ω speed of the moving walls of V_g is $d\beta_w/d\Omega < \frac{1}{2}$, where this refers to the position of the center of one of the straight potential sides. Again, the limit $\frac{1}{2}$ is reached when the system β point is far from the potential walls. (Because of the triangular symmetry, the corners of the V_g equipotential curves move outward with Ω speed $d\beta_c/d\Omega \sim 1$.) For details of the calculation of these quantities, see Misner,[9-11] MSW, and also Sec. 4 below.

2. THE FLUID CONSERVATION LAWS

We now recall two useful identities. The equations of motion for u_i in these type IX models read

$$u^0\dot{u}_i = \epsilon_{ijk}R^{-2}e^{-2\beta}_{kl}u_ju_l - (\delta^\sigma_i + u_iu^\sigma)p_{,\sigma}(\rho + p)^{-1}. \tag{2.1}$$

(Hawking[12] gives the form for the convective derivative in type IX. The general form for the equation of motion for a fluid is given by Ehlers[6] and by many others.) Because of the assumed homogeneity, p has only a time derivative. Dividing Eq. (2.1) by u^0 and multiplying by u_i, one obtains that

$$u_iu_ih^2 = A^2 \tag{2.2}$$

is constant. In Eq. (2.2), the enthalpy h is defined by

$$dh/h = dp/(\rho + p). \tag{2.3}$$

Equation (2.2) is equivalent to the statement of the evolution of the vorticity in a fluid with an equation of state.[6]

Another useful conservation law is contained in the Bianchi identity $T^{i\mu}{}_{;\mu} = 0$. This can be written

$$\begin{aligned}(R^3T_{0i})^\cdot &= -R^3\epsilon_{ijk}T_{jl}R^{-2}e^{-2\beta}_{lk}\\ &= -R^3\epsilon_{ijk}u_ju_lR^{-2}e^{-2\beta}_{kl}(\rho + p).\end{aligned}$$

Hence

$$2(R^3T_{0i})(R^3T_{0i})^\cdot = (R^6T_{0i}T_{0i})^\cdot = 0 \tag{2.4}$$

or

$$(\rho + p)^2u_0^2u_iu_i = (\rho + p)^2u_0^2A^2h^{-2} = A^2M^2R^{-6}, \tag{2.5}$$

where M is another constant. When the rotation vanishes so that $u^0 = 1$, Eq. (2.5) contains the familiar laws for adiabatic expansion: for dust $p = 0$, $\rho \propto R^{-3}$; for radiation $p = \frac{1}{3}\rho$, $\rho \propto R^{-4}$.

We shall find it useful to introduce the notation $u^2 = u_iu_i$ and $n_i = u_i/u$. Then Eq. (2.2) connects u and ρ (because we assume there is an equation of state so that $h = H[\rho]$), while Eq. (2.5) can be considered to connect u, β, and ρ, with n_i and R regarded as being externally given parameters in the relation. Hence, given R and n_i, only one of the three quantities u, β, and ρ can be varied independently and Eqs. (2.2) and (2.5) then force a variation in the other two. We shall below take β to be the freely varied quantity.

3. THE VARIATIONAL PRINCIPLE

Because of the Bianchi identities, the $G^k_k = T^k_k$ equation is satisfied once all the others are, while the $T_{0i} = G_{0i}$ equation can be viewed as a constraint which restricts only the initial conditions. The remaining equations which we have to consider can be expressed the following way, in a local Lorentz frame (orthogonal tetrad):

$${}^0G_{ik} - \tfrac{1}{3}\delta_{ik}{}^0G_{ll} = {}^0T_{ik} - \tfrac{1}{3}\delta_{ik}{}^0T_{ll}. \tag{3.1}$$

The notation "left superscript zero" indicates the components in the orthonormal tetrad $\{dt, \sigma^i = R^{-1}e^{-\beta}_{ij}\omega^j\}$. Equation (3.1), for the model we consider

described by Eqs. (1.1) and (1.3), reads

$$\dot{\sigma}_{ij} + 3\frac{\dot{R}}{R}\sigma_{ij} + \sigma_{il}\tau_{lj} - \tau_{il}\sigma_{lj} + \tfrac{3}{4}R^{-2}\frac{\partial V}{\partial \beta_{ij}} = (\rho + p)(v_i v_j - \tfrac{1}{3}\delta_{ij}v_k v_k). \quad (3.2)$$

In Eq. (2.2), $\tau_{ij} = \frac{1}{2}\{(e^{\beta})^{\cdot}e^{-\beta} - e^{-\beta}(e^{\beta})^{\cdot}\}_{ij}$, and the orthonormal components of the velocity $v_i \equiv {}^0u_i$ are introduced as a notational convenience. They satisfy

$$v_i = R^{-1}e^{-\beta}_{ij}u_j, \quad u_0^2 = 1 + v_i v_i. \quad (3.3)$$

The anisotropy-governing components of the Einstein tensor, the left side of Eq. (3.2), may be obtained by taking the variational derivative with respect to β_{ij} in the Lagrangian[10,11]

$$\mathfrak{L} = R^3(\tfrac{1}{2}\sigma_{ij}\sigma_{ij} - \rho_g V_g). \quad (3.4)$$

Here $\rho_g \equiv \frac{3}{4}R^{-2}$, and R is treated as an externally given function of time.

When there is no rotation,the traceless stresses

$${}^0T_{ij} - \tfrac{1}{3}\delta_{ij}\,{}^0T_{kk}$$

vanish, so the equation for β_{ij} is simply

$$\frac{\delta \mathfrak{L}}{\delta \beta_{ij}} = 0,$$

where the notation $\delta\beta_{ij}$ indicates a particular kind of "variation in β_{ij}" which leaves e^{β}_{ij} symmetric and traceless. As Misner[11] has discussed, one actually varies $e^{2\beta}$, but considers the coefficient of

$$\delta\beta = \tfrac{1}{2}e^{-\beta}\delta(e^{2\beta})e^{-\beta}.$$

The subject of this paper will be the modifications due to the presence of matter. We shall show that, for simple adiabatic equations of state $p = P[\rho]$, the modification consists simply of the addition of a matter Lagrangian

$$\mathfrak{L}_m = -R^3T_{00} = -R^3(\rho + p)u_0^2 + R^3p. \quad (3.5)$$

The anisotropy enters (3.5) explicitly in the definition of u_0, Eq. (3.3), and also implicitly in ρ and p because of the conservation laws (2.2) and (2.5) above.

In order to show that $\mathfrak{L}_m$ as defined by Eq. (3.5) is the correct matter Lagrangian, we now proceed to compute the variation. For later convenience, we shall compute the total variation

$$\delta T_{00} = \frac{\delta T_{00}}{\delta \Omega}\delta\Omega + \frac{\delta T_{00}}{\delta n_i}\delta n_i + \frac{\delta T_{00}}{\delta \beta_{ij}}\delta\beta_{ij}. \quad (3.6)$$

The variation of other quantities (ρ, p, and u) appearing in T_{00} are considered to be given by the variation of Ω and β, via the conservation laws, Eqs. (2.2) and (2.5).

At this point we introduce more notation and state explicitly the properties we assume the fluid to have. We use the asterisk to denote the inverse of a function: $\rho = P^*[p]$. Since the case $p = 0$ has been treated by MSW, we shall exclude it here. (It can be checked that the results found here correspond, in the limit $p \to 0$, to those found in MSW.) We shall require $0 < P' < 1 - \gamma$, where the prime denotes the derivative of a function with respect to its argument: $P'[\rho] = dP/d\rho$, and $\gamma > 0$ can be chosen arbitrarily small. We also assume $P[\rho = 0] = 0$. These are fairly restrictive requirements but admit all equations of state $p = \kappa\rho$, $\kappa < 1$, as well as polytropic equations of state for those values of the parameters that have $P' < 1$. It also includes the equations of state obtained from simple kinetic theory models, e.g., $p = \kappa(p)\rho$ as obtained for massive particles where $\kappa(p) \to 0$ as $p \to 0$ and $\kappa(p) \to \frac{1}{3}$ as $p \to \infty$.

With the assumptions made above on P and P', one finds

$$1 > \frac{d\ln H}{d\ln \rho} > 0, \quad (3.7)$$

and defining

$$Q[\rho] \equiv (\rho + p)/h, \quad (3.8)$$

one has

$$1 > \frac{d\ln Q}{d\ln \rho} = \frac{\rho}{\rho + p} > 0. \quad (3.9)$$

Note that $Q'H = 1$. Because both Q' and H' are positive, the inverses Q^* and H^* are well defined. It is straightforward to show that

$$d\ln Q^*[x]/d\ln x > 1. \quad (3.10)$$

Now,

$$\delta T_{00} = \delta\{(\rho + p)h^{-1}u_0(hu_0) - p\} = 3(\rho + p)u_0^2\delta\Omega + \tfrac{1}{2}(\rho + p)\delta(u_0^2) + (u_0^2 - 1)\delta p, \quad (3.11)$$

where we grouped terms to take advantage of Eq. (2.5) and used the definition of h.

We use Eq. (2.5) again, since

$$p = P[\rho] = P[Q^*[M/(R^3u_0)]]$$

yields

$$\delta p = \frac{P'}{Q'}\left(\frac{M}{R^3u_0}\right)\left\{3\delta\Omega - \frac{1}{2u_0^2}\delta(u_0^2)\right\}.$$

Use Eq. (2.5) to eliminate M, and remember $Q'h = 1$. Then we can rewrite Eq. (3.11):

$$\delta T_{00} = 3(\rho + p)u_0^2\delta\Omega + 3P'(u_0^2 - 1)(\rho + p)\delta\Omega + \tfrac{1}{2}(\rho + p)(u_0^2 - u_0^2P' + P')u_0^{-2}\delta(u_0^2). \quad (3.12)$$

Now

$$\begin{aligned}\tfrac{1}{2}\delta(u_0^2) &= \tfrac{1}{2}\delta(1 + R^{-2}e_{ij}^{-2\beta}u^2n_in_j)\\ &= (u_0^2 - 1)\delta\Omega - R^{-2}e_{il}^{-\beta}e_{jk}^{-\beta}u_iu_k\delta\beta_{ij}\\ &\quad + R^{-2}e_{ij}^{-2\beta}u^2n_i\delta n_j + (u_0^2 - 1)\tfrac{1}{2}u^{-2}\delta(u^2).\end{aligned} \tag{3.13}$$

The variation $\delta(u^2)$ is constrained by the conservation laws [Eqs. (2.2) and (2.5)]. We have $h = H[\rho] = A/u$, so that $\rho = H^*[A/u]$. We equate this $\rho = Q^*[M/(R^3u_0)]$, and,forming the variation of each side, obtain

$$\frac{M}{Q'}\,\delta\left(\frac{1}{R^3u^0}\right) = \frac{A}{H'}\,\delta\left(\frac{1}{u}\right).$$

Carrying out the indicated variations, and using Eqs. (2.2) and (2.5) to eliminate M and A, one obtains

$$\tfrac{1}{2}u^{-2}\delta(u^2) = \tfrac{1}{2}P'u_0^{-2}\delta(u_0^2) - 3P'\delta\Omega. \tag{3.14}$$

To obtain Eq. (3.14), we also used $Q'h = 1$ and $H'(\rho + p) = HP'$.

Equation (3.13) now becomes

$$\begin{aligned}\tfrac{1}{2}u_0^{-2}\delta(u_0^2)(u_0^2 - u_0^2P' + P')&\\ = (1 - 3P')(u_0^2 - 1)\delta\Omega - v_iv_j\delta\beta_{ij}&\\ + R^{-2}e_{ij}^{-2\beta}u^2n_i\delta n_j.&\end{aligned} \tag{3.15}$$

So we have, finally,

$$\begin{aligned}\delta T_{00} = (\rho + p)(4u_0^2 - 1)\delta\Omega - v_iv_i\delta\beta_{ij}(\rho + p)&\\ + R^{-2}e_{ij}^{-2\beta}u^2n_i\delta n_j(\rho + p).&\end{aligned} \tag{3.16}$$

We must of course always take variations δn_i such that $n_i\delta n_i = 0$. If we recall the traceless nature of $\delta\beta_{ij}$,we see from Eqs.(3.16) and (3.2) that the Lagrangian for the anisotropy in these fluid-filled models can be written

$$\mathfrak{L} = R^3(\tfrac{1}{2}\sigma_{ij}\sigma_{ij} - \rho_gV_g - T_{00}), \tag{3.17}$$

where R and n_i are considered given functions of time. (R is given by the $T_{00} = G_{00}$ equation and n_i is given by the equation of motion.)

The Lagrangian of Eq. (3.17) differs from the form previously suggested by Hawking[12] for radiation ($p = \frac{1}{3}\rho$) and by this author[13] for general fluids with $p = \kappa\rho$. That previous form was

$$\mathfrak{L}_m = -[(\rho + p)/(1 - \kappa)]u_0^2R^3. \tag{3.18}$$

Equation (3.18) was not satisfactory because it ignored the constraint on u^2 given by Eq. (2.2). In addition, it only worked for constant κ and did not lead to as simple or useful forms for the quantities discussed in Eqs. (4.5) and (4.6) below.

That T_{00} acts as a potential in the anisotropic motion obviously agrees with the form ρu_0^2 found by MSW for dust. It should be recalled that the potential found by Misner[11] in nonrotating type I universes for collisionless radiation (neutrinos) was also, aside from additive terms independent of β, given by T_{00}.

There is an even closer analogy with the collisionless case, as we can see when we consider the asymptotic large behavior of T_{00}. During the early parts of the cosmological evolution, when the anisotropy is large, it is only when T_{00} itself is large that we can expect it will be significant in the evolution of the model. We shall now make precise just what we mean by "T_{00} large." We shall find that "T_{00} large" always implies $|\beta| \gg 1$, although the converse is not true.

Since $Q'[\rho] > 0$ and Eq. (2.5) shows that $Q[\rho] < MR^{-3}$, we find that, near the singularity,

$$\rho = Q^*[M/(R^3u_0)] < Q^*[MR^{-3}], \tag{3.19}$$

no matter how large the anisotropy becomes. Equation (3.19) gives us the basis for our characterization of "T_{00} large"; it means

$$T_{00} \gg Q^*[MR^{-3}]. \tag{3.20}$$

(If we were discussing dust, this would be the requirement $T_{00} \gg M/R^3$, while for radiation with $p = \rho/3$, it reads $T_{00} \gg M^{\frac{4}{3}}/R^4$.)

Because of (3.19), T_{00} can satisfy Eq. (3.20) only if $u_0^2 \gg 1$. We now show that T_{00} does in fact become large if $u_0^2 \gg 1$. The dominant term in T_{00} (for large u_0^2) gives

$$T_{00} \simeq (\rho + p)u_0^2 \simeq (\rho + p)u_0un_0, \tag{3.21}$$

where in the last term we write

$$u_0 \simeq un_0, \tag{3.22}$$

with

$$n_0 = R^{-1}(e_{ij}^{-2\beta}n_in_j)^{\frac{1}{2}}. \tag{3.23}$$

Equation (3.22), hence also Eq. (3.21), holds when $u_0 \gg 1$. Now $(\rho + p)uu_0 = AMR^{-3}$, so

$$T_{00} = -R^{-3}\mathfrak{L}_m \simeq AMR^{-4}(e_{ij}^{-2\beta}n_in_j)^{\frac{1}{2}}, \tag{3.24}$$

when

$$e_{ij}^{-2\beta}n_in_j \gg 1.$$

From the first member of Eq. (3.19) we see that $T_{00} \to \infty$ at $R = 0$ if u_0 is bounded, and Eq. (3.24) gives $T_{00} \to \infty$ at $R = 0$ for $u_0 \gg 1$. We have just shown, therefore, that $R = 0$ gives a singularity in T_{00}. In the Appendix we will show that in fact $\rho \to \infty$ as $R \to 0$, so there is a true matter singularity.

The form (3.24) compares directly to the form found by Misner[11] for collisionless radiation in a nonrotating model. Misner's result was

$$T_{00} = a_\nu R^{-4} \frac{1}{4\pi} \int (e_{ij}^{-2\beta} n_i n_j)^{\frac{1}{2}} \, d\Omega, \qquad (3.25)$$

with a_ν constant. Aside from additive terms independent of β, Misner had

$$\mathfrak{L}_m = -R^3 T_{00}.$$

Misner's potential form (in a nonrotating solution) is just the average over the sphere of the asymptotic form we obtained in rotating models, with a fluid source, when $u_0 \gg 1$.

This $u_0 \gg 1$ regime is just where we expect matter to act like radiation, since it is then moving (relative to our $\{dt, \omega^i\}$ Lorentz frame) with a speed near the speed of light. The matter potentials which have been called "rotation potentials" by MSW and by Ryan[8] appear only when there is rotation in fluid-filled type IX models because only then is there a component of the velocity which can be blue-shifted by the anisotropy. When this matter is blue-shifted by an amount sufficient to give it a large velocity, one obtains the result expected from a (directed) stream of radiation traveling in the same direction.

In Eq. (3.25) for collisionless radiation appears the quantity $a_\nu R^{-4}$, which is defined as the energy density if β is instantaneously zero. It is interesting that, on the other hand, $\rho + p$ appears in Eq. (3.21). Apparently, pressure and matter density enter equally into the matter potential.

4. COMMENTS ON DYNAMICS

If the anisotropy is small, approximation methods can give an accurate description of the anisotropy behavior. Discussions of this type are found in Ref. 12 and for dust in MSW. (Detailed numerical calculations for the behavior near the maximum are also given in graphical form by MSW.)

On the other hand, when the anisotropy is large, the matter potential for any fluid is (to within a multiplicative constant) the same as it is for dust. Since the dust potentials have been extensively discussed by MSW, and in more detail by Ryan,[8] we shall confine ourselves to only general comments.

We can get a general idea of the behavior of the solution by considering the region of β-space that the solution is allowed to occupy. Hence, we will concentrate on the motion of the potential "walls," assuming large anisotropy. For the large anisotropy case, we can define a "matter potential" $V_m(\beta, n_i)$ by

$$T_{00} \simeq AMR^{-4} V_m(\beta, n_i),$$
$$V_m(\beta, n_i) = (e_{ij}^{-2\beta} n_i n_j)^{\frac{1}{2}}. \qquad (4.1)$$

This definition does not work when T_{00} is small, but it will give an adequate description of the behavior of the matter potential walls.

It is useful to write Eq. (1.5) as

$$3\dot{\Omega}^2 = \rho_T - \rho_g, \qquad (4.2)$$

where

$$\rho_T = \tfrac{1}{2}\sigma_{ij}\sigma_{ij} + \rho_g V_g + T_{00}. \qquad (4.3)$$

The evolution equation for ρ_T is

$$R^{-6} \frac{d}{d\Omega} R^6 \rho_T = \dot{\Omega}^{-1} \Big[\sigma_{ij}\dot{\sigma}_{ij} - 3\dot{\Omega}\sigma_{ij}\sigma_{ij} + \rho_g \frac{\partial V_g}{\partial \beta_{ij}} \sigma_{ij} - (\rho + p) v_i v_j \sigma_{ij} \Big] - 4\rho_g V_g - (2u_0^2 + 1)(\rho + p) + 6p. \qquad (4.4)$$

To obtain this form we used Eq. (3.16) for δT_{00}. The term in n_i vanishes in virtue of the equation of motion (2.1). (This is a nonintegrable constraint, so we made no attempt to insert it previously.) The quantity multiplying $\dot{\Omega}^{-1}$ in Eq. (4.4) vanishes in virtue of Eq. (3.2), and

$$\frac{d}{d\Omega} \ln (\rho_T R^6) = -\frac{4\rho_g V_g}{\rho_T} - \frac{(2u_0^2 + 1(\rho) + p)}{\rho_T} + \frac{6p}{\rho_T} < 0. \qquad (4.5)$$

This reduces to the form found by MSW for dust. Its accuracy can also be checked for an *isotropic* model ($\beta = 0$ and $u_0 = 1$) with $p = \kappa\rho$. Then Eq. (2.5) gives

$$\rho_T = \rho \propto R^{-3-3\kappa} \quad \text{or} \quad R^{-6} \frac{d}{d\Omega}(\rho_T R^6) = (3\kappa - 3)\rho.$$

Inserting $p = \kappa\rho$ and $u_0^2 = 1$ into (4.5), one verifies this relationship.

We have seen that when the matter terms are important in the anisotropy motion, $u_0^2 \gg 1$. Hence, for large anisotropy situations, the matter terms on the right in Eq. (4.5) are negligible except when $u_0^2 \gg 1$. The matter potential terms rise exponentially with β in that case, as does V_g. So, for large anisotropy

$$\frac{d}{d\Omega} \ln (\rho_T R^6) \simeq -\frac{4\rho_g V_g}{\rho_T} - \frac{2(\rho + p)u_0^2}{\rho_T} \simeq -\frac{4\rho_g V_g}{\rho_T} - \frac{2AMR^{-4} V_m(\beta, n_i)}{\rho_T}. \qquad (4.6)$$

Because of the exponential steepness of V_m and V_g, $\Lambda \equiv \rho_T R^6$ is approximately constant except during approximately impulsive collisions with the potential walls, and all the potentials are negligible except for the occasional collisions.

We shall find it useful to give a derivation of the limit $|d\beta/d\Omega| < 1$ of Eq. (1.12). We define

$$\beta = O^{\mathrm{T}} b O, \tag{4.7}$$

where O is an orthogonal matrix, and b is a 3×3 *diagonal* matrix whose components are the eigenvectors of β. The quantity $\frac{1}{2}\sigma_{ij}\sigma_{ij}$ which appears in the Lagrangian is

$$\tfrac{1}{2}\sigma_{ij}\sigma_{ij} = \tfrac{1}{2}\dot{b}_{ij}\dot{b}_{ij} + \tfrac{1}{4}S_{mk}S_{km} - \tfrac{1}{4}e^{-2b}_{kl}S_{lm}e^{2b}_{mp}S_{pk}, \tag{4.8}$$

where $S_{lm} = \dot{O}_{ls}O^{\mathrm{T}}_{sm}$ is an antisymmetric 3×3 matrix. We introduce $S_{kl} = \epsilon_{klm}S_m$, where $S_i = Ss_i$ gives the angular velocity S and the direction s_i ($s_i s_i = 1$) of the rotation described by O_{lm}. The direction s_i is intimately related to the direction of the fluid flow, since Eq. (1.4) can be rewritten (using the diagonal traceless nature of b)

$$G_{0i} = 2O^{\mathrm{T}}_{ij}L_{ja}S_a, \tag{4.9}$$

where L_{lm} is a diagonal positive-semidefinite matrix:

$$L_{lm} = \mathrm{diag}\,\{\sinh^2[3\beta_+ - (\sqrt{3})\beta_-], \sinh^2[3\beta_+ + (\sqrt{3})\beta_-], \sinh^2[(2\sqrt{3})\beta_-]\}. \tag{4.10}$$

Equation (4.9) is reminiscent of the relation between angular velocity and angular momentum in a tumbling body.

Using the definitions of s_i, S, and L_{lm}, we find, for $\frac{1}{2}\sigma_{ij}\sigma_{ij}$,

$$\begin{aligned}\tfrac{1}{2}\sigma_{ij}\sigma_{ij} &= \tfrac{1}{2}\dot{b}_{ij}\dot{b}_{ij} + L_{lm}s_l s_m S^2 \\ &= 3(\dot{\beta}_+^2 + \dot{\beta}_-^2) + L_{lm}s_l s_m S^2 \\ &= 3\left|\frac{d\beta}{dt}\right|^2 + \frac{L_{lm}s_l s_m}{L^2_{ab}s_a s_b}\frac{A^2M^2}{4R^6}.\end{aligned} \tag{4.11}$$

This last form uses Eqs. (4.9) and (2.5). Hence, so long as ρ_g is negligible, Eq. (1.12) follows from Eqs. (4.11) and (4.2). Inserting the large anisotropy behavior for T_{00}, we rewrite Eq. (4.2), using Eq. (4.3):

$$1 \simeq \left|\frac{d\beta}{d\Omega}\right|^2 + \frac{\rho_g V_g}{\rho_T} + \frac{AMR^{-4}}{\rho_T}V_m + \frac{L_{lm}s_l s_m}{L^2_{ab}s_a s_b}\frac{A^2M^2}{4\Lambda}. \tag{4.12}$$

To discuss the motion of the potential "walls," we define β_w for each of the potentials. For instance, using the asymptotic form (1.9) for V_g, define β_g by

$$\rho_T = \rho_g \tfrac{1}{3}e^{8\beta_g} = \tfrac{1}{4}R^{-2}e^{8\beta_g}.$$

Thus,

$$\tfrac{1}{8}\ln(4\Lambda/R_m^4) + \tfrac{1}{2}\Omega = \beta_g, \tag{4.13}$$

for the distance β_g of the center of the wall from the origin. One can also define the location of the triangular corner of the potential given by the triangular geometry $\beta_c = 2\beta_g$.

A similar discussion can be carried out for the asymptotic parts of V_m. In the frame in which β is instantaneously diagonal, one defines the β_+, β_- coordinates of the "matter wall" by

$$\rho_T = AMR^{-4}(e^{-2\beta_+ - (2\sqrt{3})\beta_-}n_1^2 + e^{-2\beta_+ + (2\sqrt{3})\beta_-}n_2^2 + e^{4\beta_+}n_3^2)^{\frac{1}{2}}.$$

Not all components of n can vanish simultaneously since then the solution must be nonrotating. By suitable relabeling of the axes, we can make n_3^2 nonzero. Then one has

$$\begin{aligned}\Lambda R^{-6} &= AMR^{-4}e^{2\beta_{m+}}|n_3|, \\ \tfrac{1}{2}\ln[\Lambda/(AMR_m^2)] + \Omega &= \beta_{m+} + \tfrac{1}{4}\ln(n_3^2),\end{aligned} \tag{4.14}$$

for the position β_{m+} of the matter wall across the positive β_+ axis. If the other components of n_i are nonzero, then one has similar formulas for the walls in the other two (triangularly symmetric) directions. Notice that if n_3, say, goes to zero, one has $\beta_{m+} \to +\infty$; the wall moves out as n_3 vanishes, and disappears completely when $n_3^2 = 0$. A particularly interesting subset of rotating models which has been investigated by MSW and by Ryan[8] has $n_3 = 1$; it is called nontumbling because one of the principal directions of β remains parallel to the 3-direction, and the other two principal directions rotate around this 3-direction. β has a block diagonal form, with off-diagonal terms only in the $(1, 2)$ plane. Hence, s_i has only a 3-component. We will restrict ourselves to these special models, for the rest of this section.

We have just seen from Eq. (4.5) that $d\ln\Lambda/d\Omega < 0$, so when $n_3^2 = 1$, the wall of the matter potential moves inward, into the central part of the potential [compare β_m from (4.14) with β_c from (4.13)], as we follow a solution toward the singularity. On the other hand, we have seen that $d\Lambda/d\Omega$ is on the average quite slow, while $d\beta_c/d\Omega \simeq 1$. Hence, the *relative* distance from the matter potential wall to the corner of V_g decreases and for a sufficiently large Ω, a sketch of the potential would show β_m lying exactly on and across the corner of the potential, as accurately as the thickness of the lines in the sketch allows.

In general the matter potential has very little effect on the dynamics of the models near the singularity. This is because there is a "kinematic" effect introduced via the term $L_{lp}s_l s_p S^2$ in the Lagrangian. This term gives rise to an effective centrifugal potential, which keeps the system away from the β_+ axis (in these

nontumbling models). From Eq. (4.12), for the nontumbling case,

$$1 \gtrsim A^2M^2[4\Lambda \sinh^2 (2\sqrt{3})\beta_-]^{-1}.$$

The limit, unity, describes the centrifugal potential wall around the β_+ axis. Now Λ decreases toward the singularity, so we assume that $A^2M^2/\Lambda > 4$. (Jacobs, Misner, and Zapolosky[14] have shown $\Lambda \propto \Omega^{-2}$ for typical motion in the potential V_g.) We use the exponential approximation for $\sinh (2\sqrt{3})\beta_-$ and define the wall radius, β_r:

$$\beta_r \simeq -\frac{1}{4\sqrt{3}} \ln \left(\frac{4\Lambda}{R_m^4}\right) - \frac{1}{4\sqrt{3}} \ln \left(\frac{R_m^4}{4A^2M^2}\right). \quad (4.15)$$

On the other hand, straightforward geometry gives the equation

$$\beta_+ = 2\beta_g - (\sqrt{3})\beta_-, \quad (4.16)$$

with β_g given by Eq. (4.13), for the equipotential contour of V_g. These two equipotentials will intersect at a β_+ coordinate (β_{+i}) given by

$$\beta_{+i} = \tfrac{1}{2} \ln (4\Lambda/R_m^4) + \Omega + \tfrac{1}{4} \ln [R_m^4/(4A^2M^2)]. \quad (4.17)$$

(There is a second intersection at $\beta_+ \simeq -\beta_g$, but we shall not be concerned with that intersection.)

The system β_+ coordinate therefore cannot exceed β_{+i}.

Equation (4.17) should be compared with the result of Eq. (4.14) which shows

$$\beta_{m+} = \beta_{+i} - \tfrac{1}{2} \ln 2.$$

Because two quantities differ only by a small constant, the matter wall potential is comparable to the other potentials affecting the motion at the corner of the region allowed by V_g and the rotation terms, but only at the corner. The V_g potential and the kinematic "centrifugal repulsion" keep the system point from getting very close to the wall of V_m.

Thus one expects that the matter potential terms will in general be unimportant except for very particular initial conditions, because the matter potential affects only the motion very near the corner. In these nontumbling cases at least, the chief effect of the rotation appears in the initial conditions, which permit an "angular momentum" of the system point in β space. This "angular momentum" introduces the centrifugal terms, a kinematic effect which keeps the system away from the β_+ axis. Once the initial conditions start the system into its rotating condition (and the presence of matter is necessary for these initial conditions to be allowed) the further evolution is simply that given to a very good approximation by the equations without the matter terms.

For a more detailed discussion of the motion of these models, we refer the reader to Ref. 8, which contains a detailed discussion of these questions for dust, including tumbling models. We have shown that the conclusions for dust hold, in the large anisotropy regime, for any fluid.

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APPENDIX: $R = 0$ IS AN INFINITE-DENSITY SINGULARITY

Shepley[2] showed that for a dust-filled type IX cosmology, the instant when $R = 0$ is a singularity, but the nature of the singularity (i.e., incompleteness, infinite density, or whatever) was not specified.

Hawking and Ellis[15] generalized this result to all spatially-homogeneous fluid-filled cosmologies with any transitive group of motions acting on 3-dimensional hypersurfaces. All such models are singular at $R = 0$ (i.e., where the time lines normal to the invariant hypersurfaces intersect). Again, however, the nature of the singularity was not specified.

Shepley[16] has presented a model in which the matter (dust) behaves in a perfectly regular way through the surface $R = 0$. There are, however, some incomplete null geodesics in that null surface. Shepley[17] discusses the relation between his and Hawking and Ellis' proofs, and his example. The behavior of the matter near the singularity must apparently be investigated in each model. MSW showed that $R = 0$ is in fact an infinite-density singularity for dust-filled type IX models. We say in the text that $R = 0$ is a matter singularity for the fluid solutions with pressure, since $T_{00} \to \infty$ there. We show here that in this case also, the singularity is one of infinite density, $\rho \to \infty$, so long as the pressure obeys $P = P[\rho] > 0$, $P[\rho = 0] = 0$, and $0 < P' < 1 - \gamma$. The proof uses a generalization of the method found in MSW for dust.

Recall Eq. (3.10):

$$\frac{d \ln Q^*[x]}{d \ln x} > 1. \quad (A1)$$

Since $u_0 > 1$, we have then

$$\rho u_0^2 = Q^*[M/(R^3u_0)]u_0^2 > N \frac{M}{R^3u_0} u_0^2 > \frac{NM}{R^3} \quad (A2)$$

as $R \to 0$, for some constant N. Thus for any ϵ one chooses, there is a value R_ϵ such that for all $R < R_\epsilon$,

$$\rho u_0^2 - \rho_g = \rho u_0^2 - \tfrac{3}{4}R^{-2} > \rho u_0^2(1 - \epsilon). \quad (A3)$$

Inserting this relationship into the T_{00} equation (1.5), one finds that for R sufficiently small

$$3(\dot{R}/R)^2 > \tfrac{1}{2}\sigma_{ij}\sigma_{ij}. \tag{A4}$$

If we define $l_{ij} = \sigma_{ij} - \dot{\Omega}\delta_{ij}$, then Eq. (A4) implies

$$3\,|\dot{\Omega}| > |l_{ij}|, \quad i,j = 1,2,3. \tag{A5}$$

Then $|l_{ij}v_iv_j| < 3\,|\dot{\Omega}|\,(u_0^2 - 1)$.

From Eq. (3.15), we have

$$\tfrac{1}{2}(u_0^2)^{\cdot} = [1 - P'(u_0^2 - 1)/u_0^2]^{-1} \times [-l_{ij}v_iv_j - 3P'(u_0^2 - 1)\dot{\Omega}]. \tag{A6}$$

Suppose $\dot{\Omega} < 0$; then, using Eq. (A5), we find

$$\tfrac{1}{2}(u_0^2)^{\cdot} > 3\dot{\Omega}u_0^2[u_0^2 - P'(u_0^2 - 1)]^{-1} \times [u_0^2 - 1 - P'(u_0^2 - 1)] \tag{A7a}$$

$$= 3\dot{\Omega}u_0^2\{1 - [u_0^2 - P'(u_0^2 - 1)]^{-1}\} \tag{A7b}$$

$$> 3\dot{\Omega}u_0^2, \tag{A7c}$$

since the right side of (A7b) is negative. Hence, dividing by $\dot{\Omega} < 0$, we find $du_0^2/d\Omega < 6u_0^2$, or

$$|u_0| < KR^{-3} \tag{A8}$$

near the singularity, for some constant K. (The same result is found, of course, if one assumes $\dot{\Omega} > 0$.) With this, we have

$$Q[\rho] = M/(R^3u_0) > M/(R^3KR^{-3}) > 0, \tag{A9}$$

so ρ does not vanish as $R \to 0$.

To get some information about the behavior of the metric, we make use of the R_{00} equation (see Hawking[12]). Using the T_{00} equation (1.5) to eliminate $\sigma_{ij}\sigma_{ij}$, it reads

$$3(\dot{R}/R)^{\cdot} = -9(\dot{R}/R)^2 + 2\rho_g V_g + \{(\rho + p)u_0^2 + \tfrac{1}{2}\rho - \tfrac{5}{2}p\} - 2\rho_g. \tag{A10}$$

The bracket on the right is bounded below by

$$(\rho + p)(u_0^2 - 1) + \tfrac{3}{2}\gamma\rho > 0, \text{ where } 0 < P' < 1 - \gamma.$$

It is easy to see that this lower bound always dominates ρ_g near the origin $R = 0$. Thus we find

$$-3(\dot{R}/R)^{\cdot} < 9(\dot{R}/R)^2$$

or

$$\frac{d}{dt}\{(\dot{R}/R)^{-1}\} < 3.$$

Hence $3(\dot{R}/R) > t^{-1}$. (We take $t = 0$ to correspond to the singularity $R = 0$.) Therefore as $t \to 0$,

$$R^3 \propto t^{\nu}, \quad \nu > 1,$$

and

$$\frac{d}{dt}R^3 < H \text{ for some constant } H. \tag{A11}$$

The proof can now be given. As in the MSW dust proof, we shall prove by contradiction that ρ is unbounded. We shall thus assume that ρ is bounded above. To show the contradiction, we return to the T_{00} equation (1.5). For $R < R_\epsilon$, it gives

$$\frac{l_{ij}l_{ij}}{(3\dot{\Omega})^2} < 1 - \frac{2\rho u_0^2}{(3\dot{\Omega})^2}(1 - \epsilon). \tag{A12}$$

Now,

$$\rho u_0^2 = \{u_0Q^*[M/(R^3u_0)]\}^2\rho^{-1}$$

and, because of Eq. (A1), we have

$$Q^*[M/R^3u_0] = (M/R^3u_0)^{1+r}, \quad r > 0. \tag{A13}$$

Hence

$$(Q^*u_0)^2 = (M/R^3)^{2+2r}u_0^{-2r}. \tag{A14}$$

Suppose that $\epsilon < \frac{1}{2}$; then

$$\frac{l_{ij}l_{ij}}{(3\dot{\Omega})^2} < 1 - \frac{(M/R^3)^2(M/R^3u_0)^{2r}}{(3\dot{\Omega})^2\rho} = 1 - M^2\frac{(M/R^3u_0)^{2r}}{\rho}\left(\frac{dR^3}{dt}\right)^{-2}. \tag{A15}$$

Now Eq. (A9) shows $M/(R^3u_0)$ is bounded below, and we have just seen in Eq. (A11) that dR^3/dt is bounded above, near the singularity. Thus,

$$|l_{ij}|/|3\dot{\Omega}| < 1 - \eta, \tag{A16}$$

where $1 > \eta > 0$ is a fixed number.

With Eq. (A16) in place of Eq. (A5), the procedure used above to prove Eq. (A8) can now be used to show that

$$|u_0| < KR^{-3(1-\eta)}.$$

But this last inequality requires

$$\rho = Q^*\left[\frac{M}{R^3u_0}\right] > Q^*\left[\frac{M}{R^3KR^{-3}}R^{-3\eta}\right] \to \infty,$$

since

$$\frac{dQ^*[x]}{dx} > 0.$$

This contradicts the assumption that ρ is bounded.

The proof originally given by Shepley[2] showed that a singularity exists (although he did not specify the nature of the singularity as we have done here) so long as $(\rho + p) > 0$ at $R = 0$. Our discussion has been limited to a rather more restricted class of models, since we had to require $p < \rho$ and the invertability of Q. In addition, attention should eventually be given to nonadiabatic equations of state, since these are much more realistic from a physical point of view and allow dissipative mechanisms which may be extremely important in a thorough description of the universe.

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[1] C. W. Misner, Essay Submitted to the Gravity Foundation Competition (1967).
[2] L. C. Shepley, Ph.D. thesis, Princeton University, 1965.
[3] H. Flanders, *Differential Forms* (Academic Press, New York, 1963).
[4] C. W. Misner, J. Math. Phys. **4**, 924 (1963).
[5] A. H. Taub, Ann. Math. **53**, 472 (1951).
[6] J. Ehlers, Abhandl. Akad. Wiss. Mainz, No. 11 (1961).
[7] R. A. Matzner, L. C. Shepley, and James B. Warren, Ann. Phys. (N.Y.) **57**, 401 (1970). This paper will be referred to as "MSW" in the text.
[8] M. P. Ryan, Ph.D. thesis, University of Maryland, 1970.
[9] C. W. Misner, Phys. Rev. **186**, 1319 (1969). Note that these definitions differ by a factor of 2 from those in MSW.
[10] C. W. Misner, Phys. Rev. Letters **22**, 1071 (1969).
[11] C. W. Misner, Astrophys. J. **151**, 431 (1968).
[12] S. W. Hawking, Monthly Notices Roy. Astron. Soc. **142**, 127 (1969).
[13] R. A. Matzner, Talk at Stevens Institute of Technology Relativity Seminar, 1969.
[14] K. C. Jacobs, C. W. Misner, and H. S. Zapolsky, Lecture Notes, University of Maryland (1969).
[15] S. W. Hawking and G. F. R. Ellis, Phys. Letters **17**, 246 (1965).
[16] L. C. Shepley, Phys. Letters **28**, 695 (1968).
[17] L. C. Shepley, *Homogeneous Cosmologies* (Princeton U.P., Princeton, N.J., to appear).

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Complex 2-Dimensional Internal Space in General Relativity*

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A calculus of vectors in 2-dimensional symplectic spaces is developed from the concept of existence of local basis systems. The similarities, as well as the differences, of this calculus with the tetrad formulation of 4-dimensional curved spaces are discussed. The affinity and curvature of the symplectic space are derived and its relationships with the affinity and curvature of the usual spinor formalism are given. A system of hybrid geometrical objects displaying a tensor and a spinor index take over the role of the usual Hermitian matrices $\sigma_{\mu}^{K\dot{M}}(x)$.

INTRODUCTION

The use of basis systems in the spinor calculus was suggested in connection with its applications to the theory of special relativity.[1] Presently, we extend the applicability of this concept to spaces with curvature. In this way, it is possible to construct, in the 2-dimensional complex spaces with skew-symmetric metrics, a formalism of local basis systems which displays several similarities with the tetrad formulation on curved manifolds. The term complex 2-legs is used for characterizing the geometrical objects which correspond to the tetrad in 4-dimensional spaces.

However, the geometrical object which corresponds formally to the tetrad in the usual formalism is not the complex 2-leg but, instead, a linear combination of these components. Such a combination involves a spinor and a tensor index. From the point of view of the 4-dimensional space, such an object behaves as a set of four null complex vectors.

The notation used in this paper follows the usual conventions of the tetrad calculus, denoting local degrees of freedom by means of the same letter as the "coordinate" index, but inside a bracket. Here, both types of indices are spinor indices so that the above term "coordinate index" is purely formal. All types of spinor indices are denoted by capital Latin letters. Indices corresponding to the 4-dimensional space are denoted by Greek letters.

1. RECIPROCAL BASIS SYSTEM IN S_2

Let S_2 be a 2-dimensional symplectic space, that is, a linear vector space over the field of the complex numbers in which there exists a nondegenerate skew-symmetric bilinear inner product. Explicitly, given u, $v \in S_2$ and α a complex number, we have the following axioms:

$$u \cdot v = -v \cdot u,$$

$$(\alpha u) \cdot v = \alpha u \cdot v, \quad u \cdot (\alpha v) = \alpha(u \cdot v),$$

$$(u + v) \cdot w = u \cdot w + v \cdot w,$$

$$u \cdot (v + w) = u \cdot v + u \cdot w,$$

$$u \cdot v = 0, \quad \text{for all} \quad v \in S_2, \quad \text{implies} \quad u = 0.$$

We introduce into S_2 a system of basis vectors $h_{(1)}$ and $h_{(2)}$ such that

$$h_{(1)} \cdot h_{(2)} = 1. \tag{1}$$

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[7] R. A. Matzner, L. C. Shepley, and James B. Warren, Ann. Phys. (N.Y.) **57**, 401 (1970). This paper will be referred to as "MSW" in the text.
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[15] S. W. Hawking and G. F. R. Ellis, Phys. Letters **17**, 246 (1965).
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$$u \cdot v = -v \cdot u,$$

$$(\alpha u) \cdot v = \alpha u \cdot v, \quad u \cdot (\alpha v) = \alpha(u \cdot v),$$

$$(u + v) \cdot w = u \cdot w + v \cdot w,$$

$$u \cdot (v + w) = u \cdot v + u \cdot w,$$

$$u \cdot v = 0, \quad \text{for all} \quad v \in S_2, \quad \text{implies} \quad u = 0.$$

We introduce into S_2 a system of basis vectors $h_{(1)}$ and $h_{(2)}$ such that

$$h_{(1)} \cdot h_{(2)} = 1. \tag{1}$$

In this paper, we use explicitly the index notation since this is important for our purposes, as will become clear during the treatment. The realization of the above relations in this notation is obtained by introducing a skew-symmetric ϵ_{AB}, playing the same role as the symmetric metric tensor in 4-dimensional space:

$$u \cdot v = \epsilon_{AB} u^A v^B = u_B v^B. \tag{2}$$

The quantities $h_{(1)}$ and $h_{(2)}$ have contravariant indices,

$$h_{(A)} = (h^B_{(A)}),$$

but they may also be given covariant indices according to

$$h_{B(R)} = h^A_{(R)} \epsilon_{AB}.$$

Relation (1) then reads as

$$h_{(1)} \cdot h_{(2)} = \epsilon_{AB} h^A_{(1)} h^B_{(2)} = h_{B(1)} h^B_{(2)} = 1.$$

A reciprocal basis system may be introduced as the set of two vectors of S_2 which satisfy

$$h^{(A)} \cdot h_{(B)} = -h_{(B)} \cdot h^{(A)} = \delta^{(A)}_{(B)}; \tag{3}$$

that is, we have

$$h^{(1)}_A = -h_{A(2)}, \tag{4a}$$

$$h^{(2)}_A = h_{A(1)}. \tag{4b}$$

It is possible to construct a unimodular matrix with the components of the vectors $h_{(1)}$ and $h_{(2)}$,

$$M = \begin{pmatrix} h^1_{(1)} & h^1_{(2)} \\ h^2_{(1)} & h^2_{(2)} \end{pmatrix}, \tag{5}$$

since

$$|M| = h_{(1)} \cdot h_{(2)} = 1.$$

Note that

$$h_{1(A)} = -h^2_{(A)}, \quad h_{2(A)} = h^1_{(A)}. \tag{6}$$

As a result of (1), (4), and (6), we get

$$h^A_{(1)} h^{(1)}_B + h^A_{(2)} h^{(2)}_B = \delta^A_B. \tag{7}$$

The inverse matrix of (5) is

$$M^{-1} = \begin{pmatrix} h^2_{(2)} & -h^1_{(2)} \\ -h^2_{(1)} & h^1_{(1)} \end{pmatrix} = \begin{pmatrix} h^{(1)}_1 & h^{(1)}_2 \\ h^{(2)}_1 & h^{(2)}_2 \end{pmatrix}. \tag{8}$$

It should be noted that

$$h^A_{(1)} = \begin{pmatrix} h^1_{(1)} \\ h^2_{(1)} \end{pmatrix} = \begin{pmatrix} h_{2(1)} \\ -h_{1(1)} \end{pmatrix},$$

$$h^{(1)}_A = \begin{pmatrix} h^{(1)}_1 \\ h^{(1)}_2 \end{pmatrix} = \begin{pmatrix} -h_{1(2)} \\ -h_{2(2)} \end{pmatrix} = \begin{pmatrix} h^2_{(2)} \\ -h^1_{(2)} \end{pmatrix},$$

$$h^A_{(2)} = \begin{pmatrix} h^1_{(2)} \\ h^2_{(2)} \end{pmatrix} = \begin{pmatrix} h_{2(2)} \\ -h_{1(2)} \end{pmatrix},$$

$$h^{(2)}_A = \begin{pmatrix} h^{(2)}_1 \\ h^{(2)}_2 \end{pmatrix} = \begin{pmatrix} h_{1(1)} \\ h_{2(1)} \end{pmatrix} = \begin{pmatrix} -h^2_{(1)} \\ h^1_{(1)} \end{pmatrix}.$$

Since the $h_{(A)}$ and the $h^{(A)}$ are basis vectors, we have, for any vector of S_2,

$$u = u^{(A)} h_{(A)} = u_{(A)} h^{(A)}, \tag{9}$$

where

$$u^{(A)} = h^{(A)} \cdot u,$$

$$u_{(A)} = u \cdot h_{(A)}.$$

In index notation, for u a contravariant vector, these relations read

$$u^A = u^{(B)} h^A_{(B)} = u_{(B)} h^{(B)A}, \tag{10}$$

$$u^{(A)} = h^{(A)}_B u^B, \tag{11}$$

$$u_{(A)} = h^B_{(A)} u_B. \tag{12}$$

As is clear from the foregoing, all vector indices are raised and lowered by the skew-symmetric matrices ϵ^{AB} and ϵ_{AB} which are given by

$$\epsilon^{AB} = \epsilon_{AB} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

and all indices between brackets, denoting the different elements of the basis, are raised and lowered by means of the skew-symmetric matrices $\epsilon^{(A)(B)}$ and $\epsilon_{(A)(B)}$, with matrix elements

$$\epsilon^{(A)(B)} = \epsilon_{(A)(B)} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

We may interpret the matrices $\epsilon^{(A)(B)}$ and $\epsilon_{(A)(B)}$ as the operators which transform the basis $h_{(B)}$ into the reciprocal basis $h^{(B)}$, and vice versa:

$$h^{(B)}_C = \epsilon^{(B)(M)} h_{(M)C}, \tag{13}$$

$$h_{(B)C} = \epsilon_{(M)(B)} h^{(M)}_C. \tag{14}$$

These equations may be written in the free-index notation as

$$h^{(B)} = \epsilon^{(B)(M)} h_{(M)},$$

$$h_{(B)} = \epsilon_{(M)(B)} h^{(M)}.$$

Multiplying the first on the left-hand side by $h^{(N)}$, and the second on the left-hand side by $h_{(N)}$, we obtain

$$\epsilon^{(B)(N)} = h^{(N)} \cdot h^{(B)}, \tag{15}$$

$$\epsilon_{(B)(N)} = h_{(N)} \cdot h_{(B)}, \tag{16}$$

from which follow the matrix elements of the previous equation. Similarly, we obtain

$$\epsilon^{BM} = h^M_{(A)} h^{B(A)} = -h^{M(A)} h^B_{(A)}, \tag{17}$$

$$\epsilon_{BM} = h_{M(A)} h^{(A)}_B = -h^{(A)}_M h_{B(A)}, \tag{18}$$

which give the matrix elements written before. It should be noted that Eq. (7), which was used in the proof of (17), may be written in two forms which

differ by a sign:

$$h^A_{(K)}h^{(K)}_B = -h^{A(K)}h_{(K)B} = \delta^A_B.$$

We can present Eqs. (15) and (16) and, similarly, (17) and (18), using again the fact that the ϵ_{AB} and the ϵ^{AB} lower and raise vector indices, in the form

$$\epsilon^{(B)(M)} = h^{(M)}_A h^{(B)}_R \epsilon^{AR}, \tag{19a}$$

$$\epsilon_{(B)(M)} = h^A_{(M)} h^R_{(B)} \epsilon_{AR}, \tag{19b}$$

$$\epsilon^{BM} = h^M_{(A)} h^B_{(R)} \epsilon^{(A)(R)}, \tag{19c}$$

$$\epsilon_{BM} = h^{(A)}_M h^{(R)}_B \epsilon_{(A)(R)}. \tag{19d}$$

Clearly, Eqs. (10)–(12) and (19) present the same behavior as the equations which define a set of tetrad vectors in 4-dimensional space. The only differences are that we deal here with an antisymmetric ϵ playing the role of a "metric tensor," and the $h_{(A)}$ and the $h^{(A)}$ are complex vectors with two components. We may call them "complex 2-legs" instead of tetrads.

2. AFFINITIES AND CURVATURE IN S_2

Following the usual method of tetrad calculus, we may interpret Eqs. (10) and (11) as defining two vector spaces spanned, respectively, by the basis vectors $h_{(A)}$ and h_A with components

$$h_{(A)} = (h_{(1)}, h_{(2)}),$$

$$h_{(1)} = \begin{pmatrix} h^1_{(1)} \\ h^2_{(1)} \end{pmatrix}, \quad h_{(2)} = \begin{pmatrix} h^1_{(2)} \\ h^2_{(2)} \end{pmatrix},$$

$$h_A = (h_1, h_2),$$

$$h_1 = \begin{pmatrix} h^{(1)}_1 \\ h^{(2)}_1 \end{pmatrix}, \quad h_2 = \begin{pmatrix} h^{(1)}_2 \\ h^{(2)}_2 \end{pmatrix}.$$

The elements of these vector spaces are the vectors $u = (u^A)$ and $u^* = (u^{(A)})$. In order to distinguish one from the other, we use the symbol * for the latter. In free-index notation, we have

$$u = u^{(A)} h_{(A)},$$

$$u^* = u^A h_A.$$

Therefore, we may define the covariant derivatives[2] of both u^A and $u^{(A)}$ by the usual method:

$$u^A_{;\mu} = u^A_{,\mu} + \Gamma^A_{\mu B} u^B, \tag{20}$$

$$u^{(A)}_{;\mu} = u^{(A)}_{,\mu} + \Lambda^{(A)}_{\mu(B)} u^{(B)}. \tag{21}$$

From Eq. (3), we obtain

$$h^{(A)}_{B;\mu} = -h^{(C)}_B h^D_{(C);\mu} h^{(A)}_D. \tag{22}$$

Thus, the vanishing of $h^A_{(B);\mu}$ is implied by the vanishing of $h^{(A)}_{B;\mu}$. We have

$$h^A_{(B);\mu} = h^A_{(B),\mu} + \Gamma^A_{\mu R} h^R_{(B)} - \Lambda^{(R)}_{\mu(B)} h^A_{(R)}. \tag{23}$$

Imposing the condition $h^A_{(B);\mu} = 0$, we can solve (23) for the Λ_μ. We find

$$\Lambda^{(R)}_{\mu(B)} = h^M_{(B)} h^{(R)}_A \Gamma^A_{\mu M} + h^{(R)}_A h^A_{(B),\mu}. \tag{24}$$

Formula (24) closely resembles the relations which exist between the affinity Γ_μ and the Christoffel symbols.[3] Indeed, the conditions which leads to those relationships, namely, $\sigma_{\mu;\nu} = 0$, are formally similar to our conditions $h^A_{(B);\mu} = 0$. In passing, we note that the condition that the $h^A_{(B)}$ are constant under covariant differentiation implies, through (22), that the internal metric components may be considered constant under the operation of covariant differentiation:

$$\epsilon^{AB}_{;\mu} = \epsilon_{AB;\mu} = 0, \tag{25a}$$

$$\epsilon^{(A)(B)}_{;\mu} = \epsilon_{(A)(B);\mu} = 0. \tag{25b}$$

This, in turn, implies that the two matrices $\Gamma_{\mu AB}$ and $\Lambda_{\mu(A)(B)}$ are symmetric. A direct inspection of (24) shows that this symmetry property is satisfied for Λ_μ, if Γ_μ is symmetric. The symmetry of Γ_μ can be obtained from its explicit representation in terms of the matrices σ_λ.[3]

Still, from (23), we may write

$$h^A_{(B),\mu} = -\Gamma^A_{\mu R} h^R_{(B)} + \Lambda^{(R)}_{\mu(B)} h^A_{(R)}. \tag{26}$$

Since the left-hand side of this equation is a gradient, the 4-dimensional curl of the right-hand side vanishes. This furnishes us with an integrability condition for the existence of solutions of (26). A direct calculation gives

$$S^{(K)}_{\mu\nu(B)} = h^{(K)}_A h^R_{(B)} P^A_{\mu\nu R}, \tag{27}$$

where

$$P^A_{\mu\nu R} = -\frac{\partial \Gamma^A_{\mu R}}{\partial x^\nu} - \frac{\partial \Gamma^A_{\nu R}}{\partial x^\mu} + \Gamma^A_{\nu S}\Gamma^S_{\mu R} - \Gamma^A_{\mu S}\Gamma^S_{\nu R}, \tag{28}$$

$$S^{(A)}_{\mu\nu(R)} = \frac{\partial \Lambda^{(A)}_{\mu(R)}}{\partial x^\nu} - \frac{\partial \Lambda^{(A)}_{\nu(R)}}{\partial x^\mu} + \Lambda^{(A)}_{\nu(S)}\Lambda^{(S)}_{\mu(R)} - \Lambda^{(A)}_{\mu(S)}\Lambda^{(S)}_{\nu(R)}. \tag{29}$$

But these geometrical objects are just the internal curvatures defined by

$$u^A_{;\mu\nu} - u^A_{;\nu\mu} = P^A_{\mu\nu B} u^B, \quad u^{(A)}_{;\mu\nu} - u^{(A)}_{;\nu\mu} = S^{(A)}_{\mu\nu(B)} u^{(B)},$$

and we have the result that $S^{(A)}_{\mu\nu(B)}$ is the projection of $P^A_{\mu\nu B}$ over the space of the vectors $u^{(A)}$, according to the usual relations of the tetrad calculus. (By tetrad

calculus, we mean the calculus of point-dependent basis systems in four dimensions.) Obviously, we could have obtained Eq. (27) by using (24), (28), and (29), but we feel that our present method is more elegant.

We finish this section by recalling that $\Lambda^{(A)}_{\mu(B)}$ and $S^{(A)}_{\mu\nu(B)}$ may be written in terms of the 4-dimensional objects $\{^{\mu}_{\nu\alpha}\}$ and $R_{\mu\nu\rho\sigma}$ by using the formulas which connect $\Gamma^{A}_{\mu B}$ and $P^{A}_{\mu\nu B}$ with $\{^{\mu}_{\nu\alpha}\}$ and $R_{\mu\nu\rho\sigma}$.

3. CONNECTION WITH THE METRIC IN 4-DIMENSIONAL SPACE

We may use the two vectors on S_2 defined by

$$J^A = h^A_{(1)}, \quad L^A = h^A_{(2)}. \tag{30}$$

According to condition (1), they satisfy

$$J \cdot L = J_A L^A = 1. \tag{31}$$

With the vectors J and L, we form the mixed quantities

$$K^A_\mu = \sigma^{A\dot{B}}_\mu J_{\dot{B}} = \sigma^{A\dot{B}}_\mu \bar{J}_B, \tag{32}$$

$$M^A_\mu = \sigma^{A\dot{B}}_\mu L_{\dot{B}} = \sigma^{A\dot{B}}_\mu \bar{L}_B, \tag{33}$$

where a bar over J_B and L_B means the complex conjugate of those quantities. The two separate relations (32) and (33) may be written in a column as

$$\phi^A_{(\dot{R})\mu} = \begin{pmatrix} \phi^A_{(\dot{1})\mu} \\ \phi^A_{(\dot{2})\mu} \end{pmatrix} = \begin{pmatrix} K^A_\mu \\ M^A_\mu \end{pmatrix} = \sigma^{A\dot{B}}_\mu \bar{h}_{B(R)}.$$

From (32) and (33), we get

$$K^A_{(\mu}K^B_{\nu)} = \sigma^{A\dot{R}}_{(\mu}\sigma^{B\dot{S}}_{\nu)} J_{\dot{R}}J_{\dot{S}}, \quad M^A_{(\mu}M^B_{\nu)} = \sigma^{A\dot{R}}_{(\mu}\sigma^{B\dot{S}}_{\nu)} \bar{L}_{\dot{R}}\bar{L}_{\dot{S}}, \tag{34}$$

$$K^A_{(\mu}M^B_{\nu)} = \sigma^{A\dot{R}}_{(\mu}\sigma^{B\dot{S}}_{\nu)} J_{\dot{R}}\bar{L}_{\dot{S}}. \tag{35}$$

Using the equations

$$\sigma^{\dot{R}}_{\mu B}\sigma^{B\dot{S}}_{\nu} + \sigma^{\dot{R}}_{\nu B}\sigma^{B\dot{S}}_{\mu} = 2g_{\mu\nu}\epsilon^{\dot{R}\dot{S}}, \tag{36}$$

for (34) and (35), we get

$$K_\mu \cdot K_\nu = -K_\nu \cdot K_\mu,$$
$$M_\mu \cdot M_\nu = -M_\nu \cdot M_\mu,$$
$$K_\mu \cdot M_\nu + K_\nu \cdot M_\mu = 2g_{\mu\nu}.$$

These equations show that $(K^A_\mu) = K_\mu$ and $(M^A_\mu) = M_\mu$ are a set of eight vectors of S_2. The symmetrized scalar product of the vector K_μ by the vector M_ν gives $2g_{\mu\nu}$ as a result. Multiplying (34) and (35) by $g^{\mu\nu}$, we obtain

$$K^\mu_A K^B_\mu = M^\mu_A M^B_\mu = 0, \tag{37}$$

$$K_{A\mu}M_{B\nu}g^{\mu\nu} = 2\epsilon_{AB}. \tag{38}$$

Equations (37) show that the M^μ_A and the K^μ_A are a set of 4-vectors of the 4-dimensional space with a null form. Each one of those vectors is a complex vector, so that we have, in all, four complex null vectors.

Finally, we may write

$$K^A_\mu = H^{(\alpha)}_\mu {}^0\sigma^{C\dot{S}}_\alpha \bar{J}_S, \tag{39}$$

$$M^A_\mu = H^{(\alpha)}_\mu {}^0\sigma^{C}_\alpha \bar{L}_S, \tag{40}$$

where the ${}^0\sigma_\alpha$ are the Pauli matrices for $\alpha = 1, 2, 3$ and the 2×2-identity matrix for $\alpha = 4$. The $H^{(\alpha)}_\mu$ are the tetrad components in 4-dimensional space, satisfying

$$H^{(\alpha)}_\mu H^{(\lambda)}_\nu {}^0g_{\alpha\lambda} = g_{\mu\nu}, \tag{41}$$

where ${}^0g_{\alpha\lambda}$ is the metric of special relativity.

From the definition (32), or similarly from (33), we may re-obtain directly the relationship between the curvature tensor $R^\lambda_{\mu\nu\alpha}$ and the $P^A_{\mu\nu B}$ as the integrability condition for the existence of solutions of

$$K^A_{\mu;\nu} = 0. \tag{42}$$

(This condition follows from $\sigma^{K\dot{M}}_{\mu;\nu} = 0$, together with our conditions $h^A_{(B);\nu} = 0$.) Indeed, from (42), we get

$$K^A_{\mu,\nu} = \begin{Bmatrix} \lambda \\ \mu\nu \end{Bmatrix} K^A_\lambda - \Gamma^A_{\nu R}K^R_\mu,$$

and the condition that $K^A_{\mu,\nu\beta} = K^A_{\mu,\beta\nu}$ gives as a result

$$R^\lambda_{\mu\nu\beta}K^A_\lambda + P^A_{\beta\nu R}K^R_\mu = 0.$$

After some calculation, using (32) again, we find

$$P^A_{\beta\nu B} = \tfrac{1}{4}R^\lambda_{\mu\beta\nu}\sigma^{A\dot{S}}_\lambda \sigma^\mu_{B\dot{S}}, \tag{43}$$

which is the well-known relationship between these two curvatures.[4]

4. THE RELATIONS WITH THE TETRAD FORMULATION IN THE 4-DIMENSIONAL SPACE

So far, we have established a calculus of local basis systems in S_2, with the same general properties of the tetrad calculus in 4-dimensional space. However, such similarities are only possible to a certain extent. In the usual tetrad calculus, the role of the metric is assumed by the tetrad. In our present formulation, the substitute for the metric is not the tetrad (or, more properly, the complex 2-legs), but a combination of these quantities, as is shown by Eqs. (32), (33), and (38). That is, the role of the metric is taken over by a set of hybrid quantities displaying a vector and a

spinor index. Such quantities are complex 4-vectors with a null norm, and are simultaneously vectors on the symplectic space. If we write

$$K_\mu^A = V_\mu^A + iJ_\mu^A,$$
$$M_\mu^A = F_\mu^A + iW_\mu^A,$$

we obtain, from (37),

$$V_A^\mu V_\mu^B - J_A^\mu J_\mu^B = 0,$$
$$V_A^\mu J_\mu^B + J_A^\mu V_\mu^B = 0,$$
$$F_A^\mu F_\mu^B - W_A^\mu W_\mu^B = 0,$$
$$W_A^\mu W_\mu^B + W_A^\mu W_\mu^B = 0,$$

which are relations limiting the total number of independent components in the K_μ^A and M_μ^A.

It is also interesting to note that we may construct a new set of null 4-vectors by taking the scalar product of the K_μ and the M_μ with the 2-legs

$$a_\mu = J \cdot K_\mu = \sigma_\mu^{A\dot{B}} J_A J_{\dot{B}},$$
$$b_\mu = L \cdot K_\mu = \sigma_\mu^{A\dot{B}} L_A J_{\dot{B}},$$
$$c_\mu = L \cdot M_\mu = \sigma_\mu^{A\dot{B}} L_A L_{\dot{B}}.$$

All those 4-vectors are null 4-vectors, since the matrices multiplying $\sigma_\mu^{A\dot{B}}$ in the above equations are singular Hermitian matrices.

We now establish the relation existing between the present formalism and the usual tetrad formalism. This relationship is established by means of formulas relating the curvatures of both formalisms.

Starting from (43), using the formula from the tetrad calculus which relates the Riemann tensor to the curvature in terms of tetrads and making use of the quantity $T_{\mu\nu(\beta)}^{(\alpha)}$, which is defined by

$$A_{;\mu\nu}^{(\alpha)} - A_{;\nu\mu}^{(\alpha)} = T_{\mu\nu(\beta)}^{(\alpha)} A^{(\beta)}$$

and which has the form

$$R_{\sigma\mu\nu}^{\rho} = H_{(\alpha)}^{\rho} H_\sigma^{(\beta)} T_{\mu\nu(\beta)}^{(\alpha)}, \tag{44}$$

we get

$$P_{\mu\nu R}^{A} = \tfrac{1}{4}\, {}^0\sigma^{\lambda A\dot{S}}\, {}^0\sigma_{\alpha\dot{S}R} T_{\mu\nu(\lambda)}^{(\alpha)}. \tag{45}$$

From (27), we have

$$P_{\mu\nu R}^{A} = h_{(C)}^{A} h_R^{(M)} S_{\mu\nu(M)}^{(C)}. \tag{46}$$

These last two equations allow us to express the cvrvature $S_{\mu\nu(M)}^{(C)}$ in terms of $T_{\mu\nu(\beta)}^{(\alpha)}$, which is the relation we want to obtain:

$$S_{\mu\nu(M)}^{(C)} = \tfrac{1}{4} h_A^{(C)} h_{(M)}^{B}\, {}^0\sigma^{\beta A\dot{S}}\, {}^0\sigma_{\alpha\dot{S}B} T_{\mu\nu(\beta)}^{(\alpha)}. \tag{47}$$

As we can show (see the Appendix),

$$h_A^{(B)}\, {}^0\sigma_\lambda^{A\dot{S}} = -M_{(\lambda)}^{(B)} \bar{J}^S + K_{(\lambda)}^{(B)} \bar{L}^S, \tag{48}$$

so that

$$S_{\mu\nu(M)}^{(C)} = \tfrac{1}{4}(K^{(C)(\beta)} M_{(M)(\alpha)} - M^{(C)(\beta)} K_{(M)(\alpha)}) T_{\mu\nu(\beta)}^{(\alpha)},$$

with

$$M^{(C)(\beta)} = {}^0g^{\beta\sigma} M_\sigma^{(C)},$$
$$M_{(M)(\alpha)} = M_{(\alpha)}^{(B)} \epsilon_{(B)(M)}.$$

Similar formulas hold for the $K^{(C)(B)}$ and $K_{(M)(\alpha)}$.

APPENDIX

From Eq. (32), by taking the projection on the 2-legs, we obtain

$$K_\mu^{(B)} = h_A^{(B)} K_\mu^A = h_A^{(B)} \sigma_\mu^{A\dot{R}} J_{\dot{R}},$$

which gives

$$K_\mu^{(B)} = h_A^{(B)}\, {}^0\sigma_\alpha^{A\dot{R}} H_\mu^{(\alpha)} \bar{h}_{R(1)}.$$

Thus,

$$K_{(\lambda)}^{(B)} = H_{(\lambda)}^{\mu} K_\mu^{(B)} = h_A^{(B)}\, {}^0\sigma_\lambda^{A\dot{R}} \bar{h}_{R(1)}. \tag{A1}$$

Similar calculations, starting with (33), give

$$M_{(\lambda)}^{(B)} = h_A^{(B)}\, {}^0\sigma_\lambda^{A\dot{R}} \bar{h}_{R(2)}. \tag{A2}$$

Multiplying (A1) by $\bar{h}^{S(1)}$ on the right-hand side and (A2) by $\bar{h}^{S(2)}$ (also on the right-hand side) and adding up both relations, we obtain

$$K_{(\lambda)}^{(B)} \bar{h}^{S(1)} + M_{(\lambda)}^{(B)} \bar{h}^{S(2)} = h_A^{(B)}\, {}^0\sigma_\lambda^{A\dot{R}} \bar{h}_{R(M)} \bar{h}^{S(M)}.$$

Since

$$h_{R(M)} h^{S(M)} = -\delta_R^S,$$

we get

$$h_A^{(B)}\, {}^0\sigma_\lambda^{A\dot{R}} = -(K_{(\lambda)}^{(B)} \bar{h}^{R(1)} + M_{(\lambda)}^{(B)} \bar{h}^{R(2)}); \tag{A3}$$

but

$$h^{R(1)} = \epsilon^{(1)(K)} h_{(K)}^R = -h_{(2)}^R = -L^R,$$
$$h^{R(2)} = \epsilon^{(2)(K)} h_{(K)}^R = h_{(1)}^R = J^R.$$

Therefore, (A3) takes the form of Eq. (48).

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[1] C. P. Luehr and M. Rosenbaum, J. Math. Phys. **9**, 2225 (1968).

[2] In this paper, we consider the structure of internal space from the point of view of general relativity, i.e., spaces with curvature.

[3] H. S. Ruse, Proc. Roy. Soc. (Edinburgh) **57**, 97 (1937); P. Bergmann, Phys. Rev. **107**, 624 (1957).

[4] C. G. Oliveira and C. Marcio do Amaral, Nuovo Cimento **47**, 9 (1967).

Solution of the Initial-Value Neutron-Transport Problem for a Slab with Infinite Reflectors*

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The initial-value transport problem of monoenergetic neutrons migrating in a thin slab surrounded by infinitely thick reflectors is solved for isotropic scattering by using the normal-mode expansion technique of Case. The results obtained indicate that the reflector may give rise to a branch-cut integral term typical of a semi-infinite medium while the central slab may contribute a summation over discrete residue terms. Exact expressions are obtained for these discrete time eigenvalues, and sample numerical results are presented showing the behavior of real time eigenvalues as a function of the material properties of the slab and reflector. In the limit of purely absorbing reflectors or a bare slab, the present solution has the properties which have been previously reported by others who used the approach of Lehner and Wing.

1. INTRODUCTION

A few time-dependent monoenergetic neutron-transport problems in plane geometry with isotropic scattering have been solved recently by applying Case's normal-mode expansion technique[1,2] to the equation which results when the time dependence has been removed by a Laplace transformation. This approach was used by Bowden[3,4] for his analysis of time-dependent 1-speed neutron transport in a bare slab of finite thickness, a problem which had been treated extensively by Lehner and Wing.[5,6] Another successful application of this technique was made by Kuščer and Zweifel[7] to the time-dependent 1-speed albedo problem for a semi-infinite medium. Such an approach has also been utilized in one two-media time-dependent problem by Erdmann,[8,9] who investigated the time decay of a plane isotropic burst of monoenergetic neutrons introduced at the interface of two dissimilar semi-infinite media. In all of these time-dependent solutions, contributions due to various parts of the spectrum of the transport operator have been indicated by suitably deforming the integration contour of the inverse Laplace transformation. This approach is used in this paper to analyze a simple idealized two-media problem in which one would expect to find discrete time eigenvalues and to obtain some insight concerning their behavior as a function of material properties.

To be specific, consider a slab of material which scatters neutrons isotropically, extends from $x = -a$ to $x = a$, and is characterized by the nuclear properties σ_2 and c_2. This uniform slab is surrounded by uniform infinitely thick reflectors of another material characterized by the properties σ_1 and c_1 (see Fig. 1). For a physically meaningful system, these reflectors should be nonmultiplying media since they extend to infinity. Therefore, we take $c_1 < 1$. For isotropic scattering of monoenergetic neutrons in a sourceless medium and plane geometry, the neutron angular flux $\psi(x, \mu, t)$ satisfies the equation[2]

$$\left(\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x} + \sigma(x)\right)\psi(x, \mu, t) = \tfrac{1}{2}c(x)\sigma(x)\int_{-1}^{1}\psi(x, \mu', t)\,d\mu', \quad (1.1)$$

where t is the neutron speed multiplied by the real time and x and μ are shown on Fig. 1, while $\sigma(x)$ and $c(x)$ are given by

$$\sigma(x), c(x) = \sigma_1, c_1, \quad \text{for} \quad |x| > a,$$
$$= \sigma_2, c_2, \quad \text{for} \quad |x| < a. \quad (1.2)$$

We seek the solution of this equation subject to the boundary conditions

$$\lim_{|x|\to\infty}\psi(\pm x, \mu, t) = 0 \quad (1.3)$$

and the continuity conditions

$$\psi(\pm a+, \mu, t) = \psi(\pm a-, \mu, t), \quad (1.4)$$

given the initial condition

$$\psi(x, \mu, 0) = f(x, \mu). \quad (1.5)$$

The latter we assume satisfies (1.3) and is extendable without poles or branch cuts in the finite μ plane except, perhaps, for a discontinuity across the imaginary axis. When the material properties of the reflectors are taken to be those of a vacuum or a pure absorber, this problem reduces to those rigorously analyzed by the Lehner and Wing approach.[5,6,10,11] Some preliminary results for the present problem

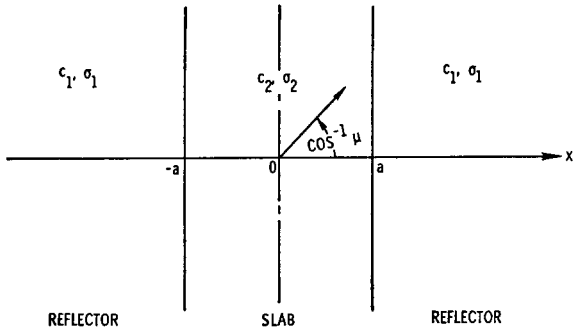

FIG. 1. Geometry of the problem.

were given in Ref. 12, while many details can be found in Ref. 13.

2. TIME REMOVAL AND ELEMENTARY SOLUTIONS

If we take the Laplace transformation of $\psi(x, \mu, t)$ as

$$\psi_s(x, \mu) = \int_0^\infty e^{-st}\psi(x, \mu, t)\, dt, \tag{2.1}$$

then the inverse transformation required to recover the t dependence is

$$\psi(x, \mu, t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{st}\psi_s(x, \mu)\, ds, \tag{2.2}$$

where γ is to the right of all singularities of $\psi_s(x, \mu)$ in the transform plane, that is, the s plane. It is expected that the path of integration in Eq. (2.2) can be deformed to indicate more precisely the character of $\psi(x, \mu, t)$. Since an arbitrary function of two variables $f(x, \mu)$ can be written as the sum of its even and odd parts, viz.,

$$f_\pm(x, \mu) = \tfrac{1}{2}[f(x, \mu) \pm f(-x, -\mu)], \tag{2.3}$$

then the symmetry of $c(x)$ and $\sigma(x)$ allows us to separate $\psi_s(x, \mu)$ into its even, $\psi_{s+}(x, \mu)$, and odd, $\psi_{s-}(x, \mu)$, parts, which can be treated separately and combined at any stage of the calculation. If we define $\psi_{j\pm}(x, \mu, s)$ and $f_{j\pm}(x, \mu)$, $j = 1, 2$, as

$$\begin{aligned}\psi_{s\pm}(x, \mu); f_\pm(x, \mu) &= \psi_{1\pm}(x, \mu, s); f_{1\pm}(x, \mu), \quad |x| > a,\\ &= \psi_{2\pm}(x, \mu, s); f_{2\pm}(x, \mu), \quad |x| < a,\end{aligned} \tag{2.4}$$

then Eqs. (1.1)–(1.5) become, under the transformation (2.1),

$$\left(\mu\frac{\partial}{\partial x} + s + \sigma_j\right)\psi_{j\pm}(x, \mu, s) = \tfrac{1}{2}c_j\sigma_j\int_{-1}^{1}\psi_{j\pm}(x, \mu', s)\, d\mu' + f_{j\pm}(x, \mu), \quad j = 1, 2, \tag{2.5}$$

$$\lim_{|x|\to\infty}\psi_{1\pm}(x, \mu, s) = 0, \tag{2.6}$$

and

$$\psi_{1\pm}(a, \mu, s) = \psi_{2\pm}(a, \mu, s). \tag{2.7}$$

The notation $g_{j\pm}(a, \mu)$ means the limit of $g_\pm(x, \mu)$ as $x \to a$ from medium j. Solutions of Eqs. (2.5) are obtained by constructing even and odd particular solutions $\psi_{jp\pm}(x, \mu, s)$ and adding to them solutions of the corresponding homogeneous equations $\psi_{jc\pm}(x, \mu, s)$, so that conditions (2.6) and (2.7) can be satisfied; i.e.,

$$\psi_{j\pm}(x, \mu, s) = \psi_{jc\pm}(x, \mu, s) + \psi_{jp\pm}(x, \mu, s), \quad j = 1, 2. \tag{2.8}$$

The functions $\psi_{jp\pm}$ and $\psi_{jc\pm}$ are constructed from Case's elementary solutions, which we denote here as $\psi_{j\nu}(x, \mu, s)$.

The elementary solutions $\psi_{j\nu}(x, \mu, s)$ are solutions of the homogeneous form of Eq. (2.5) in the form

$$\psi_{j\nu}(x, \mu, s) = \varphi_{js\nu}(\mu)e^{-(s+\sigma_j)x/\nu}, \tag{2.9}$$

where ν is a complex parameter introduced in this separation of variables and $\varphi_{js\nu}(\mu)$ is normalized as

$$\int_{-1}^{1}\varphi_{js\nu}(\mu)\, d\mu = s + \sigma_j. \tag{2.10}$$

Bowden[3,4] and Erdmann[8,9] have investigated the solutions $\varphi_{js\nu}(\mu)$ and show that they are given by

$$\varphi_{js\nu}(\mu) = \tfrac{1}{2}c_j\sigma_j\nu P(\nu - \mu)^{-1} + \lambda_{js}(\nu)\delta(\nu - \mu), \quad \nu \in (-1, +1), \tag{2.11}$$

where P denotes the Cauchy principal value, $\delta(\nu - \mu)$ is the Dirac δ function, and

$$\lambda_{js}(\nu) = s + \sigma_j - c_j\sigma_j\nu\tanh^{-1}\nu. \tag{2.12}$$

Two discrete solutions are

$$\varphi_{\pm\nu_{0j}}(\mu) = \frac{1}{2}\frac{c_j\sigma_j\nu_{0j}}{\nu_{0j} \mp \mu}, \quad s \in S_{ji}, \tag{2.13}$$

provided that the function

$$\Omega_{js}(z) = s + \sigma_j - c_j\sigma_j z\tanh^{-1} z^{-1} \tag{2.14}$$

of two complex variables s and z vanishes at the two points $\pm\nu_{0j}$. The condition for this to happen[3,4] is that s lie inside the curve C_j ($s \in S_{ji}$; see Fig. 2) defined by

$$C_j = \left\{\frac{s + \sigma_j}{c_j\sigma_j} = \alpha' + i\beta' \,\middle|\, \alpha' = \frac{2\beta'}{\pi}\tanh^{-1}\left(\frac{2\beta'}{\pi}\right)\right\}. \tag{2.15}$$

We note that ν_{0j} is an analytic function of s for $s \in S_{ji}$, except for a branch cut on the real s axis between

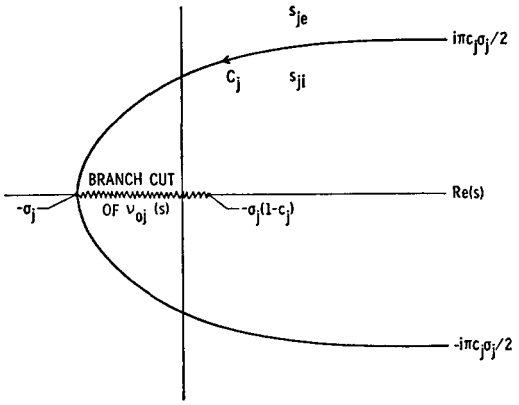

FIG. 2. Regions in a single-medium s plane. Location of Im (s) axis depends on whether $c_j \gtrless 1$.

$-\sigma_j$ and $-\sigma_j(1-c_j)$, and have denoted by $+\nu_{0j}$ that zero of $\Omega_{js}(z)$ for which $\mathrm{Re}\,(\nu_{0j}) > 0$, $s \notin [-\sigma_j, -\sigma_j(1-c_j)]$. The important result is that the general solution of the homogeneous form of Eq. (2.5) can be expressed as the linear combination

$$\psi_j(x,\mu,s) = [a_j\psi_{\nu_{0j}}(x,\mu,s) + b_j\psi_{-\nu_{0j}}(x,\mu,s)]\delta_j(s) + \int_{-1}^{1} A_j(\nu)\psi_{j\nu}(x,\mu,s)\,d\nu, \quad (2.16)$$

where we define $\delta_j(s)$ as

$$\delta_j(s) \equiv 1, \quad s \in S_{ji}, \qquad \equiv 0, \quad s \in S_{je}, \quad (2.17)$$

and the s dependence of the expansion coefficients has not been indicated. To avoid confusion with our notation, $\pm$ for parity, the customary notation for the discrete modes has not been used.

3. CONSTRUCTION OF TRANSFORMED SOLUTION

The expression (2.16) is the general solution of the homogeneous form of Eq. (2.5), but it does not have definite parity. For the slab which is symmetric about $x = 0$, $\psi_{2c\pm}(x,\mu,s)$ can be formed as

$$\psi_{2c\pm}(x,\mu,s) = a_{2\pm}[\psi_{\nu_{02}}(x,\mu,s) \pm \psi_{-\nu_{02}}(x,\mu,s)]\delta_2(s) + \int_0^1 A_{2\pm}(\nu)[\psi_{2\nu}(x,\mu,s) \pm \psi_{2(-\nu)}(x,\mu,s)]\,d\nu. \quad (3.1)$$

For the reflectors which extend to infinity, the boundary condition (2.6) requires half of the coefficients in Eq. (2.16) to vanish when $\mathrm{Re}\,(s) > -\sigma_1$. The remaining coefficients in the right reflector are related to those in the left by using the continuity condition (2.7) and the parity of $\psi_{2c\pm}(x,\mu,s)$. We have

$$\psi_{1c\pm}(x,\mu,s) = a_{1\pm}\psi_{-\nu_{01}}(x,\mu,s)\delta_1(s) + \int_0^1 A_{1\pm}(-\nu)\psi_{1(-\nu)}(x,\mu,s)\,d\nu, \quad x < -a,$$
$$= \pm a_{1\pm}\psi_{\nu_{01}}(x,\mu,s)\delta_1(s) \pm \int_0^1 A_{1\pm}(-\nu)\psi_{1\nu}(x,\mu,s)\,d\nu, \quad x > a, \quad (3.2)$$

for $\mathrm{Re}\,(s) - \sigma_1$.

As can be seen by direct substitution, explicit forms of $\psi_{2p\pm}$ and $\psi_{1p\pm}$ can be written as

$$\psi_{2p\pm}(x,\mu,s) = [F_{2\pm}(x,\nu_{02},s)\psi_{\nu_{02}}(x,\mu,s) \pm F_{2\pm}(-x,\nu_{02},s)\psi_{-\nu_{02}}(x,\mu,s)]\delta_2(s) + \int_0^1 F_{2\pm}(x,\nu,s)\psi_{2\nu}(x,\mu,s)\,d\nu \pm \int_0^1 F_{2\pm}(-x,\nu,s)\psi_{2(-\nu)}(x,\mu,s)\,d\nu \quad (3.3)$$

and

$$\psi_{1p\pm}(x,\mu,s) = \{\pm[-\tilde{F}_{\pm}(-a,\nu_{01},s) + F_{1\pm}(-x,-\nu_{01},s)]\psi_{\nu_{01}}(x,\mu,s) \pm F_{1\pm}(-x,\nu_{01},s)\psi_{-\nu_{01}}(x,\mu,s)\}\delta_1(s) \pm \int_0^1 [-\tilde{F}_{\pm}(-a,\nu,s) + F_{1\pm}(-x,-\nu,s)]\psi_{1\nu}(x,\mu,s)\,d\nu \pm \int_0^1 F_{1\pm}(-x,\nu,s)\psi_{1(-\nu)}(x,\mu,s)\,d\nu, \quad x > a, \quad (3.4)$$

for $\mathrm{Re}\,(s) > -\sigma_1$, with a similar expression for $\psi_{1p\pm}(x,\mu,s)$, $x < -a$. Here,

$$\tilde{F}_{\pm}(-a,\omega,s) \equiv F_{1\pm}(-a,-\omega,s) \mp F_{1\pm}(-a,\omega,s) \quad (3.5a)$$

and

$$F_{j\pm}(x,\omega,s) \equiv \int_{l(j)}^{x} C_{j\pm}(x_0,\omega)e^{(s+\sigma_j)x_0/\omega}\,dx_0, \quad (3.5b)$$

with

$$l(1) = -\infty \quad \text{and} \quad l(2) = -a, \quad (3.6)$$

while the $C_{j\pm}$ are full-range expansion coefficients of the function $f_{j\pm}(x,\mu)/\mu$ (e.g., see Ref. 4).

The solutions in medium 1, $|x| > a$, have been constructed so that the boundary condition (2.6) is satisfied. If we substitute $x = a$ in Eq. (2.8), apply the continuity condition (2.7), and use the explicit forms of $\psi_{jc\pm}$ given by Eqs. (3.1) and (3.2), we obtain a two-media full-range expansion involving the $\varphi_{js\nu}$

which contains unknown coefficients $a_{j\pm}$ and $A_{j\pm}$. The same expansion is, of course, obtained for $x = -a$. Erdmann[8] proved completeness theorems which apply in two-media expansions in time-dependent problems while Kuščer, McCormick, and Summerfield[14] derived orthogonality relations which are applicable to two-media expansions in time-*independent* problems. Their results are easily extended to obtain orthogonality relations in forms which are valid for all regions of the transform plane. As usual in problems involving a slab, we cannot obtain closed form solutions for the expansion coefficients. The continuum coefficients $A_{2\pm}(\nu)$ are given as the solutions of Fredholm integral equations, and all of the other coefficients are obtained from the $A_{2\pm}(\nu)$. Bowden, McCrosson, and Rhodes[15] have shown how the normal-mode expansion coefficients such as $A_j(\nu)$ in Eq. (2.16) are related to a function which can be extended to the complex plane ($\nu \to z'$). More specifically, we define

$$E_{2\pm}(\nu, s) \equiv A_{2\pm}(\nu)\Omega_{2s}^{+}(\nu)\Omega_{2s}^{-}(\nu)e^{(s+\sigma_2)a/\nu} \tag{3.7a}$$

and

$$E_{1\pm}(\nu, s) \equiv A_{1\pm}(-\nu)\Omega_{1s}^{+}(\nu)\Omega_{1s}^{-}(\nu)e^{-(s+\sigma_1)a/\nu}, \tag{3.7b}$$

where

$$\Omega_{js}^{\pm}(\nu) = \lambda_{js}(\nu) \pm \tfrac{1}{2}i\pi c_j\sigma_j\nu, \quad -1 \leq \nu \leq 1, \tag{3.8}$$

are the limiting values of the function $\Omega_{js}(z)$ of Eq. (2.14) on the real z axis $(-1, 1)$. Throughout, we use $+$ and $-$ superscripts to denote the limiting values of a function on its branch cut as the argument approaches the cut from the upper $(+)$ and lower $(-)$ half-planes. We use orthogonality relations and obtain the following list of equations for Re $(s) > -\sigma_m$:

$$E_{2\pm}(z, s) = I_{2\pm}(z, s) \pm \frac{k_s}{c_2\sigma_2}\frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)}\frac{X_0(-z, s)}{2\pi i} \times \int_{C'} \frac{E_{2\pm}(z', s)X_0(-z', s)e^{-2(s+\sigma_2)a/z'}}{\Omega_{2s}(z')(z' + z)}\, dz', \tag{3.9}$$

$$E_{1\pm}(z, s) = I_{1\pm}(z, s) \pm \frac{c_1\sigma_1}{c_2\sigma_2}E_{2\pm}(z, s)e^{-2(s+\sigma_2)a/z} \mp \frac{k_s}{c_2\sigma_2X_0(-z, s)2\pi i} \times \int_{C'} \frac{E_{2\pm}(z', s)X_0(-z', s)e^{-2(s+\sigma_2)a/z'}}{\Omega_{2s}(z')(z' - z)}\, dz', \tag{3.10}$$

$$I_{2\pm}(z, s) = \frac{c_2\sigma_2}{c_1\sigma_1}L_{1\pm}(-a, z, s) + \left(\frac{k_s}{2\pi i}\frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)}X_0(-z, s)\right) \times \left(\pm\int_{C'} \frac{L_{2\pm}(a, z', s)X_0(-z', s)}{c_2\sigma_2\Omega_{2s}(z')(z' + z)}\, dz' + \frac{\Omega_{1s}(\infty)}{\Omega_{2s}(\infty)}\int_{C'} \frac{L_{1\pm}(-a, z', s)\, dz'}{c_1\sigma_1X_0(-z', s)\Omega_{1s}(z')(z' - z)}\right), \tag{3.11}$$

and

$$I_{1\pm}(z, s) = \mp L_{1\pm}(-a, z, s)e^{-2(s+\sigma_1)a/z} \pm \frac{c_1\sigma_1}{c_2\sigma_2}L_{2\pm}(a, z, s) - \left(\frac{k_s}{2\pi iX_0(-z, s)}\right) \times \left(\pm\int_{C'} \frac{L_{2\pm}(a, z', s)X_0(-z', s)}{c_2\sigma_2\Omega_{2s}(z')(z' - z)}\, dz' + \frac{\Omega_{1s}(\infty)}{\Omega_{2s}(\infty)}\int_{C'} \frac{L_{1\pm}(-a, z', s)\, dz'}{c_1\sigma_1X_0(-z', s)\Omega_{1s}(z')(z' + z)}\, dz'\right), \tag{3.12}$$

where, for Re $(s) > -\sigma_j$,

$$L_{j\pm}(x, z, s) = \int_{l(j)}^{x} e^{-(s+\sigma_j)(x-x_0)/z}\left(\tfrac{1}{2}c_j\sigma_j\int_0^1 f_{j\pm}(x_0, -\mu)\frac{d\mu}{\mu + z} - \tfrac{1}{2}c_j\sigma_j\int_0^1 f_{j\pm}(x_0, \mu)\frac{d\mu}{\mu - z} + \frac{1}{z}f_{j\pm}(x_0, z)\Omega_{js}(z)\right) dx_0, \tag{3.13}$$

with $l(j)$ given by Eq. (3.6). In the above equations, z does not lie outside the contour C' which encircles ν_{0j} as shown in Fig. 3, and σ_m is defined as

$$\sigma_m \equiv \min(\sigma_1, \sigma_2). \tag{3.14}$$

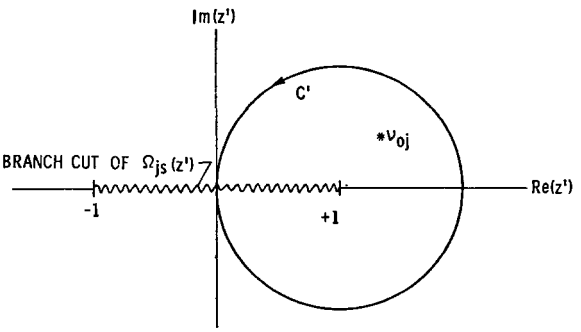

FIG. 3. The contour C' in the z' plane.

The restriction Re $(s) > -\sigma_m$ is discussed in the next section. The $L_{j\pm}$ functions were introduced as

$$L_{j\pm}(x, \nu, s) = F_{j\pm}(x, \nu, s)\Omega_{js}^{+}(\nu)\Omega_{js}^{-}(\nu)e^{-(s+\sigma_j)x/\nu}, \quad 0 \leq \nu \leq 1. \quad (3.15)$$

In addition, we have used the X_{0j} functions which, as Kuščer and Zweifel[7] have shown, are continuous across the curves C_j in the s plane (see Fig. 2). For two material media, we take the ratio of their single-medium X_{0j} functions,

$$X_0(z, s) = X_{02}(z, s)/X_{01}(z, s), \quad (3.16)$$

where

$$X_{0j}(z, s) = (\nu_{0j} - z)X_{js}(z), \quad s \in S_{ji}, \\ = (1 - z)X_{js}(z), \quad s \in S_{je}, \quad (3.17)$$

and

$$X_{js}(z) = \frac{1}{1 - z} \exp\left[\frac{1}{2\pi i}\int_0^1 \ln\left(\frac{\Omega_{js}^{+}(\nu)}{\Omega_{js}^{-}(\nu)}\right)\frac{d\nu}{\nu - z}\right]. \quad (3.18)$$

For Re $(z) < 0$, $X_0(z, s)$ given by Eq. (3.16) is a non-vanishing analytic function of z and s provided that $s \notin [-\sigma_j, -\sigma_j(1 - c_j)]$, the branch cuts of $\nu_{0j}(s)$, $j = 1, 2$. The quantity

$$k_s = s(c_1\sigma_1 - c_2\sigma_2) + \sigma_1\sigma_2(c_1 - c_2) \quad (3.19)$$

is related to the difference between medium 1 and medium 2 continuum solutions.

Noting that, if $s \in S_{ji}$, then $[\Omega_{js}(z)]^{-1}$ has a pole at $z = \nu_{0j}$ whose residue leads to a discrete term, we obtain the usual expressions for $E_{j\pm}(\nu, s)$, $\nu \in (0, 1)$ [and hence $A_{j\pm}(\nu)$], when the contour C' is collapsed onto the branch cut $(0, 1)$. When $s \in S_{je}$, $\Omega_{js}(z)$ does not vanish. The discrete coefficients $a_{j\pm}$ are obtained from

$$E_{2\pm}(\nu_{02}, s) = \tfrac{1}{2}c_2\sigma_2\nu_{02}\Omega_{2s}'(\nu_{02})e^{(s+\sigma_2)a/\nu_{02}}a_{2\pm}, \quad s \in S_{2i}, \quad (3.20a)$$

and

$$E_{1\pm}(\nu_{01}, s) = \tfrac{1}{2}c_1\sigma_1\nu_{01}\Omega_{1s}'(\nu_{01})e^{-(s+\sigma_1)a/\nu_{01}}a_{1\pm}, \quad s \in S_{1i}, \quad (3.20b)$$

where

$$\Omega_{js}'(z) = \frac{d}{dz}\,\Omega_{js}(z). \quad (3.21)$$

The solutions $\psi_{jc\pm}(x, \mu, s)$ and $\psi_{jp\pm}(x, \mu, s)$ can now be written similarly as

$$\psi_{2c\pm}(x, \mu, s) = \frac{1}{2\pi i}\left(\int_{C'} \frac{E_{2\pm}(z', s)e^{-(s+\sigma_2)(a+x)/z'}}{\Omega_{2s}(z')(z' - \mu)}\,dz' \pm \int_{C'} \frac{E_{2\pm}(z', s)e^{-(s+\sigma_2)(a-x)/z'}}{\Omega_{2s}(z')(z' + \mu)}\,dz'\right), \quad |x| < a, \quad (3.22)$$

for Re $(s) > -\sigma_m$,

$$\psi_{1c\pm}(x, \mu, s) = \frac{1}{2\pi i}\int_{C'} \frac{E_{1\pm}(z', s)e^{(s+\sigma_1)(x+a)/z'}}{\Omega_{1s}(z')(z' + \mu)}\,dz', \quad x < -a, \\ = \frac{\pm 1}{2\pi i}\int_{C'} \frac{E_{1\pm}(z', s)e^{-(s+\sigma_1)(x-a)/z'}}{\Omega_{1s}(z')(z' - \mu)}\,dz', \quad x > a, \quad (3.23)$$

for Re $(s) > -\sigma_m$,

$$\psi_{2p\pm}(x, \mu, s) = \frac{1}{2\pi i}\left(\int_{C'} \frac{L_{2\pm}(x, z', s)}{\Omega_{2s}(z')(z' - \mu)}\,dz' \pm \int_{C'} \frac{L_{2\pm}(-x, z', s)}{\Omega_{2s}(z')(z' + \mu)}\,dz'\right), \quad |x| < a, \quad (3.24)$$

for Re $(s) > -\sigma_2$, and

$$\psi_{1p\pm}(x, \mu, s) = \frac{1}{2\pi i}\left(\int_{C'} \frac{L_{1\pm}(x, z', s)}{\Omega_{1s}(z')(z' - \mu)}\,dz' + \int_{C'} \frac{M_{\pm}(x, z', s) \pm L_{1\pm}(-a, z', s)e^{-(s+\sigma_1)(a-x)/z'}}{\Omega_{1s}(z')(z' + \mu)}\,dz'\right), \quad x < -a, \\ = \frac{1}{2\pi i}\left(\int_{C'} \frac{L_{1\pm}(-a, z', s)e^{-(s+\sigma_1)(a+x)/z'} \pm M_{\pm}(x, z', s)}{\Omega_{1s}(z')(z' - \mu)}\,dz' \pm \int_{C'} \frac{L_{1\pm}(-x, z', s)}{\Omega_{1s}(z')(z' + \mu)}\,dz'\right), \quad x > a, \quad (3.25)$$

for Re $(s) > -\sigma_1$. The functions $M_{\pm}(x, z, s)$ are also integrations over the initial distribution $f_{1\pm}(x, \mu)$ and are given by

$$M_{\pm}(x, z, s) = \int_{-|x|}^{-a} e^{-(s+\sigma_1)(|x|+x_0)/z}\left(\tfrac{1}{2}c_1\sigma_1\int_0^1 f_{1\pm}(x_0, \mu)\frac{d\mu}{\mu + z} - \tfrac{1}{2}c_1\sigma_1\int_0^1 f_{1\pm}(x_0, -\mu)\frac{d\mu}{\mu - z} + \frac{1}{z}f_{1\pm}(x_0, -z)\Omega_{1s}(z)\right)dx_0, \quad |x| > a, \quad (3.26)$$

for Re $(s) > -\sigma_1$ and z not outside C'. Again, the discrete and continuum terms which appear in Eqs. (3.1)–(3.4) are due to the zeros and branch cuts of $\Omega_{js}(z)$ which appear in the integrands of Eqs. (3.22)–(3.25).

4. PROPERTIES OF TRANSFORMED SOLUTION

Analytic properties of $\psi_{s\pm}(x, \mu)$ as a function of s must be investigated before we can recover the time-dependent solution $\psi(x, \mu, t)$ according to the

inverse Laplace transformation given by Eq. (2.2). We need to know the behavior of $\psi_{s\pm}$ in some right half s plane. First note that, for arbitrary initial distributions $f(x, \mu)$, $\psi_{s\pm}(x, \mu)$ is not analytic for Re $(s) < -\sigma_m$. This is true since each of the inhomogeneous terms $I_{j\pm}$ of Eqs. (3.9) and (3.10) contains both $L_{1\pm}$ and $L_{2\pm}$, as can be seen from Eqs. (3.11) and (3.12), and therefore, in general, is not analytic for Re $(s) < -\sigma_m$, where σ_m is given by Eq. (3.14). In particular, note that, for $|x| > a$, $\psi_{1\pm}(x, \mu, s)$ never appears to be analytic for Re $(s) < -\sigma_m$. However, for special cases of material properties and initial distributions, $\psi_{2\pm}(x, \mu, s)$ can be shown to be analytic for $-\sigma_2 <$ Re $(s) < -\sigma_1$ except perhaps for poles.

We now look at the behavior of $\psi_{s\pm}$ for Re $(s) > -\sigma_m$. Observe that the transform plane for the present problem must be taken as a superposition of two "single-medium" planes, that is, one for each material medium in the problem. The expressions (3.1)–(3.4) for the transformed solution were not defined for $s \in C_j$ and outwardly appear to be discontinuous at $s \in C_j$. However, this is not the case. The complex representation of $E_{j\pm}$ given by Eqs. (3.9) and (3.10) shows that such coefficients are continuous across the curves C_j. Thus, it is seen from the representation of $\psi_{s\pm}$ given in Eqs. (3.22)–(3.25) that $\psi_{s\pm}$ is indeed continuous across the curves C_j.

It is convenient to introduce at this point the solution of the associated eigenvalue problem, that is, the solution of Eq. (2.5) subject to the boundary conditions (2.6) and (2.7) with $f_{j\pm}(x, \mu) \equiv 0$. Such solutions, denoted with a bar, have the form

$$\begin{aligned}
&\bar{\psi}_{s\pm}(x, \mu) \\
&= \bar{b}_{1\pm}\psi_{-\nu_{01}}(x, \mu, s)\delta_1(s) + \int_0^1 \bar{B}_{1\pm}(-\nu)\psi_{1(-\nu)}(x, \mu, s)\, d\nu, \\
&\qquad\qquad x < -a, \\
&= [\psi_{\nu_{02}}(x, \mu, s) \pm \psi_{-\nu_{02}}(x, \mu, s)]\delta_2(s) \\
&\quad + \int_0^1 \bar{B}_{2\pm}(\nu)[\psi_{2\nu}(x, \mu, s) \pm \psi_{2(-\nu)}(x, \mu, s)]\, d\nu, \\
&\qquad\qquad |x| < a, \\
&= \pm\bar{b}_{1\pm}\psi_{\nu_{01}}(x, \mu, s)\delta_1(s) \pm \int_0^1 \bar{B}_{1\pm}(-\nu)\psi_{1\nu}(x, \mu, s)\, d\nu, \\
&\qquad\qquad x > a, \qquad (4.1)
\end{aligned}$$

where, obviously, $\bar{B}_{j\pm}$ and $\bar{b}_{1\pm}$ can be obtained from the $E_{j\pm}$ given by Eqs. (3.9) and (3.10) for $f_{j\pm}(x, \mu) \equiv 0$. As we shall see, the solution $\psi_{s\pm}$ has poles at those values of s for which the associated eigenvalue problem has nontrivial solutions. It can be shown[13] that, as the slab thickness becomes very large, this eigenvalue problem has only trivial solutions for Re $(s) > -\sigma_2$ except, perhaps, on the branch cuts of $\nu_{0j}(s)$. Since in previously solved time-dependent problems, singularities of the transformed solution always occur on these cuts, we assume for *all* values of a that the singularities of $\psi_{s\pm}$ occur on the branch cuts of $\nu_{0j}(s)$. In any case, we show that the only other singularities of $\psi_{s\pm}$, Re $(s) > -\sigma_m$, which could occur off the branch cuts of $\nu_{0j}(s)$ are poles whose residue could readily be added to the time-dependent solution.

In order to see the behavior of $\psi_{s\pm}$ on the branch cuts of $\nu_{0j}(s)$, we first look at $\bar{\psi}_{s\pm}$ in the region $s \in S_{1i} \cap S_{2i}$. For this region, the expansion coefficients are given by the equations

$$\begin{aligned}
\bar{B}_{2\pm}(\mu) &= \pm\tfrac{1}{2}k_s \frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)} \frac{(\nu_{02}^2 - \mu^2)}{(\nu_{01}^2 - \mu^2)} \frac{h_2(\mu)}{g_2(\mu)} \\
&\quad \times \left(\frac{h_2(\nu_{02})}{\mu + \nu_{02}} \pm \frac{h_2(-\nu_{02})}{\mu - \nu_{02}} \right. \\
&\quad \left. + \int_0^1 \bar{B}_{2\pm}(\nu)h_2(\nu) \frac{d\nu}{\nu + \mu} \right), \quad 0 \le \mu \le 1, \qquad (4.2)
\end{aligned}$$

$$\begin{aligned}
\bar{B}_{1\pm}(-\mu) &\mp \frac{c_2\sigma_2}{c_1\sigma_1} \bar{B}_{2\pm}(\mu)e^{(\sigma_1-\sigma_2)a/\mu} \\
&= \pm\tfrac{1}{2}k_s \frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)} \frac{h_1(\mu)}{g_1(\mu)} \left(\frac{h_2(\nu_{02})}{\mu - \nu_{02}} \pm \frac{h_2(-\nu_{02})}{\mu + \nu_{02}} \right. \\
&\quad \left. + \int_0^1 \bar{B}_{2\pm}(\nu)h_2(\nu) \frac{2\varphi_{1s\mu}(\nu)}{c_1\sigma_1\mu}\, d\nu \right), \qquad (4.3)
\end{aligned}$$

and

$$\begin{aligned}
&\mp h_1(-\nu_{01})\bar{b}_{1\pm} \\
&\quad = h_2(\nu_{02}) \pm h_2(-\nu_{02}) \\
&\qquad + (\nu_{02}^2 - \nu_{01}^2) \int_0^1 \bar{B}_{2\pm}(\nu)h_2(\nu) \frac{d\nu}{\nu^2 - \nu_{01}^2}, \qquad (4.4)
\end{aligned}$$

where

$$h_2(\omega) = \omega \frac{X_{2s}(-\omega)}{X_{1s}(-\omega)} e^{-(s+\sigma_2)a/\omega}, \qquad (4.5a)$$

$$h_1(\omega) = \frac{\Omega_{1s}(\infty)}{\Omega_{2s}(\infty)} \omega \frac{X_{1s}(-\omega)}{X_{2s}(-\omega)} e^{(s+\sigma_1)a/\omega}, \qquad (4.5b)$$

and

$$g_j(\mu) = \mu\Omega_{js}^+(\mu)\Omega_{js}^-(\mu). \qquad (4.5c)$$

In addition, the eigenvalue condition

$$0 = \frac{h_2(\nu_{02})}{\nu_{01} + \nu_{02}} \pm \frac{h_2(-\nu_{02})}{\nu_{01} - \nu_{02}} + \int_0^1 \bar{B}_{2\pm}(\nu)h_2(\nu) \frac{d\nu}{\nu + \nu_{01}} \qquad (4.6)$$

must be satisfied. Since the eigenvalue condition (4.6) has different limiting values as s approaches the branch cut of $\nu_{01}(s)$, we conclude that there are only trivial solutions of the associated eigenvalue problem on the $\nu_{01}(s)$ cut. When s belongs to the branch cut of $\nu_{02}(s)$,

which is not also part of the $\nu_{01}(s)$ cut, i.e., when $\mathrm{Re}\,(\nu_{02}) = \mathrm{Im}\,(\nu_{01}) = 0$, it appears that nontrivial solutions of the associated eigenvalue problem may exist. From the results for the bare slab,[3-6] it is expected that Eqs. (4.2) and (4.6) are satisfied only at isolated points $\{s_n\}$.

If material properties are such that $-\sigma_2 < -\sigma_1$, then a portion of the branch cut of $\nu_{02}(s)$ lies in $s \in S_{2i} \cap S_{1e}$. In this region, however, $s < -\sigma_m = -\sigma_1$ and, for such values, the solution $\bar{\psi}_{s\pm}(x, \mu)$, $|x| > a$, that is, $\bar{\psi}_{1\pm}$, is not bounded as $|x| \to \infty$. However, $\bar{\psi}_{2\pm}$ may have nontrivial solutions on such a portion of the branch cut of $\nu_{02}(s)$. The equations for $\bar{B}_{2\pm}$ and the additional constraint for this region are

$$\bar{B}_{2\pm}(\mu) = \pm\tfrac{1}{2}k_s \frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)}(\nu_{02}^2 - \mu^2)\frac{h_2(\mu)}{g_2(\mu)}\frac{X_{1s}(-\mu)}{X_{01s}(-\mu)} \times \left(\frac{h_2(\nu_{02})}{\mu + \nu_{02}}\frac{X_{1s}(-\nu_{02})}{X_{01s}(-\nu_{02})} \pm \frac{h_2(-\nu_{02})}{\mu - \nu_{02}}\frac{X_{1s}(\nu_{02})}{X_{01s}(\nu_{02})} + \int_0^1 \bar{B}_{2\pm}(\nu)h_2(\nu)\frac{X_{1s}(-\nu)}{X_{01s}(-\nu)}\frac{d\nu}{\nu + \mu}\right), \quad 0 \le \mu \le 1, \tag{4.7}$$

and

$$0 = h_2(\nu_{02})\frac{X_{1s}(-\nu_{02})}{X_{01s}(-\nu_{02})} \pm h_2(-\nu_{02})\frac{X_{1s}(\nu_{02})}{X_{01s}(\nu_{02})} + \int_0^1 \bar{B}_{2\pm}(\nu)h_2(\nu)\frac{X_{1s}(-\nu)}{X_{01s}(-\nu)}\,d\nu. \tag{4.8}$$

The zeros of Eq. (4.8) can, under some conditions, be poles of $\psi_{2\pm}$ and, therefore, may contribute discrete modes in $\psi(x, \mu, t)$, $|x| < a$. For this reason, we are interested in where these zeros lie and refer to them as pseudoeigenvalues.

We now indicate how the solution of the associated eigenvalue problem $\bar{\psi}_{s\pm}$ is contained in the inhomogeneous solution $\psi_{s\pm}$. The original expansion coefficients of Eqs. (3.1) and (3.2) can be written as

$$A_{j\pm}(\mu) = [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\bar{B}_{j\pm}(\mu) + B_{j\pm}(\mu) \tag{4.9a}$$

and

$$a_{1\pm} = [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\bar{b}_{1\pm} + b_{1\pm}, \quad s \in S_{1i} \cap S_{2i}, \tag{4.9b}$$

where $\bar{B}_{j\pm}$ and $\bar{b}_{1\pm}$ are given by Eqs. (4.2)–(4.4). The coefficients $B_{j\pm}$ and $b_{1\pm}$ are given by

$$B_{2\pm}(\nu) = \frac{c_1\sigma_1}{c_2\sigma_2}F_{1\pm}(-a, \nu, s)e^{(\sigma_1-\sigma_2)a/\nu} \pm \tfrac{1}{2}k_s\frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)}\frac{(\nu_{02}^2 - \nu^2)}{(\nu_{01}^2 - \nu^2)}\frac{h_2(\nu)}{g_2(\nu)} \times \left[\int_0^1 B_{2\pm}(\mu)h_2(\mu)\frac{d\mu}{\mu + \nu} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)\left(\frac{h_2(\nu_{02})}{\nu + \nu_{02}} \mp \frac{h_2(-\nu_{02})}{\nu - \nu_{02}}\right) + \int_0^1 F_{2\pm}(a, \mu, s)h_2(\mu)\frac{d\mu}{\mu + \nu} \mp \int_0^1 F_{1\pm}(-a, \mu, s)h_1(\mu)\frac{\nu_{01}^2 - \mu^2}{\nu_{02}^2 - \mu^2}\frac{2\varphi_{2sv}(\mu)}{c_2\sigma_2\nu}\,d\mu\right], \tag{4.10}$$

$$B_{1\pm}(-\nu) \mp \frac{c_2\sigma_2}{c_1\sigma_1}B_{2\pm}(\nu)e^{(\sigma_1-\sigma_2)a/\nu} = \pm\tfrac{1}{2}k_s\frac{\Omega_{2s}(\infty)}{\Omega_{1s}(\infty)}\frac{h_1(\nu)}{g_1(\nu)} \times \left[\tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)\left(\frac{h_2(\nu_{02})}{\nu - \nu_{02}} \mp \frac{h_2(-\nu_{02})}{\nu + \nu_{02}}\right) + \int_0^1 [B_{2\pm}(\mu) + F_{2\pm}(a, \mu, s)]h_2(\mu)\frac{2\varphi_{1sv}(\mu)}{c_1\sigma_1\nu}\,d\mu \mp \int_0^1 F_{1\pm}(-a, \mu, s)h_1(\mu)\frac{(\nu_{01}^2 - \mu^2)}{(\nu_{02}^2 - \mu^2)}\frac{d\mu}{\mu + \nu}\right] \mp \left[F_{1\pm}(-a, \nu, s) - \frac{c_2\sigma_2}{c_1\sigma_1}F_{2\pm}(a, \nu, s)e^{(\sigma_1-\sigma_2)a/\nu}\right], \tag{4.11}$$

and

$$\mp h_1(-\nu_{01})[b_{1\pm} - \tilde{F}_{\pm}(-a, \nu_{01}, s)] = \beta_{1\pm}. \tag{4.12}$$

The coefficient $[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]$ is given by

$$[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)] = \frac{-\nu_{01}\beta_{1\pm} + \beta_{2\pm}}{(\nu_{01}\alpha_{1\pm} - \alpha_{2\pm})}. \tag{4.13}$$

In these equations, $\alpha_{j\pm}$ and $\beta_{j\pm}$ are

$$\alpha_{1\pm} = h_2(\nu_{02}) \pm h_2(-\nu_{02}) + (\nu_{02}^2 - \nu_{01}^2)\int_0^1 \bar{B}_{2\pm}(\mu)h_2(\mu)\frac{d\mu}{\mu^2 - \nu_{01}^2}, \tag{4.14a}$$

$$\alpha_{2\pm} = \nu_{02}h_2(\nu_{02}) \mp \nu_{02}h_2(-\nu_{02}) + (\nu_{02}^2 - \nu_{01}^2)\int_0^1 \bar{B}_{2\pm}(\mu)h_2(\mu)\frac{\mu\,d\mu}{\mu^2 - \nu_{01}^2}, \tag{4.14b}$$

$$\beta_{1\pm} = \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s) \times [h_2(\nu_{02}) \mp h_2(-\nu_{02})] + (\nu_{02}^2 - \nu_{01}^2) \times \int_0^1 [B_{2\pm}(\mu) + F_{2\pm}(a, \mu, s)]h_2(\mu)\frac{d\mu}{\mu^2 - \nu_{01}^2} \pm (\nu_{01}^2 - \nu_{02}^2)\int_0^1 F_{1\pm}(-a, \mu, s)h_1(\mu)\frac{d\mu}{\mu^2 - \nu_{02}^2} \pm [F_{1+}(-a, \nu_{01}, s)h_1(\nu_{01}) + F_{1\pm}(-a, -\nu_{01}, s)h_1(-\nu_{01})], \tag{4.15a}$$

and

$$\beta_{2\pm} = \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)\nu_{02} \times [h_2(\nu_{02}) \pm h_2(-\nu_{02})] + (\nu_{02}^2 - \nu_{01}^2) \times \int_0^1 [B_{2\pm}(\mu) + F_{2\pm}(a, \mu, s)]h_2(\mu)\frac{\mu\, d\mu}{\mu^2 - \nu_{01}^2} \mp (\nu_{01}^2 - \nu_{02}^2)\int_0^1 F_{1\pm}(-a, \mu, s)h_1(\mu)\frac{\mu\, d\mu}{\mu^2 - \nu_{02}^2} \mp [\nu_{01}F_{1\pm}(-a, \nu_{01}, s)h_1(\nu_{01}) - \nu_{01}F_{1\pm}(-a, -\nu_{01}, s)h_1(-\nu_{01})]. \quad (4.15b)$$

In terms of these quantities, the solutions $\psi_{j\pm}$ can be written as

$$\psi_{2\pm}(x, \mu, s) = [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\bar{\psi}_{2\pm}(x, \mu, s) + \int_0^1 B_{2\pm}(\nu)[\psi_{2\nu}(x, \mu, s) \pm \psi_{2(-\nu)}(x, \mu, s)]\, d\nu + \int_0^1 [F_{2\pm}(x, \nu, s)\psi_{2\nu}(x, \mu, s) \pm F_{2\pm}(-x, \nu, s)\psi_{2(-\nu)}(x, \mu, s)]\, d\nu + \tfrac{1}{2}[F_{2\pm}(x, \nu_{02}, s) \pm F_{2\pm}(-x, -\nu_{02}, s)] \times \psi_{\nu_{02}}(x, \mu, s) + \tfrac{1}{2}[F_{2\pm}(x, -\nu_{02}, s) \pm F_{2\pm}(-x, \nu_{02}, s)] \times \psi_{-\nu_{02}}(x, \mu, s), \quad |x| < a, \quad (4.16)$$

and

$$\psi_{1\pm}(x, \mu, s) = [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\bar{\psi}_{1\pm}(x, \mu, s) \pm [b_{1\pm} - \tilde{F}_{\pm}(-a, \nu_{01}, s) + F_{1\pm}(-x, -\nu_{01}, s)]\psi_{\nu_{01}}(x, \mu, s) \pm F_{1\pm}(-x, \nu_{01}, s)\psi_{-\nu_{01}}(x, \mu, s) \pm \int_0^1 [B_{1\pm}(-\nu) - \tilde{F}_{\pm}(-a, \nu, s) + F_{1\pm}(-x, -\nu, s)]\psi_{1\nu}(x, \mu, s) \pm \int_0^1 F_{1\pm}(-x, \nu, s)\psi_{1(-\nu)}(x, \mu, s)\, d\nu, \quad x > a. \quad (4.17)$$

The solution $\psi_{1\pm}(x, \mu, s)$ for $x < -a$ has a similar form. In these equations, $\bar{\psi}_{j\pm}(x, \mu, s)$ are the parts of $\bar{\psi}_{s\pm}(x, \mu)$ which are given by Eq. (4.1). Equation (4.4) is written in terms of $\alpha_{1\pm}$ as

$$\mp h_1(-\nu_{01})\bar{b}_{1\pm} = \alpha_{1\pm}. \quad (4.18)$$

Consider now what happens on the branch cut of $\nu_{01}(s)$, where $\nu_{01} = i\,|\nu_{01}|$ for Im $(s) = 0^-$ and $\nu_{01} = -i\,|\nu_{01}|$ for Im $(s) = 0^+$. From the above equations, it can be seen that the quantities $\bar{B}_{2\pm}$, $\bar{B}_{1\pm}$, $B_{2\pm}$, $B_{1\pm}$, $\alpha_{1\pm}$, $\alpha_{2\pm}$, $\beta_{1\pm}$, and $\beta_{2\pm}$ do not inherit the branch cut of $\nu_{01}(s)$. Equations (4.18) and (4.12) show that $\bar{b}_{1\pm}$ and $b_{1\pm}$ have branch cuts due to that of $\nu_{01}(s)$. Equation (4.13) indicates that $[a_{2\pm} + \frac{1}{2}F_{2\pm}(a, \nu_{02}, s)]$ has the branch cut due to $\nu_{01}(s)$ unless $\alpha_{1\pm}/\alpha_{2\pm}$ is equal to $\beta_{1\pm}/\beta_{2\pm}$. In general, this will not be true, since $\beta_{1\pm}/\beta_{2\pm}$ depends on the arbitrary initial distribution $f_{\pm}(x, \mu)$, whereas $\alpha_{1\pm}/\alpha_{2\pm}$ does not. Therefore, it is concluded that both $\psi_{1\pm}$ and $\psi_{2\pm}$ inherit the branch cut of $\nu_{01}(s)$.

On the branch cut of $\nu_{02}(s)$, the quantities $B_{2\pm}$, $B_{1\pm}$, $b_{1\pm}$, $\beta_{1\pm}$, and $\beta_{2\pm}$ are single valued. Since the quantities $\alpha_{1\pm}$ and $\alpha_{2\pm}$ of Eq. (4.14) are related above and below the branch cut of $\nu_{02}(s)$ by

$$[\alpha_{j\pm}]^+ = \pm[\alpha_{j\pm}]^-, \quad (4.19)$$

it follows from Eq. (4.13) that, on that part of the branch cut of $\nu_{02}(s)$ which is not also part of the $\nu_{01}(s)$ cut, i.e., for Re $(\nu_{02}) =$ Im $(\nu_{01}) = 0$, we have

$$[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]^+ = \pm[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]^-, \quad (4.20)$$

if the denominator of the rhs of Eq. (4.13) does not vanish. It is seen from Eqs. (4.1)–(4.4) that, for this same region,

$$[\bar{\psi}_{s\pm}(x, \mu)]^+ = \pm[\bar{\psi}_{s\pm}(x, \mu)]^-. \quad (4.21)$$

Hence, the product

$$[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\bar{\psi}_{s\pm}(x, \mu), \quad (4.22)$$

which appears in $\psi_{s\pm}$, does not inherit the branch cut of $\nu_{02}(s)$. However, the denominator of

$$[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)],$$

namely, $(\nu_{01}\alpha_{1\pm} - \alpha_{2\pm})$, is equivalent to the eigenvalue condition (4.6). Thus, if the associated eigenvalue problem has a nontrivial solution at $s = s_n$, Re $(s) > -\sigma_m$, then $\psi_{s\pm}$ has a pole there.

We briefly summarize the analytic properties of the transformed solution $\psi_{s\pm}(x, \mu)$. For arbitrary initial distributions $f_{\pm}(x, \mu)$, $\psi_{s\pm}$ is not analytic to the left of Re $(s) = -\sigma_m$ in the s plane, whereas, to the right of Re $(s) = -\sigma_m$, it is analytic except for the branch cut along $[-\sigma_m, -\sigma_1(1 - c_1)]$ [due to the branch cut of $\nu_{01}(s)$] if $\sigma_m > \sigma_1(1 - c_1)$ and except for poles at the values of s at which the associated eigenvalue problem has nontrivial solutions $\bar{\psi}_{s\pm}$. We have assumed that, for arbitrary slab thicknesses a, these poles, if they exist, lie on the branch cut of $\nu_{02}(s)$, since this is the rigorous result obtained for the case when $c_2\sigma_2 a$ is large and by others[5,6,10,11] for several special cases of the present problem. For special values of material properties and initial data, $\psi_{s\pm}(x, \mu)$ for $|x| < a$ (that is, $\psi_{2\pm}$) may be analytic in the region $-\sigma_2 <$ Re $(s) < -\sigma_1$, except perhaps for poles.

5. RECOVERY OF TIME-DEPENDENT SOLUTION

The time-dependent solution $\psi(x, \mu, t)$ is obtained from the inverse Laplace transformation (2.2), where γ is to the right of all singularities of $\psi_s(x, \mu)$ in the s plane. From the analysis of the preceding section, we expect that we can choose any

$$\gamma > \max\,[-\sigma_1(1 - c_1), -\sigma_2(1 - c_2)].$$

In order to show the time dependence of the solution $\psi(x, \mu, t)$ more explicitly, we deform the inversion contour as far as possible to the left in the s plane by making use of the analytic properties of $\psi_s(x, \mu)$ obtained in Sec. 4.

The contour Re $(s) = \gamma$ crosses both of the curves C_j, and it has been shown that $\psi_{s\pm}$ is continuous across these curves. As $|s| \to \infty$ on such a contour, $s \in S_{1\epsilon} \cap S_{2\epsilon}$, and it is readily seen that $\psi_{s\pm}$ is not necessarily $O(s^{-1})$. However, the parts which are not can be easily inverted as follows. We define *for all s* the function $\psi_{us\pm}(x, \mu)$ as that part of $\psi_{s\pm}$ which is not $O(s^{-1})$ and, upon making the substitution

$$\begin{aligned} x - x_0 &= \mu t, \quad \mu > 0, \\ x_0 - x &= |\mu|\, t, \quad \mu < 0, \end{aligned} \tag{5.1}$$

we see that $\psi_{us\pm}(x, \mu)$ can be written as

$$\psi_{us\pm}(x, \mu) = \int_0^\infty e^{-st}[\psi_{u\pm}(x, \mu, t)]\, dt. \tag{5.2}$$

That is, the parts of $\psi_{s\pm}$ which do not behave as $O(s^{-1})$ as $|s| \to \infty$, Re $(s) = \gamma$, can be inverted by inspection. The solution $\psi_{u\pm}(x, \mu, t)$ is given by

$$\begin{aligned} &\psi_{u\pm}(x, \mu, t) \\ &= e^{-\sigma_2 t} f_{2\pm}(x - \mu t, \mu), && t < (a + x)/\mu, \\ &= e^{-\sigma_1 t} e^{-(\sigma_2 - \sigma_1)(a+x)/\mu} f_{1\pm}(x - \mu t, \mu), && t > (a + x)/\mu, \end{aligned} \tag{5.3}$$

for $|x| < a$ and $\mu > 0$,

$$\begin{aligned} &\psi_{u\pm}(x, \mu, t) \\ &= e^{-\sigma_2 t} f_{2\pm}(x - \mu t, \mu), && t < (a - x)/|\mu|, \\ &= e^{-\sigma_1 t} e^{(\sigma_2 - \sigma_1)(a-x)/\mu} f_{1\pm}(x - \mu t, \mu), && t > (a - x)/|\mu|, \end{aligned} \tag{5.4}$$

for $|x| < a$ and $\mu < 0$,

$$\begin{aligned} &\psi_{u\pm}(x, \mu, t) \\ &= e^{-\sigma_1 t} f_{1\pm}(x - \mu t, \mu), && t < (x - a)/\mu, \\ &= e^{-\sigma_2 t} e^{(\sigma_2 - \sigma_1)(x-a)/\mu} f_{2\pm}(x - \mu t, \mu), \\ & && (x - a)/\mu < t < (x + a)/\mu, \\ &= e^{-\sigma_1 t} e^{-(\sigma_2 - \sigma_1)2a/\mu} f_{1\pm}(x - \mu t, \mu), && t > (x + a)/\mu, \end{aligned} \tag{5.5}$$

for $x > a$ and $\mu > 0$, and

$$\psi_{u\pm}(x, \mu, t) = e^{-\sigma_1 t} f_{1\pm}(x - \mu t, \mu), \tag{5.6}$$

for $x > a$ and $\mu < 0$. That $\psi_{u\pm}$ describes the motion of uncollided neutrons from the initial distribution can be seen by direct substitution into the equation

$$\frac{\partial \psi_{u\pm}}{\partial t} + \mu \frac{\partial \psi_{u\pm}}{\partial x} + \sigma(x)\psi_{u\pm} = 0. \tag{5.7}$$

In the limit $t \to 0$, we note that

$$\psi_{u\pm}(x, \mu, 0) = f_\pm(x, \mu). \tag{5.8}$$

For an arbitrary $f(x, \mu)$ which vanishes as $|x| \to \infty$, $\psi_{us\pm}(x, \mu)$ as it is given by Eqs. (5.2) and (5.3)–(5.6) is an analytic function of s for Re $(s) > -\sigma_m$ for almost all x and μ. If $f_{1\pm} \equiv 0$ ($f_{2\pm} \equiv 0$), then $\psi_{us\pm}$ is an analytic function of s for Re $(s) > -\sigma_2$ [Re $(s) > -\sigma_1$]. Therefore, the function $\Phi_{s\pm}(x, \mu)$ defined as

$$\Phi_{s\pm}(x, \mu) \equiv \psi_{s\pm}(x, \mu) - \psi_{us\pm}(x, \mu), \quad \text{Re } (s) > -\sigma_m, \tag{5.9}$$

has the same analytic properties as $\psi_{s\pm}$ in the right half-plane Re $(s) > -\sigma_m$, except that it is $O(s^{-1})$ as $|s| \to \infty$.

The definite parity parts of the time-dependent solution, therefore, can be written from Eq. (2.2) as

$$\psi_\pm(x, \mu, t) = \psi_{u\pm}(x, \mu, t) + \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} \Phi_{s\pm}(x, \mu) e^{st}\, ds. \tag{5.10}$$

Now, using the analytic properties, we can deform the contour to the left and obtain, in general,

$$\begin{aligned} &\psi_\pm(x, \mu, t) \\ &= \psi_{u\pm}(x, \mu, t) + \sum_{s=s_n} \text{Res}\,[\psi_{s\pm}(x, \mu)e^{st}] \\ &\quad + \frac{1}{2\pi i}\int_{-\sigma_m}^{-\sigma_1(1-c_1)} \{[\psi_{s\pm}(x, \mu)]^- - [\psi_{s\pm}(x, \mu)]^+\} e^{st}\, ds \\ &\quad + \frac{1}{2\pi i}\int_{-\sigma_m - i\infty}^{-\sigma_m + i\infty} [\psi_{s\pm}(x, \mu) - \psi_{us\pm}(x, \mu)] e^{st}\, ds \\ &\quad + \frac{1}{2\pi i}\lim_{\rho \to 0}\int_{C_\rho} \psi_{s\pm}(x, \mu) e^{st}\, ds, \\ &\qquad\qquad -\sigma_m < -\sigma_1(1 - c_1) < s_n, \end{aligned} \tag{5.11}$$

where C_ρ is a small circular contour of radius ρ with center at $s = -\sigma_1(1 - c_1)$. Generally, the point $s = -\sigma_1(1 - c_1)$ will not satisfy the eigenvalue condition (4.6), and the contribution from the contour C_ρ vanishes as $\rho \to 0$. If, however, $s = -\sigma_1(1 - c_1)$ happens to satisfy Eq. (4.6), the contribution from the contour C_ρ has the form of a discrete residue term.

Equation (5.11) is the solution of the time-dependent problem written in a form in which the uncollided portion of the initial distribution $f(x, \mu)$ has been separated. For arbitrary $f(x, \mu)$, the contour cannot

be deformed further to the left. In the final section, it is shown how this solution reduces to those obtained previously by others for special cases of the present problem.

We close this section by indicating the form of some parts of Eq. (5.11). The uncollided term $\psi_{u\pm}(x, \mu, t)$ is given explicitly by Eqs. (5.3)–(5.6). The form of $\psi_{s\pm}(x, \mu)$ on the branch cut $[-\sigma_m, -\sigma_1(1 - c_1)]$ was given in Sec. 4. From those results, it is seen that, on this branch cut, $[\psi_{s\pm}(x, \mu)]^- - [\psi_{s\pm}(x, \mu)]^+$ can be written from Eqs. (4.16) and (4.17) as

$$[\psi_{s\pm}(x, \mu)]^- - [\psi_{s\pm}(x, \mu)]^+ = \{[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]^- - [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]^+\}\bar{\psi}_{2\pm}(x, \mu, s), \quad (5.12)$$

for $|x| < a$, and as

$$[\psi_{s\pm}(x, \mu)]^- - [\psi_{s\pm}(x, \mu)]^+ = [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]^-[\bar{\psi}_{1\pm}(x, \mu, s)]^- - [a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]^+[\bar{\psi}_{1\pm}(x, \mu, s)]^+ \pm \{[b_{1\pm} - \tilde{F}_{\pm}(-a, \nu_{01}, s)]^-\psi_{\nu_{01}}(x, \mu, s) - [b_{1\pm} - \tilde{F}_{\pm}(-a, \nu_{01}, s)]^+\psi_{-\nu_{01}}(x, \mu, s)\}, \quad (5.13)$$

for $x > a$, where $[a_{2\pm} + \frac{1}{2}F_{2\pm}(a, \nu_{02}, s)]$ is given by Eq. (4.13), $\bar{\psi}_{j\pm}(x, \mu, s)$ by Eq. (4.1), and

$$[b_{1\pm} - \tilde{F}_{\pm}(-a, \nu_{01}, s)]$$

by Eq. (4.12). The solution $\psi_{s\pm}(x, \mu)$ has poles at $s = s_0, \cdots, s_N$ due to the poles of

$$[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\nu_{02}^{\frac{1}{2}(1\mp1)}.$$

Again, from the results given in Sec. 4, it follows that

$$\text{Res } [\psi_{s\pm}(x, \mu)e^{st}]_{s_n} = e^{s_n t}\{\bar{\psi}_{s\pm}(x, \mu)[\nu_{02}^{-\frac{1}{2}(1\mp1)}]\}_{s_n} \times \text{Res } \{\nu_{02}^{\frac{1}{2}(1\mp1)}[a_{2\pm} + \tfrac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\}_{s_n}. \quad (5.14)$$

Note that the factor $\nu_{02}^{\frac{1}{2}(1\mp1)}$ is introduced so that $\bar{\psi}_{s\pm}\nu_{02}^{-\frac{1}{2}(1\mp1)}$ and $[a_{2\pm} + \frac{1}{2}F_{2\pm}(a, \nu_{02}, s)]\nu_{02}^{\frac{1}{2}(1\mp1)}$ are single valued on the branch cut of ν_{02} [cf. Eqs. (4.20) and (4.21)]. These terms have an exponential time dependence $e^{s_n t}$, and we have obtained the implicit equations, viz., Eqs. (4.2) and (4.6), from which the eigenvalues $\{s_n\}$ can be computed. Since information concerning the behavior of eigenvalues (e.g., number, location, etc.) as a function of material properties is not readily obtained analytically from such expressions, we have made a numerical study of real time eigenvalues, and the results are discussed in the next section.

6. CALCULATION OF REAL TIME EIGENVALUES

We first note that the eigenvalues and pseudo-eigenvalues depend on five parameters (c_1, σ_1, c_2, σ_2, and a) and, therefore, many numerical computations would be required in order to see the specific dependence on each parameter. As we shall see, the bare-slab results of Bowden,[3,4] the theorems of Hintz[11] for slabs surrounded by pure absorbers, and some observations of the present numerical results for a few reflected slab cases allow us to speculate about the behavior of eigenvalues for reflected slabs as a function of the slab half-thickness a. However, rather than compute eigenvalues $\{s_n\}$ in terms of c_1, σ_1, c_2, σ_2, and a, we define a nondimensional variable ζ and nondimensional parameters σ_R, σ_D, and A as

$$\zeta = \frac{s + \sigma_2}{c_2\sigma_2}, \quad \sigma_R = \frac{c_1\sigma_1}{c_2\sigma_2}, \quad \sigma_D = \frac{\sigma_1 - \sigma_2}{c_2\sigma_2}, \quad \text{and} \quad A = c_2\sigma_2 a. \quad (6.1)$$

In terms of these quantities, the branch cut of ν_{02} becomes the real interval (0, 1) and the branch cut of ν_{01} becomes the real interval $(-\sigma_D, -\sigma_D + \sigma_R)$. Since σ_j and c_j are nonnegative, it follows that

$$-\sigma_D \leq 1/c_2, \quad (6.2)$$

where the equality holds only if $\sigma_1 = 0$. Also, we have restricted $c_1 < 1$ so that $-\sigma_D + \sigma_R \geq 1$ implies that $c_2 < 1$. Obviously, $\sigma_R = 0$ when the reflector is a pure absorber or a vacuum and $\sigma_D = 0$ when the total macroscopic cross sections of the two media are the same. We have seen from the last section that, in general, the inversion contour can be deformed to the left only as far as Re $(s) = -\sigma_m$, which corresponds to Re $(\zeta) = \max(-\sigma_D, 0)$. However, there are no eigenvalues on the branch cut of ν_{01} so that the region of the real ζ axis where the eigenvalues $\{\zeta_n\}$ should appear is

$$\max(-\sigma_D + \sigma_R, 0) < \zeta_n < 1. \quad (6.3)$$

This interval corresponds to $s \in S_{1i} \cap S_{2i}$, and Eqs. (4.2) and (4.6), written in terms of the quantities of Eq. (6.1), are solved numerically to obtain the real eigenvalues $\{\zeta_n\}$ for specified σ_R, σ_D, and A. In addition, the pseudoeigenvalues are obtained numerically by solving Eqs. (4.7) and (4.8), also written in terms of the quantities of Eq. (6.1). Details concerning numerical procedures and computational equations are given in Ref. 13. The calculations were done on a Control Data 6600 computer system at NASA Langley Research Center.

The time dependence of discrete modes is seen from Eqs. (5.11) and (5.14) to be

$$e^{s_n t} = e^{(c_2\zeta_n - 1)\sigma_2 t}. \tag{6.4}$$

Now $\zeta_n = -\sigma_D + \sigma_R$ implies that

$$s_n = -\sigma_1(1 - c_1) \leq 0$$

since $c_1 < 1$ and the equality holds only if $\sigma_1 = 0$. Therefore, such ζ_n correspond to time-decaying modes regardless of the value of c_2. For values of ζ_n within the interval (6.3), the time decay or growth depends on whether $c_2\zeta_n$ is less than or greater than unity, as can be seen from Eq. (6.4). A discrete mode represents a critical system if $c_2\zeta_n = 1$.

Many different combinations of material parameters could be considered, but here we restrict our study of the eigenvalue behavior to the case of overlapping branch cuts. As σ_R departs from zero, we would like to see how the eigenvalues depart from those previously reported[3,4] for a bare slab. The present eigenvalues $\{\zeta_n\}$ for vacuum reflectors, i.e., $\sigma_R = 0$, and those of Bowden[3,4] are in good agreement. In addition, critical dimensions obtained for bare slabs, spheres, and infinitely reflected slabs are also in good agreement with those previously reported by others.[16–18]

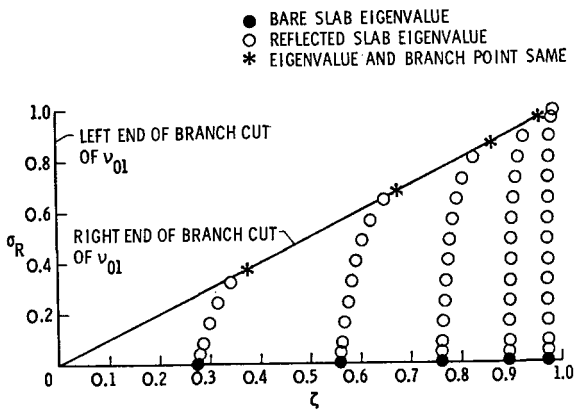

FIG. 4. Dependence of eigenvalues ζ_n on σ_R; $\sigma_D = 0$, $A = 5$.

The results presented here were computed for $A = 5$. A bare slab of such thickness has five eigenvalues[3,4] which were investigated as σ_R departs from zero for several values of σ_D. In Fig. 4, results are given for $\sigma_D = 0$. Our calculations show that the largest eigenvalue ζ_0 is present up to $\sigma_R = 0.9999$. Apparently, this eigenvalue remains up to $\sigma_R = 1$, which is only obtained for $c_2 < 1$. All other eigenvalues disappear into the branch cut of ν_{01} at $\zeta_n = \sigma_R$, labeled with an asterisk, which corresponds to a time-decaying mode, regardless of the value of c_2. In fact, on Figs. 4–6, we indicate the points at which an

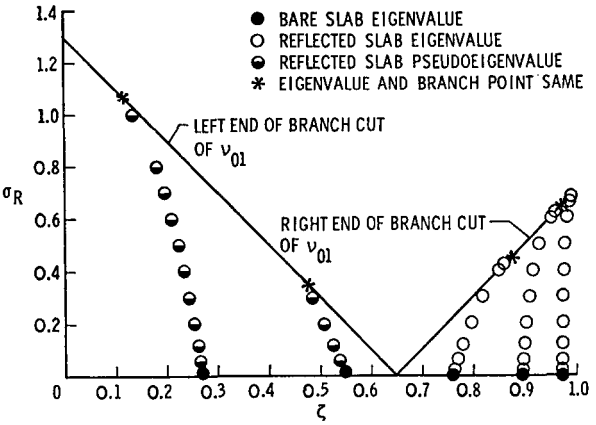

FIG. 5. Dependence of eigenvalues ζ_n on σ_R; $\sigma_D = 0.5\sigma_R - 0.65$, $A = 5$.

eigenvalue or pseudoeigenvalue coincides with the branch points of ν_{01} by an asterisk. Even though such points appear to have a discrete eigenvalue type of time dependence, we feel that they are properly part of the branch-cut integral contribution. We note that the branch points of ν_{01} are located at $\zeta = -\sigma_D$ and $\zeta = -\sigma_D + \sigma_R$ and find that the limiting form of the condition which determines whether or not such points are eigenvalues (or pseudoeigenvalues) no longer depends explicitly on σ_R or σ_D. The theorems of Lehner[10] apply for $\sigma_R = 0$ in Fig. 4.

In Fig. 5, results are presented for $\sigma_D = -0.65 + 0.5\sigma_R$. These typify results for $-\sigma_D$ values in the range between zero and $[\zeta_0]_{\sigma_R=0}$, where the notation $[\zeta_n]_{\sigma_R=0}$ means bare-slab eigenvalue, which we note depends on c_2, σ_2, and a. The open and closed circles represent eigenvalues as in Fig. 4 while the half-closed circles are pseudoeigenvalues corresponding to $s < -\sigma_m = -\sigma_1$. Again, the largest eigenvalue ζ_0 appears to remain provided that $c_2 > 1$. Here, as in Fig. 6, results for $\sigma_R = 0$ agree with the theorems of Hintz[11] which apply only for $c_1 = 0$. Basically, his result is

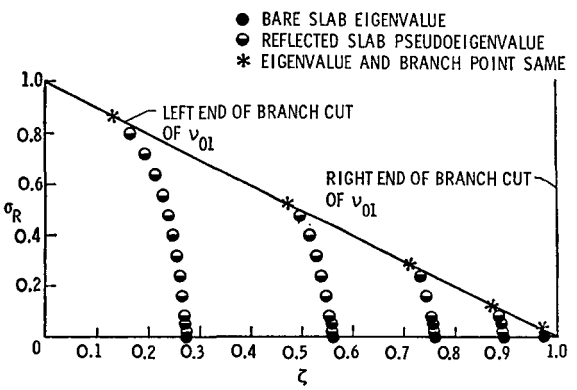

FIG. 6. Dependence of eigenvalues ζ_n on σ_R; $\sigma_D = \sigma_R - 1$, $A = 5$.

that the strip Re (ζ) between 0 and $-\sigma_D$ belongs to the continuous spectrum and that the bare-slab eigenvalues lying in this interval are not eigenvalues of the slab surrounded by perfect absorbers. He finds that there are no eigenvalues if $-\sigma_D > [\zeta_0]_{\sigma_R=0}$, but says nothing about the physical significance. It is seen from Eq. (6.2) that for such cases $\zeta_0 < 1/c_2$ and corresponds, therefore, to a time-decaying mode. In other words, stationary (critical) or time-increasing modes cannot disappear into the continuous spectrum as material properties are varied. In fact, we have seen that, when $\sigma_R \neq 0$, such modes cannot disappear into the branch cut of ν_{01} either. In Fig. 6, results are given for $-\sigma_D + \sigma_R = 1$, which we recall implies $c_2 < 1$. For this case, all of the bare-slab eigenvalues lie in the continuous spectrum found by Hintz when $\sigma_R = 0$. In both Figs. 5 and 6, $s = -\sigma_m$ corresponds to $\zeta = -\sigma_D$.

All numerical results indicate that real time eigenvalues $\{\zeta_n\}$ for material reflectors are finite in number and tend to eigenvalues previously obtained for a vacuum as $\sigma_R \to 0$, as do the pseudoeigenvalues for $s < -\sigma_m$. If the set $\{\zeta_n\}$ is empty, then the neutron density is necessarily decaying in time. Conversely, if the neutron density is stationary or increasing in time, then the set $\{\zeta_n\}$ is *not* empty. As expected, if $c_2 > 1$, then a critical thickness can be found, i.e., the largest eigenvalue ζ_0 must be present for large enough slab thicknesses for the given $c_2 > 1$.

As pointed out at the beginning of this section, we can draw some conclusions concerning the behavior of $\{\zeta_n\}$ for reflected slabs as a function of the slab half-thickness a. We base the following conclusions on the observation that, if ζ_0 at $\sigma_R = 0$ lies to the right of $-\sigma_D$, then it appears to remain to the right of $-\sigma_D + \sigma_R$ as σ_R increases until $-\sigma_D + \sigma_R = 1$. (See Figs. 4 and 5.) The dependence of $[\zeta_0]_{\sigma_R=0}$ on slab half-thickness is given in Ref. 3. First, if $-\sigma_D + \sigma_R \geq 1$ (recall that this implies $c_2 < 1$), then the set $\{\zeta_n\}$ is empty for all a. However, there may be pseudoeigenvalues if $-\sigma_D > 0$. Next, if $-\sigma_D + \sigma_R < 1$, then two cases arise, depending on the value of σ_D:

(a) When $-\sigma_D > 0$, then, regardless of the value of c_2, we can find an a^* such that $a < a^*$ implies that the set $\{\zeta_n\}$ is empty, whereas $a > a^*$ implies that the set $\{\zeta_n\}$ is not empty. The number a^* is obtained from the bare-slab result $[\zeta_0]_{\sigma_R=0}$ as

$$[\zeta_0(c_2, \sigma_2, a^*)]_{\sigma_R=0} = -\sigma_D. \tag{6.5}$$

(b) When $-\sigma_D \leq 0$, the set $\{\zeta_n\}$ is never empty. Thus, given c_j, σ_j, and a and the bare-slab eigenvalues corresponding to c_2, σ_2, and a, we can say whether or not the set $\{\zeta_n\}$ is empty. Furthermore, the number of eigenvalues $\{\zeta_n\}$ will not exceed the number of bare-slab eigenvalues $\{[\zeta_n]_{\sigma_R=0}\}$ which are greater than $-\sigma_D$. Finally, the number of real reflected-slab eigenvalues and pseudoeigenvalues does not exceed the number of bare-slab eigenvalues.

7. CONCLUDING REMARKS

It has been shown by using Case's method that the solution to the initial value problem of monoenergetic neutrons migrating in a finite slab (properties c_2, σ_2) with infinite reflectors (properties c_1, σ_1) can be written in the form

$$\begin{aligned}\psi(x, \mu, t) &= \psi_u(x, \mu, t) + \sum_{s=s_n} \text{Res}\,[\psi_s(x, \mu)]_{s_n} e^{s_n t} \\ &\quad + \frac{1}{2\pi i}\int_{-\sigma_m}^{-\sigma_1(1-c_1)} \{[\psi_s(x, \mu)]^- - [\psi_s(x, \mu)]^+\} e^{st}\, ds \\ &\quad + \frac{1}{2\pi i}\int_{-\sigma_m - i\infty}^{-\sigma_m + i\infty} [\psi_s(x, \mu) - \psi_{us}(x, \mu)] e^{st}\, ds, \\ &\qquad -\sigma_m < -\sigma_1(1 - c_1) < s_n. \end{aligned} \tag{7.1}$$

Some terms of the solution (7.1) will not be present if $-\sigma_m \not< -\sigma_1(1 - c_1) \not< s_n$. That is, if $-\sigma_1(1 - c_1) < -\sigma_m$, then the branch-cut integral does not appear. Likewise, if all $s_n < -\sigma_1(1 - c_1)$, then there are not residue terms. These discrete eigenvalue terms are characteristic of a finite slab while the branch-cut integral term is typical of a semi-infinite medium. The term $\psi_u(x, \mu, t)$ describes the behavior of neutrons from the initial distribution $f(x, \mu)$, which have not suffered a scattering collision, and its definite parity parts are given in Eqs. (5.3)–(5.6). The discrete eigenvalue terms in Eq. (7.1) are given by Eq. (5.14), while the integrand of the branch-cut integral is given by Eqs. (5.12) and (5.13). The definite parity parts of the last integrand are given by Eqs. (5.2) and Eqs. (3.22)–(3.25). The eigenvalues $\{s_n\}$ can be computed, as was demonstrated in the last section; thus, everything which appears in Eq. (7.1) can be calculated.

In all special cases of the present problem, which have been solved by using the approach of Lehner and Wing,[5,6,10,11] $c_1 = 0$. Thus, in these cases, there is no branch cut due to $\nu_{01}(s)$ and the branch-cut integral is not present in Eq. (7.1). It was shown that as $c_1 \to 0$ the eigenvalues $\{s_n\}$ which are greater than $-\sigma_m$ approach those for a bare slab, as do the pseudoeigenvalues for $s < -\sigma_m$. The solution $\psi_{s\pm}$ has the proper behavior as $c_1 \to 0$ since those terms of Eq. (3.11) and (3.12) which appear to blow up in such a limit actually cancel when the contour C' is

collapsed onto the portion of the branch cut of $\Omega_{js}(z')$, $0 \leq z' \leq 1$. When the uncollided term is combined with the last integral, it is then seen that the solution (7.1) and the eigenvalues $\{s_n\}$ have the behavior required by the theorems of Lehner[10] and Hintz.[11] The present problem reduces to those considered by Lehner and Hintz when

$$c_1 = 0, \quad \sigma_1 = \sigma_2 \quad \text{(Lehner[10])} \tag{7.2a}$$

and

$$c_1 = 0, \quad \sigma_1 \neq \sigma_2 \quad \text{(Hintz[11])}. \tag{7.2b}$$

In order to describe the same physical problem in the slab as that solved by Lehner and Wing,[5,6] we must not only have

$$c_1 = 0 \quad \text{and} \quad \sigma_1 = 0, \tag{7.3}$$

but also

$$f(x, \mu) = 0, \quad \text{for} \quad x < -a, \quad \mu > 0, \quad \text{and} \quad x > a, \quad \mu < 0. \tag{7.4}$$

In other words, neutrons from the initial distribution outside the slab cannot impinge on the slab faces at times $t > 0$. Lehner and Wing solved the time-dependent problem with boundary conditions

$$\psi(\pm a, \mu, t) = 0, \quad \mu \lessgtr 0, \quad t > 0. \tag{7.5}$$

Restrictions (7.3) and (7.4) in the present solution make $I_{2\pm}(\mu, s)$ and, therefore, $A_{2\pm}(\mu)$ depend only on properties of the slab. Then, in looking for solutions inside the slab ($|x| < a$), the inversion contour along Re $(s) = -\sigma_m$ can be deformed back to Re$(s) = -\sigma_2$, and we pick up a residue contribution from any pseudoeigenvalue in the region and thus obtain the Lehner–Wing results. That is, the solution has the proper form, and all bare-slab eigenvalues are recovered.

The analogous problem for $c_1 \neq 0$ in which the inversion contour can be deformed to the left of Re $(s) = -\sigma_m$ for $|x| < a$ is obtained when $\sigma_2 > \sigma_1$ and $f_1(x, \mu) \equiv 0$. That is, if

$$f(x, \mu) \equiv 0, \quad |x| > a \quad \text{and} \quad \sigma_2 > \sigma_1, \tag{7.6}$$

then all terms in $I_{2\pm}(\mu, s)$ which contain $(s + \sigma_1)$ factors in the exponentials are identically zero; this allows us to deform the contour along Re $(s) = -\sigma_m$ back to Re $(s) = -\sigma_2$ when $|x| < a$. Such a deformation is not possible for $|x| > a$; for this latter range of x, we must stop at Re $(s) = -\sigma_m = -\sigma_1$. If there are pseudoeigenvalues in $-\sigma_2 <$ Re $(s) < -\sigma_1 = -\sigma_m$ (see, for example, Fig. 5), they will appear in the solution for $|x| < a$ as residue terms which have the exponential time dependence. They are not eigenvalues for the reflected slab though, since such terms do not appear for $|x| > a$. Erdmann[8,9] solved the time-dependent problem for two semi-infinite media, where an isotropic pulse of neutrons was introduced at the interface, and found that the inversion contour for $x \in$ medium j could be deformed to the left as far as Re $(s) = -\sigma_j$. In the present problem, such deformations can be made only when conditions (7.6) are satisfied. It appears that the contour Re $(s) = -\sigma_m$ cannot be deformed to the left of Re $(s) = -\sigma_2$, since the equations which determine $A_{2\pm}(\mu)$ (Sec. 4) require Re $(s) \geq -\sigma_2$. Apparently, Re $(s) = -\sigma_2$ is the edge of a continuous spectrum in all cases for the reflected slab.

We briefly summarize the results which have been obtained. The present solution has been shown to have the required properties in all special cases which have been solved previously by others using the approach of Lehner and Wing. However, in all of these rigorous solutions, there was no scattering outside the slab. We have seen that, with infinite reflectors on the slab and neutrons anywhere outside the slab initially, it is possible for some neutrons which have spent their entire history in the reflector to impinge on the slab faces at times $t > 0$. Such neutrons have a collision rate which is characteristic of reflector properties and this, in general, restricts us from deforming the inversion contours to the left of Re $(s) = -\sigma_m$. We have illustrated two cases in which a further deformation is possible for $|x| < a$, by eliminating neutrons outside the slab initially which can later impinge on the slab faces. This is equivalent to a further restriction on the Hilbert space which has been used in some of the above-mentioned rigorous solutions. The exact eigenvalue condition has been obtained, and real time eigenvalues have been calculated for a number of combinations of material parameters.

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[1] K. M. Case, Ann. Phys. (N.Y.) **9**, 1 (1960).
[2] K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967).
[3] R. L. Bowden, Jr., Ph.D. thesis, Virginia Polytechnic Institute, 1963.
[4] R. L. Bowden and C. D. Williams, J. Math. Phys. **5**, 1527 (1964).
[5] J. Lehner and G. M. Wing, Commun. Pure Appl. Math. **8**, 217 (1955).
[6] J. Lehner and G. M. Wing, Duke Math. J. **23**, 125 (1956).
[7] I. Kuščer and P. F. Zweifel, J. Math. Phys. **6**, 1125 (1965).
[8] R. C. Erdmann, Ph.D. thesis, California Institute of Technology, 1966.
[9] R. C. Erdmann and H. Lurie, Nucl. Sci. Eng. **28**, 190 (1967).

[10] J. Lehner, J. Math. Mech. 11, 173 (1962).
[11] G. R. Hintz, Ph.D. thesis, Purdue University, 1969.
[12] P. A. Newman and R. L. Bowden, in "Neutron Transport Theory Conference, January 20–24, 1969," ORO-3858-1, USAEC, 1969, p. 289.
[13] P. A. Newman, Ph.D. thesis, Virginia Polytechnic Institute, 1969.
[14] I. Kuščer, N. J. McCormick, and G. C. Summerfield, Ann. Phys. (N.Y.) 30, 411 (1964).
[15] R. L. Bowden, F. J. McCrosson, and E. A. Rhodes, J. Math. Phys. 9, 753 (1968).
[16] G. J. Mitsis, ANL Report No. ANL-6787, 1963.
[17] T. W. Mullikin, J. Math. Anal. Appl. 5, 184 (1962).
[18] K. Kowalska, Nucl. Sci. Eng. 24, 260 (1966).

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Curvature Collineations for Gravitational pp Waves*

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Vacuum fields which admit a covariant constant vector are investigated in order to find "curvature collineations," i.e., $\pounds R^i_{klj} = 0$. For all discussed types of pp waves it is shown that proper curvature collineations exist. We state the explicit form of these transformations.

I. INTRODUCTION

A special symmetry property of Riemannian manifolds called "curvature collineations" (CC's) was recently proposed.[1] This symmetry is defined by $\pounds_\xi R^i_{klj} = 0$ for infinitesimal transformations $\bar{x}^i = x^i + \xi^i\delta\epsilon$, where $\pounds_\xi$ denotes the Lie derivative and R^i_{klj} denotes the mixed Riemann tensor. The importance of CC symmetries for general relativity was pointed out and the close connection with covariant conservation laws stated.

In this paper, we investigate CC's admitted by vacuum fields, i.e., $R_{ik} = 0$, which possess a covariant constant vector. Such fields are called plane-fronted waves with parallel rays or pp waves. There are several reasons why we turn our attention to pp waves. First, they have been extensively studied so that all possible occurring isometry groups together with a representative metric are known.[2,3] Second, for vacuum fields the more familiar symmetries such as projective collineations and conformal collineations are subcases of CC's. Finally, pp waves are gravitational null fields for which a covariant conservation law follows if they admit a CC.

So we start with a brief summary of CC's and related symmetries for the case of vacuum fields. Section III is devoted to the definition of pp waves, the general form of the metric and components of the Riemann tensor.

In Sec. IV, we write down the explicit equations for the vectors ξ^i defining CC's. Formally, we get 20 coupled partial differential equations of first degree with nonconstant coefficients. However, by pure algebraic manipulations, it is possible to reduce them into two sets. One set (10 equations) are relations only between the partial derivatives of the vector ξ^i itself, not containing the unspecified function of the pp waves, while the other set, depending on the special structure of these functions, can be reduced to two. We can then integrate the first 10 equations to obtain the necessary structure of the vectors ξ^i for CC's. We then give the solutions of the second set of equations for five types of pp waves. The result is that general pp wave admits CC's only in the lightlike direction of the covariant constant vector. For plane, cylindrically symmetric, and screw-symmetric waves, more general CC's exist. For all types, we give the form of the vectors ξ^i and compare them with their corresponding Killing vectors (Table I, Sec. V).

In Sec. VI, we show that all the types discussed admit, in general, proper CC's, i.e., the ξ^i satisfy CC's but not a higher symmetry.

Finally, we discuss the covariant conservation law following from a CC. We do not attempt in this paper to give a physical interpretation to the CC's found.

II. CURVATURE COLLINEATIONS AND RELATED SYMMETRIES

A Riemann space–time admits a CC if, for infinitesimal transformations $\bar{x}^i = x^i + \xi^i\delta\epsilon$, the Lie derivative of the Riemann tensor R^i_{klj} in the direction of ξ^i vanishes:

$$\pounds_\xi R^i_{klj} = 0. \tag{1}$$

[10] J. Lehner, J. Math. Mech. 11, 173 (1962).
[11] G. R. Hintz, Ph.D. thesis, Purdue University, 1969.
[12] P. A. Newman and R. L. Bowden, in "Neutron Transport Theory Conference, January 20–24, 1969," ORO-3858-1, USAEC, 1969, p. 289.
[13] P. A. Newman, Ph.D. thesis, Virginia Polytechnic Institute, 1969.
[14] I. Kuščer, N. J. McCormick, and G. C. Summerfield, Ann. Phys. (N.Y.) 30, 411 (1964).
[15] R. L. Bowden, F. J. McCrosson, and E. A. Rhodes, J. Math. Phys. 9, 753 (1968).
[16] G. J. Mitsis, ANL Report No. ANL-6787, 1963.
[17] T. W. Mullikin, J. Math. Anal. Appl. 5, 184 (1962).
[18] K. Kowalska, Nucl. Sci. Eng. 24, 260 (1966).

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Vacuum fields which admit a covariant constant vector are investigated in order to find "curvature collineations," i.e., $\pounds R^i_{klj} = 0$. For all discussed types of pp waves it is shown that proper curvature collineations exist. We state the explicit form of these transformations.

I. INTRODUCTION

A special symmetry property of Riemannian manifolds called "curvature collineations" (CC's) was recently proposed.[1] This symmetry is defined by $\pounds_\xi R^i_{klj} = 0$ for infinitesimal transformations $\bar{x}^i = x^i + \xi^i\delta\epsilon$, where $\pounds_\xi$ denotes the Lie derivative and R^i_{klj} denotes the mixed Riemann tensor. The importance of CC symmetries for general relativity was pointed out and the close connection with covariant conservation laws stated.

In this paper, we investigate CC's admitted by vacuum fields, i.e., $R_{ik} = 0$, which possess a covariant constant vector. Such fields are called plane-fronted waves with parallel rays or pp waves. There are several reasons why we turn our attention to pp waves. First, they have been extensively studied so that all possible occurring isometry groups together with a representative metric are known.[2,3] Second, for vacuum fields the more familiar symmetries such as projective collineations and conformal collineations are subcases of CC's. Finally, pp waves are gravitational null fields for which a covariant conservation law follows if they admit a CC.

So we start with a brief summary of CC's and related symmetries for the case of vacuum fields. Section III is devoted to the definition of pp waves, the general form of the metric and components of the Riemann tensor.

In Sec. IV, we write down the explicit equations for the vectors ξ^i defining CC's. Formally, we get 20 coupled partial differential equations of first degree with nonconstant coefficients. However, by pure algebraic manipulations, it is possible to reduce them into two sets. One set (10 equations) are relations only between the partial derivatives of the vector ξ^i itself, not containing the unspecified function of the pp waves, while the other set, depending on the special structure of these functions, can be reduced to two. We can then integrate the first 10 equations to obtain the necessary structure of the vectors ξ^i for CC's. We then give the solutions of the second set of equations for five types of pp waves. The result is that general pp wave admits CC's only in the lightlike direction of the covariant constant vector. For plane, cylindrically symmetric, and screw-symmetric waves, more general CC's exist. For all types, we give the form of the vectors ξ^i and compare them with their corresponding Killing vectors (Table I, Sec. V).

In Sec. VI, we show that all the types discussed admit, in general, proper CC's, i.e., the ξ^i satisfy CC's but not a higher symmetry.

Finally, we discuss the covariant conservation law following from a CC. We do not attempt in this paper to give a physical interpretation to the CC's found.

II. CURVATURE COLLINEATIONS AND RELATED SYMMETRIES

A Riemann space–time admits a CC if, for infinitesimal transformations $\bar{x}^i = x^i + \xi^i\delta\epsilon$, the Lie derivative of the Riemann tensor R^i_{klj} in the direction of ξ^i vanishes:

$$\pounds_\xi R^i_{klj} = 0. \tag{1}$$

The Lie derivative can be written explicitly either in terms of partial or covariant differentiation[4]

$$\pounds_\xi R^i_{klj} = R^i_{klj,m}\xi^m - R^m_{klj}\xi^i_{,m} + R^i_{mlj}\xi^m_{,k} + R^i_{kmj}\xi^m_{,l} + R^i_{klm}\xi^m_{,j}, \quad (2)$$

where, as usual, a comma indicates partial differentiation and a semicolon covariant differentiation. From the relation (we drop the ξ, since it is always understood)

$$\pounds R^i_{klj} = \pounds(g^{im}R_{mklj}) = (\pounds g^{im})R_{mklj} + g^{im}\pounds R_{mklj},$$

we note that, if $\pounds g^{ik} = 0$, then $\pounds R^i_{klj} = 0$ is equivalent to $\pounds R_{iklj} = 0$. We assume that g_{ik} has signature $(+++-)$.

Following Ref. 1, a CC is called proper if it does not imply one of the following higher symmetries:

conformal collineations (Conf C's) given by

$$\pounds\Gamma^i_{jh} = (\delta^i_j\xi^l_{;lh} + \delta^i_h\xi^l_{;lj} - g_{jh}g^{is}\xi^l_{;ls})n^{-1},$$

$n = 4$ dimension of the space,

projective collineations (PC's)

$$\pounds\Gamma^i_{jh} = (\delta^i_j\xi^l_{;lh} + \delta^i_h\xi^l_{;lj})(n+1)^{-1},$$

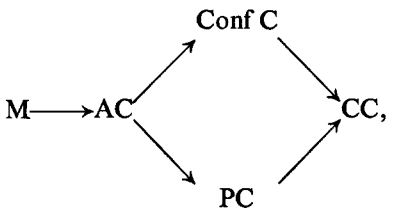
affine collineations (AC's)

$$\pounds\Gamma^i_{jk} = 0,$$

and *motions* (M's) which are defined by the Killing equations

$$\pounds g_{ik} = 0.$$

For vacuum fields $R_{ik} = 0$, every PC and Conf C is a CC; we thus have, in order of decreasing symmetry,



where the preceding symmetry always implies the following one. Therefore, a CC is proper if it is neither a Conf C nor a PC.

III. pp WAVES

If a vacuum field admits a covariant constant vector its Riemann tensor is of degenerate type[5] N and the covariant vector is necessarily lightlike. These fields are called plane-fronted waves with parallel rays or pp waves.

The metric of pp waves can always be written in the form

$$ds^2 = dx^2 + dy^2 + 2\,du\,dv + 2H(x, y, u)\,du^2, \quad (3)$$

where $H(x, y, u)$ is any arbitrary function in x, y, and u which satisfies the vacuum field equations $R_{ik} = 0$.

For the metric (3), the field equation for H reads simply

$$H_{xx} + H_{yy} = 0, \quad (4)$$

where H_{xx} and H_{yy} mean second partial derivatives with respect to x and y, respectively.[6] The covariant constant vector is $k^i \sim \delta^i_3$ with $k^i_{;j} = 0$ and $k^ik_i = 0$.

From Eq. (3), one obtains the nonvanishing Γ's to

$$\Gamma^1_{00} = -H_1, \quad \Gamma^2_{00} = -H_2, \quad \Gamma^3_{00} = H_0, \quad \Gamma^3_{01} = H_1, \quad \Gamma^3_{02} = H_2. \quad (5)$$

If we use the notation of Ref. 2, where the sign of the Riemann tensor is defined by

$$\tfrac{1}{2}R^i_{klj} = \Gamma^i_{k[l,j]} + \Gamma^m_{k[l}\Gamma^i_{j]m},$$

where the subscript brackets mean antisymmetrization, then the tensor R_{iklj} is given by

$$R_{iklj} = H_{mn}\delta^{0m}_{ik}\delta^{0n}_{lj} \quad \text{with} \quad \delta^{ab}_{ik} = 2\delta^a_{[i}\delta^b_{k]}$$

and, for R^i_{klj}, one gets the following nonvanishing components with the help of Eq. (4):

$$R^1_{010} = -R^2_{020} = -R^3_{110} = R^3_{220} = H_{11},$$
$$R^2_{010} = R^1_{020} = -R^3_{120} = -R^3_{210} = H_{12}. \quad (6)$$

Only two of them are independent, but for CC's we need all components because they lead to different Eqs. (1).

IV. THE EQUATIONS $\pounds R^i_{klj} = 0$

From symmetry properties of Eq. (1), taking into account the cyclic identity on the mixed curvature tensor, there are formally $n^2[\frac{1}{2}n(n-1) - 1] = 80$ equations. But since only a few components of the Riemann tensor are nonzero, this number is strongly reduced. Note that zero components also contribute to Eq. (1) when three indices belong to a nonvanishing component.

Introducing the result (6) into Eqs. (2), we get first for the contributing zero components the

equations

$$\pounds R^0{}_{010} = -H_{11}\xi^0{}_{,1} - H_{12}\xi^0{}_{,2} = 0, \tag{7}$$

$$\pounds R^3{}_{010} = -H_{11}(\xi^3{}_{,1} + \xi^1{}_{,0}) - H_{12}(\xi^3{}_{,2} + \xi^2{}_{,0}) = 0, \tag{8}$$

$$\pounds R^0{}_{020} = -H_{12}\xi^0{}_{,1} + H_{11}\xi^0{}_{,2} = 0, \tag{9}$$

$$\pounds R^3{}_{020} = -H_{12}(\xi^3{}_{,1} + \xi^1{}_{,0}) + H_{11}(\xi^3{}_{,2} + \xi^2{}_{,0}) = 0, \tag{10}$$

$$\pounds R^0{}_{110} = -\pounds R^0{}_{220} = H_{11}\xi^0{}_{,3} = 0, \tag{11}$$

$$\pounds R^1{}_{110} = H_{11}(\xi^1{}_{,3} + \xi^0{}_{,1}) = 0, \tag{12}$$

$$\pounds R^2{}_{110} = -H_{11}\xi^2{}_{,3} + H_{12}\xi^0{}_{,1} = 0, \tag{13}$$

$$\pounds R^0{}_{120} = \pounds R^0{}_{210} = H_{12}\xi^0{}_{,3} = 0, \tag{14}$$

$$\pounds R^1{}_{120} = H_{12}(\xi^1{}_{,3} + \xi^0{}_{,1}) = 0, \tag{15}$$

$$\pounds R^2{}_{120} = H_{12}\xi^2{}_{,3} + H_{11}\xi^0{}_{,1} = 0, \tag{16}$$

$$\pounds R^1{}_{210} = H_{12}\xi^1{}_{,3} + H_{11}\xi^0{}_{,2} = 0, \tag{17}$$

$$\pounds R^2{}_{210} = H_{12}(\xi^2{}_{,3} + \xi^0{}_{,2}) = 0, \tag{18}$$

$$\pounds R^1{}_{220} = -H_{11}\xi^1{}_{,3} + H_{12}\xi^0{}_{,2} = 0, \tag{19}$$

$$\pounds R^2{}_{220} = -H_{11}(\xi^2{}_{,3} + \xi^0{}_{,2}) = 0. \tag{20}$$

Because, for $(H_{11})^2 + (H_{12})^2 = 0$, space is flat, which we exclude, it follows from Eqs. (11) and (14) that

$$\xi^0{}_{,3} = 0, \tag{21}$$

from Eqs. (7) and (9) that

$$\xi^0{}_{,1} = 0, \quad \xi^0{}_{,2} = 0, \tag{22}$$

and then from Eqs. (12), (15), (17), (19) and (13), (16), (18), (20) that

$$\xi^1{}_{,3} = 0, \quad \xi^2{}_{,3} = 0. \tag{23}$$

The remaining two Eqs. (8) and (10) lead finally to the relations

$$\begin{aligned} \xi^3{}_{,2} + \xi^2{}_{,0} &= 0, \\ \xi^3{}_{,1} + \xi^1{}_{,0} &= 0. \end{aligned} \tag{24}$$

For the nonvanishing components of the Riemann tensor, Eq. (1) gives

$$\begin{aligned} \pounds R^1{}_{010} &= -\pounds R^2{}_{020} \\ &= H_{11l}\xi^l + 2H_{11}\xi^0{}_{,0} - H_{12}(\xi^1{}_{,2} - \xi^2{}_{,1}) = 0, \end{aligned} \tag{25}$$

$$\begin{aligned} \pounds R^2{}_{010} &= H_{12l}\xi^l + H_{12}(2\xi^0{}_{,0} + \xi^1{}_{,1} - \xi^2{}_{,2}) \\ &\quad - 2H_{11}\xi^2{}_{,1} = 0, \end{aligned} \tag{26}$$

$$\begin{aligned} \pounds R^1{}_{020} &= H_{12l}\xi^l + H_{12}(2\xi^0{}_{,0} - \xi^1{}_{,1} + \xi^2{}_{,2}) \\ &\quad + 2H_{11}\xi^1{}_{,2} = 0, \end{aligned} \tag{27}$$

$$\begin{aligned} \pounds R^3{}_{110} &= -H_{11l}\xi^l - H_{11}(\xi^0{}_{,0} + 2\xi^1{}_{,1} - \xi^3{}_{,3}) \\ &\quad - 2H_{12}\xi^2{}_{,1} = 0, \end{aligned} \tag{28}$$

$$\begin{aligned} \pounds R^3{}_{120} &= \pounds R^3{}_{210} \\ &= -H_{12l}\xi^l - H_{12}(\xi^0{}_{,0} + \xi^1{}_{,1} + \xi^2{}_{,2} - \xi^3{}_{,3}) \\ &\quad - H_{11}(\xi^1{}_{,2} - \xi^2{}_{,1}) = 0, \end{aligned} \tag{29}$$

$$\begin{aligned} \pounds R^3{}_{220} &= H_{11l}\xi^l + H_{11}(\xi^0{}_{,0} + 2\xi^2{}_{,2} - \xi^3{}_{,3}) \\ &\quad - 2H_{12}\xi^1{}_{,2} = 0. \end{aligned} \tag{30}$$

By simple algebraic calculations

H_{11} [Eq. (26) − Eq. (27)] + H_{12} [Eq. (28) + Eq. (30)],

we get

$$\xi^2{}_{,1} + \xi^1{}_{,2} = 0 \tag{31}$$

and, from Eq. (26) − Eq. (27), then

$$\xi^1{}_{,1} - \xi^2{}_{,2} = 0. \tag{32}$$

With these results, we go back to Eqs. (25)–(30); it turns out that Eq. (26) = Eq. (27) and Eq. (28) = −Eq. (30). Adding Eq. (28) and Eq. (25), using the results obtained so far, we have

$$\xi^1{}_{,1} = \tfrac{1}{2}(\xi^0{}_{,0} + \xi^3{}_{,3}). \tag{33}$$

Now Eq. (25) = −Eq. (28) = Eq. (30) and Eq. (26) = Eq. (27) = −Eq. (29). So, finally, there remain only two coupled partial first-order differential equations

$$\begin{aligned} H_{11l}\xi^l + 2H_{11}\xi^0{}_{,0} + 2H_{12}\xi^2{}_{,1} &= 0, \\ H_{12l}\xi^l + 2H_{12}\xi^0{}_{,0} - 2H_{11}\xi^2{}_{,1} &= 0. \end{aligned} \tag{34}$$

From Eqs. (21)–(24) and (31)–(33), which do not involve the function $H(x, y, u)$, we can draw conclusions about the general form of the vectors ξ^i in order that these be CC's.

First, we see that $\xi^0 = \xi^0(u)$ is only a function of u, while ξ^1 and ξ^2 are independent of v. Equations (31) and (32) are just the Cauchy–Riemann differential equations, so that ξ^1 and ξ^2 are, in x and y, real and imaginary parts of a complex function of $z = x + iy$, also depending on u.

Using the relations (24) and the integrability condition $\xi^3{}_{,21} = \xi^3{}_{,12}$, we see that

$$\xi^1{}_{,02} = \xi^2{}_{,01} = 0.$$

An ansatz for ξ^1 and ξ^2 with the above results and with the aid of Eq. (33) leads, after a straightforward calculation, to the structure of the ξ^i:

$$\begin{aligned} \xi^0 &= \int [2c(u) - b(u)]\, du + g, \\ \xi^1 &= c(u)x + d(u) + ay, \\ \xi^2 &= c(u)y + e(u) - ax, \\ \xi^3 &= -[\tfrac{1}{2}c'(u)(x^2 + y^2) + d'(u)x + e'(u)y] \\ &\quad + b(u)v + f(u), \end{aligned} \tag{35}$$

TABLE I. Restrictions on the arbitrary functions of Eqs. (34) in order that the vectors ξ^i define CC's or M's.

Type of wave	$H(x, y, u)$	CC	Killing vectors	G_i
General pp	—	$a = g = 0$ $b(u) = c(u) = d(u) = e(u) = 0$	$f(u) = \text{const}$	G_1
Screw symmetric	$\phi(x, y)$	$a = 0$ $b(u) = c(u) = d(u) = e(u) = 0$	$f(u) = \text{const}$	G_2
Cylindrically symmetric	$\ln (x^2 + y^2)^{\frac{1}{2}}$	$b(u) = c(u)$ $d(u) = e(u) = 0$	$b(u) = c(u) = 0$ $f(u) = \text{const}$	G_3
Plane wave	$\frac{1}{2}F(u)(x^2 - y^2) + G(u)xy$ $F(u) \simeq G(u)$	$a = g = 0$ $2c(u) = b(u)$	$b(u) = c(u) = 0$ $f(u) = \text{const}$ $d(u)F + e(u)G = d''(u)$ $d(u)G - e(u)F = e''(u)$	G_5
Plane wave linearly polarized	$\frac{1}{2}(x^2 - y^2)$	$a = 0$ $2c(u) = b(u)$	$b(u) = c(u) = 0$ $f(u) = \text{const}$ $e''(u) + e(u) = 0$ $d''(u) - d(u) = 0$	G_6

where a and g are real constants, and $b(u)$, $c(u)$, $d(u)$, $e(u)$, and $f(u)$ are arbitrary functions of u only. $c'(u)$ means differentiation with respect to u.

It is easily verified that this vector actually satisfies the required relations. In order to be a CC, the ξ^i have to be a solution of the remaining two Eqs. (34). Thus, for every possible $H(x, y, u)$, the arbitrary functions in Eqs. (35) have to be chosen to satisfy Eqs. (34).

V. SPECIAL CASES FOR $H(x, y, u)$

In Ref. 2, a detailed discussion of pp waves is given. They are classified in terms of isometry groups for different types of the function $H(x, y, u)$.

We proceed to investigate possible solutions of Eqs. (34) for five of these types. The obtained vectors ξ^i define CC's and can be compared with their corresponding Killing vectors.

First, let $H(x, y, u)$ be restricted only by the vacuum field equation (4). Since the vectors ξ^i given in Eqs. (35) have a fixed x and y dependence, while $H(x, y, u)$ is arbitrary up to Eq. (4), inspection of Eqs. (34) shows us that only the trivial solution with

$$a = b(u) = c(u) = d(u) = e(u) = 0$$

is possible. The component ξ^3 does not enter in Eqs. (34), so that there is no restriction on the function $f(u)$. Therefore, general pp waves admit CC's of the form

$$\xi^i = \delta^i_3 f(u). \tag{36}$$

Because $\pounds R^i{}_{klj} = 0$ is an integrability condition for the Killing equation $\pounds g_{ik} = 0$, the Killing vectors must be obtained as special cases from the admitted CC's. In general, pp waves admit only a G_1, which acts in the direction of the covariant constant vector. Thus, the Killing vector is lightlike and in the direction of propagation, i.e., in our coordinates

$$\xi^i = \delta^i_3.$$

If one restricts $H(x, y, u)$ to special functions, then nontrivial solutions of Eqs. (34) also exist. Results for special types of pp waves are listed in Table I.[7]

The first column denotes the type of wave and the second gives the corresponding form of $H(x, y, u)$. The third column gives the restrictions on the constants a and g and the functions $b(u)$, $c(u)$, $d(u)$, $e(u)$, and $f(u)$, which occur in Eq. (35), so that the vectors ξ^i define CC's. Constants or functions not listed remain arbitrary. The fourth column states further restrictions on these functions, so that the corresponding vectors are also Killing vectors. Note that all restrictions of the preceding column must also hold here. Finally, the order of the isometry group of the Killing vector is given; e.g., we infer from the table that screw-symmetric pp waves admit CC of the form

$$\xi^i = g\delta^i_0 + f(u)\delta^i_3,$$

while the Killing vectors of the 2-parameter isotropy group are given by

$$\xi^i = g\delta^i_0 + f\delta^i_3, \quad f = \text{const}.$$

VI. PROPER CC

So far, we have seen that all listed waves admit a CC, which only for very special choices of the arbitrary functions are also M, so that, in general, $\pounds g_{ik} \neq 0$. To confirm that the CC found are proper CC, we must show that they are not Conf C's or PC's.

First we deduce that for all cases, in general, $\pounds \Gamma^i_{kl} \neq 0$, which is equivalent to

$$\xi_{i;kj} + \xi_{k;ij} \neq 0.$$

There are 40 equations, but if one component does not vanish, the vector ξ^i cannot be an AC. By looking at the $\xi_{0;0}$ term, we infer that $\xi_{0;00} \neq 0$ for each of the cases.

A necessary condition for a CC to be a PC or Conf C is that

$$\xi^i_{;ijk} = 0. \tag{37}$$

The only nonvanishing component for ξ^i from Eq. (35) is

$$\xi^0_{;000} \sim c''(u).$$

For the last three types of Table I there is no restriction on $c(u)$; $c''(u)$ is in general different from zero and thus the corresponding CC's are not PC's or Conf C's. Together with the above result that $\pounds\Gamma^i_{kl} \neq 0$, the ξ^i are proper CC's.

For the more general types, we note that $c(u) = 0$, and the necessary condition is fulfilled. However, also $\xi^i_{;i} = 0$ and, from the definitions of Conf C's and PC's in Sec. II, we see that the vectors ξ^i are then Conf C's or PC's only if the relation $\pounds\Gamma^i_{kl} = 0$ also holds, which is not true. We may thus state the following result.

Theorem: In a space with $R_{ik} = 0$, general pp waves admit lightlike *proper* CC's in the direction of the covariant constant vector.

VII. CONSERVATION LAW

It is well known that the existence of symmetry properties of the Riemannian manifold under continuous groups of motions lead to conservation laws, such as energy, linear and angular momentum.[8]

More general symmetry transformations have been discussed in connection with conservation laws, showing that, e.g., AC's or PC's are related to the existence of conserved quadratic first integrals.[9,10]

We want to discuss briefly a conservation law following from the existence of CC's for null gravitational fields. The theorem given in Ref. 1 states the following: If, in a space with $R_{ij} = 0$, a null field admits a CC, then it admits a covariant conservation law of the form

$$[(-g)^{\frac{1}{2}}T^{ikjl}\xi_j]_{;l} = 0, \tag{38}$$

where T^{ikjl} is the Bel–Robinson tensor which, for pp waves, has the structure

$$T^{ikjl} = Ik^ik^kk^jk^l, \tag{39}$$

with $k_{i;j} = 0$ and $k^ik_i = 0$, where I is a scalar depending on the function $H(x, y, u)$ of Eq. (3), and where k^i is the lightlike covariant constant Killing vector which has components $k^i \sim \delta^i_3$.

If we substitute for T^{ikjl} from Eq. (39) into Eq. (38), we obtain

$$k^jk^l\xi_{j;l} = 0.$$

This is satisfied by all CC's because of Eqs. (21) and (23).

For $k^i\xi_i \neq 0$, one deduces from Eq. (38) a conservation law which was first given by Sachs[11] for null fields:

$$[(-g)^{\frac{1}{2}}Ik^l]_{;l} = 0. \tag{40}$$

For general pp waves, the CC's have $\xi^i = \delta^i_3 f(u)$ and, therefore, $k^i\xi_i = 0$ for all such vectors ξ^i. It is, therefore, not possible to obtain in this general case the conservation law Eq. (40) from Eq. (38).

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[1] G. H. Katzin, J. Levine, and W. R. Davis, J. Math. Phys. **10**, 617 (1969).

[2] P. Jordan, W. Kundt, and J. Ehlers, Akad. Wiss. Lit. (Mainz), Abhandl. Math.-Nat. Kl. **2**, 21 (1960).

[3] J. Ehlers and W. Kundt, in *Gravitation: An Introduction to Current Research*, L. Witten, Ed. (Wiley, New York, 1962), p. 49.

[4] J. A. Schouten, *Ricci-Calculus* (Springer, Berlin, 1954), 2nd ed.

[5] For algebraic classification of the Riemann tensor in connection with radiation see F. A. E. Pirani, *Brandeis Lectures, 1964, Vol. II: General Relativity* (Prentice Hall, Englewood Cliffs, N.J., 1965).

[6] We label coordinates by $u = x^0$, $x = x^1$, $y = x^2$, $v = x^3$ so that, e.g., $H_{xy} = H_{12} = \partial^2 H/\partial x\partial y$.

[7] For details and calculations see P. C. Aichelburg, ICTP Preprint No. IC/69/80, Trieste, 1969.

[8] For a review and further references see A. Trautmann, in *Gravitation: An Introduction to Current Research*, L. Witten, Ed. (Wiley, New York, 1962), p. 169.

[9] W. R. Davis and M. K. Moss, Nuovo Cimento **38**, 1558 (1965).

[10] G. H. Katzin and J. Levine, J. Math. Phys. **9**, 8 (1968).

[11] R. K. Sachs, Z. Physik **157**, 462 (1960); for the Bel–Robinson tensor see the Appendix.

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Analytic Function Method for the Many-Body Problem

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The equivalence of analytic functions in complex variable representations with conserved functions in real variable representations is utilized to write eigenvalue equations for the energy and momentum on the complex planes. A self-consistent field method is then developed and used to study the scalar interactions of a particle gas with arbitrary coupling strength. The eigenvalue equations for momentum and energy yield equilibrium solutions which are functions only of the initial values and a renormalized coupling strength. The results are applied to the electron gas and to the Bose gas.

INTRODUCTION

In earlier studies of the analytic properties of functions of two complex variables, a self-consistent field method was developed for obtaining the energy and momentum eigenvalues for an interacting particle gas to first order in perturbation theory.[1] Subsequently, a self-consistent field method suitable for strong interactions was developed[2] and applied to the interaction of a spinor and a scalar field. We consider now a problem of interest when there are many particles interacting by means of scalar fields of arbitrary strength. It is well known that the formulation of this problem in terms of an expansion in 2-body potentials is not convergent. We consider instead a single particle interacting with the remaining particles by means of an effective field defined by the inhomogeneous wave equation. The field consists of a constant term plus a term representing the fluctuations and oscillations. The eigenvalues for the constant field are assumed known, and the wave equation is then solved self-consistently with the interacting Hamiltonian for the new eigenvalues.

Our method makes use of transformations of the form

$$\begin{aligned} P^{\dagger}(z) &= e^{z}P(z)e^{-z} \\ &= P(z) + [z, P] + \tfrac{1}{2}[z, [z, P]] + \cdots \\ &= P(z) + \sigma_z \frac{\partial P}{\partial z^*} + \frac{\sigma_z^2}{2}\frac{\partial^2 P}{\partial z^{*2}} + \cdots, \end{aligned} \tag{1}$$

where z is a normalized complex scalar and σ_z is a constant. The transformation of the second line to the third line follows from the fundamental quantum conditions taking $\mathrm{Re}\, z$ and $\mathrm{Im}\, z$ for the canonical variables.[2] We now look for values z' for which $P^{\dagger} = P$, that is, z' satisfying

$$\lim_{z \to z'} [z, P] = \sigma_{z'} \frac{\partial P}{\partial z^{*'}} \equiv 0, \tag{2}$$

and it can be shown that, if (2) holds, all the higher-order terms vanish in (1). Now $\partial P/\partial z^* = 0$ are the Cauchy–Riemann equations which give the necessary condition that P be analytic in z so that, provided P is differentiable, (2) defines the analytic region of P on the z plane. Thus the eigenvalues z' satisfying (2) define the analytic region. Also, if $P^{\dagger}(z') = P(z')$, then (1) is clearly a unitary transformation and the z' are conserved or, conversely, the z' are the conserved eigenvalues under the transformation. It follows that the analytic function $P(z')$ corresponds to a conserved function for real variables so that the problem of obtaining the new eigenvalues, in an interacting particle gas, for example, reduces to finding the analytic region, that is, the solutions of (2).

Our procedure then is to obtain equations such as (2) for all of the conserved variables, that is, momentum, energy, and particle number in an interacting system, and solve them simultaneously for the new eigenvalues. We work, therefore, entirely in momentum and energy space and, since the momentum and energy are complex, the eigenvalues k' and E' give also the interaction range and decay time of the particle excitations (we define particle excitation as a particle plus its associated *short-range* field) and the particle excitation eigenvalues give just the renormalized particle levels, including the effects of finite range and line width.

The generality of this procedure is due to two factors: (i) the use of complex variables throughout, which allows an exact solution of equations such as (1) and (2), whereas for real variables the equivalent of (2) is a minimization condition which, however, does not insure that the higher-order terms vanish; (ii) with the use of symmetry transformations such as (1), one avoids dealing with equations of motion which, of course, cannot be solved for strong coupling without additional constraints.

1. DERIVATION OF THE EIGENVALUE EQUATIONS

If we consider the stationary states of the density

$$\begin{aligned} \rho(\mathbf{x}, t) &= e^{iH(t-t_0)}\rho(\mathbf{x}, t_0)e^{-iH(t-t_0)} \\ &= \rho(\mathbf{x}, t_0), \end{aligned} \tag{3}$$

then the density equation of motion becomes

$$[H, \rho] = 0, \tag{4}$$

where

$$H(\mathbf{x}, t) = -(2m)^{-1}\nabla^2 + U(\mathbf{x}, t), \tag{5}$$

and U is defined by the inhomogeneous wave equation

$$\Box U(\mathbf{x}, t) = \lambda\rho(\mathbf{x}, t), \tag{6}$$

where λ is the coupling strength. Now (3) is evidently a conservation condition on the density; but this constraint has no great physical significance, whereas conservation conditions on H are of fundamental importance. But, if (4) holds, then $-[H, \rho]$ occurs as the first-order term in

$$H^\dagger = e^{\rho/\rho_0} H e^{-\rho/\rho_0}, \tag{7}$$

so that (4) is satisfied provided $H^\dagger = H$. In this case the density is conserved in the interacting system, and it can easily be shown that transformations such as (7) with ρ/ρ_0 replaced by k/k_0 also conserve momentum if $H^\dagger = H$. There is a similar transformation for energy conservation. The transformation (7) and similar transformations on the momentum and energy planes are obviously unitary, provided that $H^\dagger = H$ for each transformation. We must therefore obtain H as a function of momentum and energy by Fourier-transforming H and (6). We then consider the analytic properties of $H(k, E)$ after continuation onto the lower semiplanes. It is obvious from (4) that $dH/d\rho^* = 0$ so that, provided H is differentiable, H is then an analytic function of ρ and in this case the function continued into the fourth quadrant satisfies $dH^*/d\rho = 0$. Since the kinetic energy is obviously an analytic function of k and E, it follows that U is also analytic in both variables. From $dH^*/d\rho = 0$ it is evident that the continuation of the kinetic energy and U^* are also analytic in the fourth quadrant. Since H is analytic, it is invariant under all rotations if the Hamiltonian represents a rigid body, as seems evident if the density is conserved; otherwise, H is invariant under positive-sense rotations only, whereas H^* is invariant only under negative-sense rotations. That H is invariant under rotations in the positive sense, provided that H is analytic, follows from a consideration of the infinitesimal inhomogeneous rotations

$$\left(1 + z^* \frac{\partial}{\partial z^*}\right) H = (1 + \tfrac{1}{2}S_z + \tfrac{1}{2}iL_z)H \tag{7'a}$$

where, with $z = z_1 + iz_2$,

$$S_z = z_1 \frac{\partial}{\partial z_1} + z_2 \frac{\partial}{\partial z_2}, \quad L_z = z_1 \frac{\partial}{\partial z_2} - z_2 \frac{\partial}{\partial z_1} \tag{7'b}$$

are operators representing the radial deformations and pure rotations on the z plane. With the Cauchy–Riemann equations

$$\frac{\partial H}{\partial z_1} = -i \frac{\partial H}{\partial z_2}, \tag{7'c}$$

it can easily be shown that $S_z H = -iL_z H$ so that H is conserved in (7'a) but not under $1 + \frac{1}{2}S_z - \frac{1}{2}L_z$. On the other hand, the operator $z\partial/\partial z$ gives $S_z - iL_z$ so that H^* is conserved, since

$$\frac{\partial H^*}{\partial z_1} = i \frac{\partial H^*}{\partial z_2}, \tag{7'd}$$

but H is not conserved.

In order that H be a rotational invariant on the entire plane, it is necessary that H be analytic on the entire plane, that is, a constant. We therefore carry out the continuations by rotations in the positive sense, mapping the first quadrants onto the third quadrants so that $k \to -k$, $q \to -q$, and $E \to -E$. Writing $H^\dagger$ for the resulting function, we now carry out the transformation

$$\begin{aligned} H'(k, E) &= e^{\rho^*(k,E)/\rho_0} H^\dagger(-k, -E) e^{-\rho^*(k,E)/\rho_0} \\ &= H^\dagger + \rho_0^{-1}[\rho^*, H^\dagger] + \cdots \\ &= H^\dagger + \frac{\sigma_\rho^*}{\rho_0}\frac{dH^\dagger}{d\rho} + \cdots. \end{aligned} \tag{7'e}$$

The terms $\partial H^\dagger/\partial\rho$, $\partial^2 H^\dagger/\partial\rho^2, \cdots$ are obtained by taking as canonical variables the real and imaginary parts of ρ and using the fundamental quantum conditions; a general formulation for several complex variables is given in Ref. 2. We now look for eigenvalues k' and E' for which $H^\dagger = H'$, that is, for which

$$\begin{aligned} \lim_{k\to k'} \lim_{E\to E'} [\rho^*, H^\dagger] &= \sigma_\rho^* \frac{dH^\dagger}{d\rho} \\ &= \sigma_\rho^* \left(\frac{\partial H^\dagger}{\partial \rho} + \frac{dE'}{d\rho}\frac{\partial H^\dagger}{\partial E'} + \frac{dk'}{d\rho}\frac{\partial H^\dagger}{\partial k'}\right) \\ &\equiv 0. \end{aligned} \tag{8}$$

In general,

$$\frac{dE'}{d\rho} \neq 0, \quad \frac{dk'}{d\rho} \neq 0, \tag{8'}$$

since ρ is a continuous function of k and E, and ρ does not conserve momentum or energy (for complex functions $\partial E/\partial\rho = 0$ insures that $\partial\rho/\partial E = 0$). From the three terms on the rhs of (8), we obtain three eigenvalue equations which give the constants of motion for the interacting system (see Appendix).

From (9) and the second term of (8′), we obtain an eigenvalue equation for the energy,

$$\lim_{E\to E'}[E^*, H^\dagger] = \sigma^*_{E'}\frac{\partial H^\dagger}{\partial E'} = 0, \tag{9}$$

where Re E' and Im E' are canonical variables satisfying the fundamental quantum conditions. Obviously, (9) provides the condition that the E' be constants of the motion, according to the elementary definitions of the commutator of any variable with H. It is not difficult to show that (9) imposes energy conservation on $H^\dagger$. Thus, in

$$H'(-k, E) = e^{E^*/E_0}H^\dagger(-k, -E)e^{-E^*/E_0} = H^\dagger + E_0^{-1}[E^*, H^\dagger] + \cdots, \tag{9′}$$

$H^\dagger = H'$ for E' satisfying (9); then, with $H^\dagger = H_0^\dagger + U^\dagger(-k, -E)$, the E' are the new eigenvalues.

Similarly, we obtain from (8′) and the third term in (8) the eigenvalue equation for the momentum,

$$\lim_{k_\alpha\to k_{\alpha'}}[k^*_\alpha, H^\dagger] = \sigma^*_{k'\alpha}\frac{\partial H^\dagger}{\partial k'_\alpha} = 0, \tag{10}$$

which guarantees momentum conservation in H by

$$H'(k, -E) = e^{k_\alpha{}^*/k_0}H^\dagger(-k, -E)e^{-k_\alpha{}^*/k_0} = H^\dagger + k_0^{-1}[k^*_\alpha, H^\dagger] + \cdots, \tag{11}$$

where k_α is a complex scalar obtained from $\mathbf{k}\cdot\boldsymbol{\epsilon}$ with $\boldsymbol{\epsilon}$ being a vector with unity modulus. In (10) Re k'_α and Im k'_α are canonical variables satisfying $[k'_\alpha, k'^*_\alpha] = \text{const}$. As for E' in (9), Eq. (10) provides the condition that the k' be constants of the motion (see Appendix).

And, finally, the first term in (8) yields

$$\lim_{\rho\to\rho'}[\rho^*, H^\dagger] = \sigma^*_{\rho'}\frac{\partial H^\dagger}{\partial \rho'} = 0, \tag{12}$$

which conserves the number of particles in the final state equilibrium. One should note at this point that (9), (10), and (12) hold, provided that there exists only a single set of canonical variables satisfying the canonical equations (see Appendix).

Finally (9), (10), and (12) hold simultaneously so that k', E', and ρ must be simultaneous eigenvalues satisfying all three equations. For these reasons we must take $k(E)$ and $E(k)$ in (9) and (10).

2. SOLUTIONS OF THE EIGENVALUE EQUATIONS

Taking matrix elements of (4) between initial state $\mathbf{p}$ and final state $\mathbf{p}+\mathbf{q}=\mathbf{k}$, E and of (6) between $\mathbf{q}$, E, and 0, we choose U such that

$$H(k, E) = E_p - E_k + U(q, E) + \text{boundary and initial values} \tag{13}$$

where

$$U(q, E) = \lambda\Gamma(q, E)\rho(q, E) + \text{boundary and initial values}, \tag{14}$$

and where

$$\Gamma(q, E) = [(E^2/c^2) - q^2]^{-1} \tag{15}$$

is the field propagator. The kinetic energy in (13) is obviously an analytic function of the momentum and energy, and it is evident H is analytic in all variables provided that there exist k', E', and ρ' satisfying (8) and (12). Now, carrying out the analytic continuations of (13) and (14) by rotations in the positive sense, we see from the discussions of (7′a)–(7′d) that H is invariant under the rotations provided that H is analytic in all variables. Then with (9), (10), and (12) we obtain H analytic on the entire planes, so that H is invariant under all possible rotations. Now (10) gives

$$k'_\alpha = m\frac{\partial U}{\partial k'_\alpha}. \tag{16}$$

The variation with respect to k_α is finite, and (16) can be evaluated by means of (14). Thus

$$[k^{*\prime}_\alpha, U(q', E)] = \lim_{k_\alpha\to k_{\alpha'}}\sigma^*_{k_\alpha}\frac{\partial U}{\partial k_\alpha} = \sigma^*_{k_{\alpha'}}\lambda\Gamma\left[\frac{\partial\rho}{\partial k'_\alpha} + 2\left((k'_\alpha - p_\alpha) - \frac{E}{c^2}\frac{\partial E}{\partial k'_\alpha}\right)\rho\Gamma\right]. \tag{17}$$

Combining (16) and (17) gives, for the momentum eigenvalues,

$$k'_\alpha = \frac{m\lambda\Gamma}{1 - 2m\lambda\rho\Gamma^2}\left(-2p_\alpha\rho\Gamma + \frac{\partial\rho}{\partial k'_\alpha} - \frac{2E}{c^2}\rho\Gamma\frac{\partial E}{\partial k'_\alpha}\right). \tag{18}$$

The first factor gives for the renormalized propagator

$$\Gamma' = \frac{\Gamma}{1 - 2m\lambda\rho\Gamma^2} = -\left(q^2 - \frac{E^2}{c^2} - \lambda\frac{2m\rho}{q^2 - E^2/c^2}\right)^{-1}, \tag{19}$$

which has a characteristic form for a field interacting with particles; the third term in the denominator results from the interaction and may be interpreted as the eigenvalue of a mass operator inserted into the wave equation (6).

The energy eigenvalue equation (9) gives

$$k_\alpha \frac{\partial k_\alpha}{\partial E'} = m \frac{\partial U}{\partial E'} \tag{20}$$

and

$$[E^{*\prime}, U(q, E')] = \lim_{E \to E'} \sigma_E^* \frac{\partial U}{\partial E} = \sigma_{E'}^* \lambda \Gamma \left[\frac{\partial \rho}{\partial E'} + 2\left((k_\alpha - p_\alpha) \frac{\partial k_\alpha}{\partial E'} - \frac{E'}{c^2} \right) \rho \Gamma \right]. \tag{21}$$

Now combining (20) and (21) gives

$$k_\alpha \frac{\partial k_\alpha}{\partial E'} = \frac{m\lambda\Gamma}{1 - 2m\lambda\rho\Gamma^2} \left[\frac{\partial \rho}{\partial E'} + 2\left(-p_\alpha \frac{\partial k_\alpha}{\partial E'} - \frac{E'}{c^2} \right) \rho \Gamma \right], \tag{22}$$

which has the same form as (18).

Equation (22) may be written

$$\frac{\partial k_\alpha}{\partial E'} \left(k_\alpha + \frac{2m\lambda\rho p_\alpha \Gamma^2}{1 - 2m\lambda\rho\Gamma^2} \right) = \frac{m\lambda\Gamma}{1 - 2m\lambda\rho\Gamma^2} \left(\frac{\partial \rho}{\partial E'} - \frac{2E'}{c^2} \rho \Gamma \right), \tag{23}$$

but taking the limit as $k_\alpha \to k'_\alpha$ yields an identity. However, for $dk_\alpha/dE' = 0$ corresponding to free-particle excitations or zero group velocity (for complex functions, $dk_\alpha/dE' = 0$ requires also that $dE'/dk_\alpha = 0$), consistent solutions of (18) and (23) are given by

$$E'^2/c^2 = q^2 + \rho/\rho_0\Gamma_0, \tag{24}$$

which may also be written

$$\rho/\rho_0 = \Gamma_0/\Gamma, \tag{25}$$

obtained by equating the rhs of (23) to zero. In (25) the equilibrium density and propagator are taken either in the noninteracting system if $U_0 = 0$, in which case $\Gamma_0 = 1/p^2$, or in the interacting system if $U_0 \neq 0$; in the latter case, $\rho_0 = \rho_0(p, q') = \rho_0(k') - \rho_0(p)$, the difference of the excited and ground state densities, and $\Gamma_0 = (p^2 - E_0^2/c^2)^{-1}$ and E_0 is a function of the coupling strength [see discussion of Eq. (40)].

With (18) and (25) we now obtain

$$k'_\alpha = -p_\alpha [g\rho_0/(\rho - g\rho_0)] \tag{26}$$

so that

$$q'_\alpha = -p_\alpha [\rho/(\rho - g\rho_0)], \tag{27}$$

where

$$g = a_0^{-1}\rho_0\Gamma_0^2, \quad a_0 = (2\pi m\lambda)^{-1}, \tag{28}$$

a_0 is the 2-particle scattering length, g is a dimensionless renormalized coupling strength which is a function of the initial values, and we have absorbed a factor π^{-1} into λ. Note that the sign of g now depends upon ρ_0, which introduces the many-body effects, as well as upon the 2-particle scattering length a_0 so that the effective interaction may be attractive or repulsive depending upon the sign of $a_0^{-1}\rho_0$.

Writing $\rho = \rho_0 + \rho_1$, we see that (27) becomes

$$q'_\alpha = -p_\alpha \left(1 + \frac{g}{1 - g + \rho_1/\rho_0} \right) \tag{29}$$

and for $\rho_1/\rho_0 \ll 1$ the term in parentheses becomes $1/(1 - g)$ which gives an expansion in powers of $g = 1/a_0 p$, in agreement with the result obtained from perturbation theory.[1] [It can easily be shown that (27) does not diverge in equilibrium; see Eq. (40).]

Now taking the limit of (24) as $q \to q'$ gives

$$\frac{E'^2}{c^2} = p^2 \left(\frac{\rho}{\rho - g\rho_0} \right)^2 + \frac{\rho}{\rho_0\Gamma_0}, \tag{30}$$

and with these expressions the new propagator becomes

$$\Gamma' = \lim_{q \to q'} \lim_{E \to E'} \frac{\Gamma}{1 - 2m\lambda\rho\Gamma^2} = \frac{\rho_0}{\rho - g\rho_0} \Gamma_0. \tag{31}$$

Obviously, as $\rho \to \rho_0$, also $g \to 0$ and Γ' reduces to the initial propagator. From (27), (30), and (31) it is evident that all of the new variables in the interacting system are obtained as functions of the renormalization factor $\rho/(\rho - g\rho_0)$.

With $q = \pi + i\kappa$, (27) gives, for real ρ_0,

$$\pi'_\alpha = -p_\alpha \frac{\operatorname{Re}\rho(\operatorname{Re}\rho + \rho_0 \operatorname{Re} g) + \operatorname{Im}\rho(\operatorname{Im}\rho - \rho_0 \operatorname{Im} g)}{(\operatorname{Re}\rho - \rho_0 \operatorname{Re} g)^2 + (\operatorname{Im}\rho - \rho_0 \operatorname{Im} g)^2} \tag{32}$$

and

$$\kappa'_\alpha = -p_\alpha \frac{\operatorname{Im}\rho(\operatorname{Re}\rho + \rho_0 \operatorname{Re} g) - \operatorname{Re}\rho(\operatorname{Im}\rho - \rho_0 \operatorname{Im} g)}{(\operatorname{Re}\rho - \rho_0 \operatorname{Re} g)^2 + (\operatorname{Im}\rho - \rho_0 \operatorname{Im} g)^2} \tag{33}$$

so that the interaction range diverges as the coupling is switched off.

Now (25) evidently reduces the field U to the zero-order value $U_0 = \lambda\rho_0\Gamma_0$; however, by integrating (16) with k' obtained from (26), we see that U equals U_0 times a renormalization factor, which is a function of ρ, g, and the initial values, and equals Γ' times a constant. The field may now be obtained in the form

$$\begin{aligned} U &= \lambda\rho\Gamma' \\ &= [\rho/(\rho - g\rho_0)]U_0, \end{aligned} \tag{34}$$

and from (30) we obtain also

$$\Gamma_0 = (p^2 - E_0^2/c^2)^{-1} \tag{35}$$

[see discussion of Eq. (40)]. The new variables (30)–(34) are all functions of the renormalized coupling strength g and the final and initial densities.

Finally, with (27) and (34) the Hamiltonian may be written as

$$H(\rho) = \frac{p^2}{2m}\left(1 - \frac{g^2\rho_0^2}{(\rho - g\rho_0)^2}\right) + U_0\frac{\rho}{\rho - g\rho_0}, \tag{36}$$

where $\rho = \rho(k', E')$, from (26) and (30), which gives

$$\rho = g\rho_0(q'_\alpha/k'_\alpha). \tag{37}$$

We now require that the Hamiltonian (36) satisfy the third eigenvalue equation (12) in the limits $k \to k'$ and $E \to E'$. Thus

$$\begin{aligned} \lim_{k\to k'}\lim_{E\to E'} &[\rho^*(k, E), H^\dagger(k, E)] \\ &= \sigma_\rho^* \frac{\partial H^\dagger(k', E')}{\partial\rho(k', E')} = 0, \end{aligned} \tag{38}$$

so that we need to evaluate

$$\begin{aligned} \lim_{\rho\to\rho'}\frac{\partial H^\dagger}{\partial\rho} &= \frac{g\rho_0}{(\rho' - g\rho_0)^2}\left(\frac{p^2}{m}\frac{g\rho_0}{(\rho' - g\rho_0)} - U_0\right) \\ &= 0, \end{aligned} \tag{39}$$

which gives for the equilibrium density

$$\begin{aligned} \rho' &= \frac{g\rho_0}{U_0}\left(\frac{p^2}{m} + U_0\right) \\ &= (1 + g)\rho_0 \end{aligned} \tag{40}$$

with the requirement that $\rho \to \rho_0$ as $\lambda \to 0$; this requires that $\Gamma_0 = p^{-2}$ in the limit so that $E_0/c = 0$ in the limit. Note that with (27), (34), and (37) one can verify that H is invariant under the inhomogeneous rotation operator

$$1 + k^*\nabla_k = 1 + \tfrac{1}{2}(S_k + iL_k), \tag{41}$$

where S_k and L_k are defined by (7'b).

And finally, using (40), we see that the equilibrium momentum, energy, and field become

$$q'_\alpha = -p_\alpha(1 + g), \tag{42}$$

$$\frac{E'^2}{2mc^2} = \frac{p^2}{2m}(1 + g)^2 + \frac{1}{2m\Gamma_0}(1 + g), \tag{43}$$

and

$$\begin{aligned} U' &= (1 + g)U_0 \\ &= (g/2m\Gamma_0)(1 + g) \end{aligned} \tag{44}$$

so that $U_0 = g/2m\Gamma_0$ and, since $\Gamma_0 \to p^{-2}$ as $\lambda \to 0$, we find that $U_0 = 0$ in the zero coupling limit. The Hamiltonian now becomes

$$\begin{aligned} H &= E_p - E_k + U' \\ &= \frac{p^2}{2m}(1 - g^2) + \frac{g}{2m\Gamma_0}(1 + g), \end{aligned} \tag{45}$$

so that we find the following relation,

$$\frac{E'^2}{2mc^2} = \frac{p^2}{2m}(1 + g)^2 - \frac{E_0^2}{2mc^2}(1 - g^2) + H, \tag{46}$$

between the excitation energies and H. Note that the $g(1 + g)/2m\Gamma_0$ term in H appears as a function of the m^2 eigenvalue in the expression for the excitation energy.

As to the particle energies, particles in excited states obviously have kinetic energies $k'^2/2m = g^2p^2/2m$, while those in the ground state initially have kinetic energies $p^2/2m$. But the interactions between particles in excited states and antiparticles in the ground state and among particles in excited states and among particles and antiparticles in the ground state give rise to additional interactions which add terms to the initial kinetic energies. That is, the particles are "dressed" by short-range collective fields and interact also with the long-range fields. We note, however, that Eqs. (42) and (43) give the momentum and energy levels of the field so that particles with $g^2p^2/2m < U'$ or $p^2/2m < U'$ will occupy these levels. Hence, the energies and momenta of particles bound in the interacting system are given directly by (42) and (43). Moreover, if g is negative, *all* the levels $E'^2/2mc^2$ are less than the initial particle levels and, in this case, (43) gives the complete set of particle levels in the interacting system. This condition depends upon the relative occupation of the ground state and excited states, so that for $n_0(p)/n_0(k') > 1$ we find that $g < 0$, whereas for $g > 0$ we have $n_0(p)/n_0(k') < 1$. In the latter case the attractive potential between particles in excited states and the ground state and antiparticles in the ground state is less than the repulsive potential among particles in excited states and the ground state and among antiparticles so that the particle spectrum extends into the continuum.

The $(1+g)^2$ term in (43) gives the renormalized kinetic energy and $(1+g)/\Gamma_0$ is an m^2 eigenvalue resulting from the interactions. Since $U_0 < 0$, we see that, in

$$\begin{aligned}\mathcal{E}' &= \frac{E'^2}{2mc^2} - U' \\ &= \frac{p^2}{2m}(1+g)^2 + \frac{1+g}{2m\Gamma_0} - \frac{g}{2m\Gamma_0}(1+g) \\ &= \frac{p^2}{2m}(1+2g) + \frac{1}{2m\Gamma_0} + \frac{g^2E_0^2}{2mc^2}, \end{aligned} \tag{47}$$

the g/Γ_0 terms cancel in (39) and (40) and the $g^2p^2/2m$ terms cancel as well. The cancelled terms appear to be identified with long-range and short-range parts of the interactions; but U' is a functional of the distribution, whereas the long-range field is an average macroscopic field independent of the particle levels. Hence, we must assume that U' is just the average short-range field and the cancelled terms in $E'^2/2mc^2$ are average values in each order.

3. APPLICATIONS

We consider now two problems of interest: first, the electron gas with arbitrary density and coupling strength and, second, the Bose gas under the same conditions.

A. Electron Gas

We consider electrons with Coulomb interactions at arbitrary density. With $E_0/c = a_0^{-1}$, which follows from considerations of E_0 at zero group velocity, and with $\lambda = 4\pi e^2$, $a_0 = \hbar^2/me^2$, $\rho_0 = p_F^3 n_0(p,q')$, and $p = p_F$, we obtain for the coupling strength

$$g = \eta_T r_s/(1-\alpha^2 r_s^2)^2, \tag{48}$$

where $\eta_T = \alpha_T + i\beta_T$, $\alpha_T = r_0(0)p_0(T)\,\mathrm{Re}\,n_0(p,q')$, $\beta_T = r_0(0)p_0(T)\,\mathrm{Im}\,n_0(p,q')$,and

$$\mathrm{Re}\,n_0(p,q') = \mathrm{Re}\,n_0(k') - n_0(p)$$

is the difference of the Fermi functions for particles in excited states and in the ground state. We see that g is a variable coupling parameter proportional to $(1-\alpha^2r_s^2)^{-2}$ and with apparently a singularity at $\alpha r_s = 1$. We find, however, that

$$\rho_0 = \rho_0(k') - \rho_0(p) = 0$$

at this point, since $\alpha r_s = 1$ requires that the densities in the ground state and in excited states be equal; that is, the excited state density is proportional to a_0^{-3} so that $\rho_0(k')/\rho_0(p) = a_0^{-3}p_F^{-3} = \alpha^3 r_s^3$ and, when $\alpha r_s = 1$, it follows that $\rho_0(k') = \rho_0(p)$. Since $\alpha_T \sim \mathrm{Re}\,n_0(k') - n_0(p)$ in (48), it is evident that $\alpha_T \to 0$ as $\alpha r_s \to 1$.

With (42) we obtain

$$q'_F = -p_F\left(1 + \frac{\eta_T r_s}{(1-\alpha^2r_s^2)^2}\right), \tag{49}$$

$$\begin{aligned}\frac{E'^2}{c^2} &= p_F^2\left(1 + \frac{\eta_T r_s}{(1-\alpha^2r_s^2)^2}\right)^2 \\ &\quad + p_F^2(1-\alpha^2r_s^2)\left(1 + \frac{\eta_T r_s}{(1-\alpha^2r_s^2)^2}\right), \end{aligned} \tag{50}$$

and

$$\begin{aligned}U' &= \left(1 + \frac{\eta_T r_s}{(1-\alpha^2r_s^2)^2}\right)U_0 \\ &= \frac{p_F^2}{2m}\frac{\eta_T r_s}{(1-\alpha^2r_s^2)}\left(1 + \frac{\eta_T r_s}{(1-\alpha^2r_s^2)^2}\right). \end{aligned} \tag{51}$$

In the high-density region, (49) gives

$$\mathrm{Re}\,q' = \pi' = -p_F(1+\alpha_T r_s) \tag{52}$$

and

$$\mathrm{Im}\,q' = \kappa' = -p_F\beta_\pi r_s\,, \tag{53}$$

which are the momentum eigenvalues for Coulomb interactions obtained in perturbation theory.[3] Now (50) gives

$$\mathrm{Re}\,\frac{E'^2}{2mc^2} = \frac{1}{2m}(\pi'^2 - \kappa'^2 - p_F\pi') \tag{54}$$

and

$$\mathrm{Im}\,\frac{E'^2}{2mc^2} = \frac{\kappa'}{2m}(2\pi' - p_F). \tag{55}$$

These results agree with perturbation theory[1,3] also, except that the energy contains additional terms associated with the mass shift $(1+g)/\Gamma_0$, which terms are not present in the perturbation theory of the electron gas. It is evident that these are to be associated with the hole states so that $p_F^2(1+\alpha_T r_s)/2m$ gives the renormalized energy of the hole states; moreover, these hole excitations decay in $\tau = 2m/p_F\kappa'$ seconds, as the first term in (55) gives the decay time for electron excitations obtained in perturbation theory. Finally, the average field is

$$\mathrm{Re}\,U' = (2m)^{-1}[\pi'(\pi' + p_F) - \kappa'^2] \tag{56}$$

and

$$\mathrm{Im}\,U' = \kappa'(2m)^{-1}(2\pi' + p_F). \tag{57}$$

Equation (56) is a sum of attractive and repulsive potentials, with the latter evidently due to the finite effective radius of the electrons, whereas the attractive potential is associated with the oscillations of the distribution function. Obviously, U' is closely related to $E'^2/2mc^2$ and differs from it only by the $p_F\pi'$ term.

Hence we expect, as pointed out in the discussion of (47), cancellation of terms between the average contributions represented by U' and the particle excitation contributions represented by $E'^2/2mc^2$. The ground-state values for the momentum and energy have already been discussed,[3] except for the hole contribution, which adds

$$-2.21\, r_s^{-2}(1 - |\alpha_0|\, r_s)\ \text{Ry} \tag{58}$$

to the electron energy. On the other hand, the field gives

$$\lim_{T\to 0} \operatorname{Re} U' = -\frac{2.21}{r_s}|\alpha_0|\,(1 - |\alpha_0|\, r_s)\ \text{Ry}, \tag{59}$$

where $|\alpha_0| = \frac{1}{2}\alpha(\frac{3}{5})^{\frac{1}{2}}$. Adding (54) and (59) gives

$$2.21\, r_s^{-2}(2 - 2\,|\alpha_0|\, r_s)\ \text{Ry}, \tag{60}$$

so that the total excitation energy is just the free-electron energy plus the 2-particle exchange plus the free hole energy.

In the low-density region the interaction terms vary as $\alpha_T/\alpha^4 r_s^3$ and $\alpha_T > 0$ corresponding to $n_0(k')/n_0(p) > 1$, that is, more particles in excited states than in the ground state. At high density we find

$$\pi' = -p_F(1 + \alpha_T/\alpha^4 r_s^3) \tag{61}$$

and

$$\kappa' = -p_F(\beta_T/\alpha^4 r_s^3), \tag{62}$$

which reduce to $\pi' = -p_F$ and $\kappa' = 0$ in the limit. Obviously, (61) and (62) represent the momentum of excitations having very weak polarization fields; the latter are seen to vary linearly with the density, since $(\alpha r_s)^{-3} = \rho_0 a^3$ where $\rho_0 = (p_F/\alpha)^3$. Hence, at low density the momentum contribution from the polarization field decreases as ρ_0. For the excitation energy we obtain

$$\operatorname{Re}\frac{E'^2}{2mc^2} = \frac{p_F^2}{2m}\left[\left(1 + \frac{\alpha_T}{\alpha^4 r_s^3}\right)^2 - \frac{\beta_T^2}{\alpha^8 r_s^6} - \alpha^2 r_s^2\left(1 + \frac{\alpha_T}{\alpha^4 r_s^3}\right)\right] \tag{63}$$

and

$$\operatorname{Im}\frac{E'^2}{2mc^2} = \frac{p_F^2}{2m}\left[\frac{\beta_T}{\alpha^4 r_s^3}\left(1 + \frac{\alpha_T}{\alpha^4 r_s^3}\right) - \frac{\beta_T}{\alpha^2 r_s}\right]. \tag{64}$$

Even at moderate densities, say $r_s = 10$, the interaction terms in (63) contribute very small terms, except for the $\alpha^2 r_s^2$ term in (63), and also $\gamma' \simeq 0$. The leading term gives, for $\alpha r_s \gg 1$,

$$\lim_{r_s\to\infty} \operatorname{Re}\frac{E'^2}{2mc^2} = -E_F\alpha^2 r_s^2 = -0.60\ \text{Ry}, \tag{65}$$

which can be taken as the total energy for the dilute gas. Finally, the average field in the high-density region is

$$\operatorname{Re} U' = -\frac{p_F^2}{2m}\frac{1}{\alpha^2 r_s}\left[\alpha_T\left(1 + \frac{\alpha_T}{\alpha^4 r_s^3}\right) - \frac{\beta_T^2}{\alpha^6 r_s^4}\right] \tag{66}$$

and

$$\operatorname{Im} U' = -\frac{p_F^2}{2m}\frac{\beta_T}{\alpha^2 r_s}\left(1 + \frac{2\alpha_T}{\alpha^4 r_s^3}\right). \tag{67}$$

Comparing (63)–(67), we see that the lowest-order interaction term in U' is of order r_s^{-1}; but this term is exactly cancelled by the last term in the excitation energy (63) so that, after the $\alpha^2 r_s^2$ term has already been calculated, the next-lowest-order term is of order r_s^{-3}. Hence the total energy is nearly

$$(-0.60 + 2.21\, r_s^{-2})\ \text{Ry}$$

with the remaining terms of order r_s^{-5} and smaller.

B. Bose Gas

We consider boson interactions near the stationary limit. With $a_0^{-1} = \epsilon_1\rho_0 a^2$, where ϵ_1 is obtained from the 2-particle scattering length, $\rho_0' = \operatorname{Re}\,[\rho_0(p) - \rho_0(k')]$, and $E_0/c = a_0^{-1}$, we find that

$$\operatorname{Re} g = \frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1 - b/a)}{(1 - \epsilon_3\rho_0 a^3)^2}, \tag{68}$$

where $\epsilon_2 = \epsilon_1 n_0(p)$, $\epsilon_3 = \epsilon_1^2$, $b = a$, $\operatorname{Re}\, n_0(k')/n_0(p)$ is the scattering length for attractive interactions, $\rho_0(p)$ and $\rho_0(k')$ are the densities of particles in the ground state and in excited states, and a factor $(4\pi)^{\frac{1}{2}}$ has been absorbed into ϵ_1. In obtaining (68), we have evaluated p in the noninteracting ground state; that is, $p_0 = (4\pi\rho_0 a)^{\frac{1}{2}}$, where a is the hard-sphere diameter, since Γ_0 is the initial propagator. From (42) we obtain, for the real momentum,

$$\begin{aligned}\operatorname{Re} q' = \pi' &= -p(1 + \operatorname{Re} g)\\ &= -(4\pi\rho_0 a - 4\pi\rho_0 b)^{\frac{1}{2}}\\ &\quad\times\left(1 + \frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1 - b/a)}{(1 - \epsilon_3\rho_0 a^3)^2}\right),\end{aligned} \tag{69}$$

valid for $b < a$. In obtaining (69), we have added to (42) a zero-order term for attractive interactions; that is, we take $p = (4\pi\rho_0 a - 4\pi\rho_0 b)^{\frac{1}{2}}$ in order to account for the "depletion" effect in the ground state. In the case of no excited states, (69) gives, for hard-sphere interactions,

$$\pi_a' = -(4\pi\rho_0 a)^{\frac{1}{2}}\left(1 + \frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}}{(1 - \epsilon_2\rho_0 a^3)^2}\right) \tag{70}$$

and, for $\rho_0 a^3 \ll 1$ and with $\epsilon_2 = 128/30\pi^{\frac{1}{2}}$, we obtain

for the new kinetic energy a result from perturbation theory found earlier.[4,5] However, it is doubtful that this is the correct coefficient. It certainly is not at He II densities, for which the first-order perturbation term is of the order of the zero-order term; thus, at He II density, $\rho_0 a^3$ is of order 0.35 so that $128(\rho_0 a^3)^{\frac{1}{2}}/30\pi^{\frac{1}{2}}$ is larger than the zero-order term.

The appearance of $1 - b/a$ in the interaction term (the attractive term appears also in the interaction term obtained from self-consistent perturbation theory) is justified by the case of dilute-gas interactions; as $a \to 0$, corresponding to point sources, there can be no interactions unless the $(b/a)(\rho_0 a^3)^{\frac{1}{2}}$ term appears. Evidently, $b < a$ corresponds to less particles in excited states than in the ground state. But, for this condition, momentum is added to the initial particle momenta, and energy minimization requires that $b = a$. In the limit $b = a$, we get $\pi' = 0$ corresponding to equal attractive and repulsive interactions. For exact equality of particles in excited states and in the ground state, the attractive and repulsive interactions cancel, all excitation momenta are zero, and only the long-range collective excitations can occur. This is evidently the condition for the existence of the superfluid state, and it clearly requires that the densities in both states be equal, a result found already by Parry and ter Haar[6] and observed in the region $T \leq T_\lambda$.[7] Further, it is to be expected that no short-range collective excitations occur at $T = 0$ so that $\kappa' = 0$; e.g., the interaction range remains infinite. In the normal state, however, one would expect screening and finite-range effects, since it has been established that these control the density and would act to maintain equal densities in the superfluid and normal states at finite temperature. In this picture, one must regard the superfluid current as resulting from the long-range collective excitations associated with equality of the densities.

The apparent singularity as $\epsilon_2 \rho_0 a^3 \to 1$ corresponds to close packing in the ground state and, therefore, to no interactions in the ground state. No singularity occurs, however, since $b/a = 1$ in the limit, because

$$\frac{\rho_0(k')}{\rho_0(p)} \sim \frac{1}{(a_0 p)^3} = \epsilon_1^3 (\rho_0 a^3)^{\frac{3}{2}}, \tag{71}$$

so that for $\epsilon_2 \rho_0 a^3 = 1$ we find $a = b$.

The interaction range r' is obtained from κ'^{-1}, where

$$\begin{aligned} \kappa' &= -p \operatorname{Im} g \\ &= [\epsilon_2 \rho_0 a^2/(1 - \epsilon_3 \rho_0 a^3)^2] \operatorname{Im} n_0(k'), \end{aligned} \tag{72}$$

which for $\rho_0 a^3 \ll 1$ also gives the perturbation theory result, and

$$\begin{aligned} \operatorname{Im} n_0(k') &= -z \sin y/(z^2 - 2z \cos y + 1), \\ \operatorname{Re} n_0(k') &= (z \cos y + 1)/(z^2 - 2z \cos y + 1), \end{aligned} \tag{73}$$

and

$$\begin{aligned} y &= \kappa' a_0^{-1} \operatorname{Re} n_0(p, q')/mKT, \\ z &= \exp [(\operatorname{Re}^2 k' - \operatorname{Im}^2 k' - \mu)/2mKT] \end{aligned} \tag{74}$$

are obtained from the Bose distribution for complex k. Thus $\operatorname{Im} n_0(k')$ is an oscillating function of the temperature and interaction parameters. It can be shown that $\operatorname{Im} n_0(k') = 0$ at zero temperature and no screening occurs in the ground state as expected. In the normal fluid, however, we expect the thermal motions to be screened by short-range collective excitations with ranges obtained from (72).

The phase of the short-range collective excitation can be determined from (73) and (74) from the condition of equal densities and $z = 1$. Then

$$y = [2\epsilon_1 \rho_0 a (4\pi \rho_0 a^3)^{\frac{1}{2}} \log 2/mKT]^{\frac{1}{2}} \tag{75}$$

and thus

$$\operatorname{Im} n_0(k') = \left(\frac{2mKT \log 2}{\epsilon_1 \rho_0 a (4\pi \rho_0 a^3)^{\frac{1}{2}}}\right)^{\frac{1}{2}}, \tag{76}$$

so that

$$\operatorname{Im} g = \frac{n_0(p)}{(1 - \epsilon_3 \rho_0 a^3)^2} \left(\frac{2m\epsilon_1 aKT \log 2}{(4\pi \rho_0 a)^{\frac{1}{2}}}\right)^{\frac{1}{2}}. \tag{77}$$

Finally,

$$\kappa' = -\frac{n_0(p)}{(1 - \epsilon_3 \rho_0 a^3)^2} [4\pi \epsilon_1 (\rho_0 a^3/\pi)^{\frac{1}{2}} mKT \log 2]^{\frac{1}{2}}, \tag{78}$$

and the interaction range varies as $T^{-\frac{1}{2}}$. With $\rho_0 = 2.10^{22}/\text{cm}^3$ and $a = 2.6$ Å, we obtain for the interaction range

$$r' = 8.6 T^{-\frac{1}{2}} \text{ Å}. \tag{79}$$

From (73) and (74), we can also estimate T_λ from the condition of equal densities, which in the interacting system corresponds to the Bose–Einstein transition in the noninteracting system. Thus (73) gives

$$(1 + \cos y)/(1 - \cos y) = 1 \tag{80}$$

or $\cos y = 0$. This gives $\operatorname{Im} n_0(k') = -\frac{1}{2}$ and

$$\begin{aligned} \operatorname{Im} n_0(k') = -\tfrac{1}{2} &= -\frac{ymKT_\lambda a_0}{p_0} \\ &= \left(\frac{2mKT_\lambda \log 2}{\epsilon_1 \rho_0 a (4\pi \rho_0 a^3)^{\frac{1}{2}}}\right)^{\frac{1}{2}}, \end{aligned} \tag{81}$$

so that

$$\begin{aligned} T_\lambda &= \frac{1}{8} \frac{\epsilon_1 \rho_0 a (4\pi \rho_0 a^3)^{\frac{1}{2}}}{mK \log 2} \\ &= 2.1°, \end{aligned} \tag{82}$$

with the proportionality constant ϵ_1 equal to 2.8. This latter value is obtained from $a_0^{-1} = \epsilon_1 \rho_0 a^2$, where a_0 is the 2-particle scattering length, which we have taken to be 2.6 Å. While this value is about 15% higher than the observed distance of closest approach from neutron scattering, the observed value of 2.27 Å gives values of T_λ, T_Δ, and τ_{roton}, which are all consistently in error by at least 15%. On the other hand, the 2.6 Å value yields estimates within 4% of T_λ, within 8% of T_Δ, and within 11% of τ_{roton}.

The energy eigenvalues obtained from (43) and (44) are

$$\begin{aligned}\operatorname{Re}\frac{E'^2}{2mc^2} &= \frac{p^2}{2m}[(1+\operatorname{Re} g)^2 - \operatorname{Im}^2 g] \\ &\quad + \frac{1}{2m\Gamma_0}(1+\operatorname{Re} g) \\ &= \frac{2\pi(\rho_0 a - \rho_0 b)}{m}\Bigg[\left(1+\frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1-b/a)}{(1-\epsilon_3\rho_0 a^3)^2}\right)^2 \\ &\quad - \frac{n_0^2(p)}{(1-\epsilon_3\rho_0 a^3)^2}\frac{2m\epsilon_1 aKT\log 2}{(4\pi\rho_0 a)^{\frac{1}{2}}} \\ &\quad + (1-\epsilon_3\rho_0 a^3)\left(1+\frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1-b/a)}{(1-\epsilon_3\rho_0 a^3)^2}\right)\Bigg] \end{aligned} \tag{83}$$

and

$$\begin{aligned}\operatorname{Im}\frac{E'^2}{2mc^2} &= \frac{p^2}{m}(1+\operatorname{Re} g) + \frac{1}{2m\Gamma_0}\operatorname{Im} g \\ &= -\frac{2\pi(\rho_0 a - \rho_0 b)}{m} \\ &\quad \times\Bigg[\left(1+\frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1-b/a)}{(1-\epsilon_3\rho_0 a^3)^2}\right) \\ &\quad + \frac{n_0(p)}{(1-\epsilon_3\rho_0 a^3)}\left(\frac{2m\epsilon_1 aKT\log 2}{(4\pi\rho_0 a)^{\frac{1}{2}}}\right)^{\frac{1}{2}}\Bigg]. \end{aligned} \tag{84}$$

(83) has the form of Landau's dispersion equation in the roton region with

$$\Delta = (2m\Gamma_0)^{-1}(1+\operatorname{Re} g), \tag{85}$$

which is obtained at the minimum for the kinetic energy [see Eq. (83)]. With $E_0^2/p^2 \ll 1$, this gives

$$\begin{aligned} T_\Delta &= \frac{2\pi\rho_0 a}{m}\left(1+\frac{\epsilon_1(\rho_0 a^3)^{\frac{1}{2}}}{(1-\epsilon_3\rho_0 a^3)^2}\right) \\ &= 8.2°, \end{aligned} \tag{86}$$

with ϵ_1, ρ_0, and a as in the previous calculation.

For the average field we find

$$\begin{aligned}\operatorname{Re} U' &= \frac{\operatorname{Re} g}{2m\Gamma_0}(1+\operatorname{Re} g) - \frac{1}{2m\Gamma_0}\operatorname{Im}^2 g \\ &= \frac{2\pi(\rho_0 a - \rho_0 b)}{m}\Bigg[\frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1-b/a)}{1-\epsilon_3\rho_0 a^3} \\ &\quad \times\left(1+\frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1-b/a)}{(1-\epsilon_3\rho_0 a^3)^2}\right) \\ &\quad - \frac{n_0^2(p)}{(1-\epsilon_3\rho_0 a^3)^2}\frac{2m\epsilon_1 aKT\log 2}{(4\pi\rho_0 a)^{\frac{1}{2}}}\Bigg], \end{aligned} \tag{87}$$

and

$$\begin{aligned}\operatorname{Im} U' &= \frac{1}{2m\Gamma_0}[\operatorname{Im} g(1+2\operatorname{Re} g)] \\ &= -\frac{2\pi(\rho_0 a - \rho_0 b)}{m}\frac{1}{1-\epsilon_3\rho_0 a^3} \\ &\quad \times\left(\frac{2m\epsilon_2 n_0(p) aKT\log 2}{(4\pi\rho_0 a)^{\frac{1}{2}}}\right)^{\frac{1}{2}} \\ &\quad \times\left(1+\frac{2\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}(1-b/a)}{(1-\epsilon_3\rho_0 a^3)^2}\right) \end{aligned} \tag{88}$$

gives the decay time for the field.

For $b = 0$, Eq. (83) gives the excitation energy in the hard sphere case and, for $b \neq 0$, the excitation energy with attractive interactions. At low density, (83) is in agreement with earlier calculations[6,7] for the particle energies, except that additional terms appear due to the presence of b in the first-order interaction term. These appear also in the perturbation theory result obtained from self-consistent field theory and are to be associated with particles in excited states.

The decay time given by (84) is that for particle excitations, that is, for the noninteracting bosons plus their short-range polarization fields, whereas Im U' in (88) gives the decay time for the average field.

The first term in (84) is of the form $\pi'\kappa'/m$, where π' and κ' are given by (69) and (72). Thus, at low density, γ' varies as $T^{\frac{1}{2}}$, which is the same dependence obtained by Parry and ter Haar[6] from the Brueckner–Sawada theory and observed by Larsson and Otnes.[8] Thus (84) gives

$$\begin{aligned}\tau_{\text{roton}} &= \frac{m}{p^2(1+\operatorname{Re} g)\operatorname{Im} g} \\ &= \frac{m}{2\pi\rho_0 a}\Bigg[\left(1+\frac{\epsilon_2(\rho_0 a^3)^{\frac{1}{2}}}{(1-\epsilon_3\rho_0 a^3)^2}\right) \\ &\quad \times\frac{n_0(p)}{(1-\epsilon_3\rho_0 a^3)^2}\left(\frac{2m\epsilon_1 aKT\log 2}{(4\pi\rho_0 a)^{\frac{1}{2}}}\right)^{\frac{1}{2}}\Bigg]^{-1} \end{aligned} \tag{89}$$

so that, at $\rho_0 a^3 \ll 1$, $\tau_{\text{roton}} \sim T^{-\frac{1}{2}}$ and $n_0(p)$ contributes an exponential factor which, for a Boltzmann

distribution, is the factor obtained by Parry and ter Haar.[6] However, at He II densities, $\rho_0 a^3 \ll 1$ does not hold, and the strong coupling factors $(1 - \epsilon_3 \rho_0 a^3)^2$ contribute significantly. With the strong coupling factors included, (89), in fact, gives

$$\tau_{\text{roton}} = 6.7 \times 10^{-12} \text{ sec}$$

at $T = 1.8°$ and is to be compared with the value of 6.10^{-12} secs obtained by Parry and ter Haar[6] and Larsson and Otnes.[8] Near the dispersion minimum, however, we find that $1 + \text{Re}\, g = \text{Im}\, g$ so that $\tau_{\text{roton}} \sim T^{-1}$ and, with the strong coupling factors included, $\tau_{\text{roton}} = 5.10^{-11}$ sec.

Finally, we should note that, with the interacting density ρ' given by (40), we are able to calculate the expectation values of the remaining observables by means of the familiar formula

$$X' = \int d^3x\, X \rho'(x), \tag{90}$$

where X is an operator corresponding to an observable in the noninteracting system.

APPENDIX: CANONICAL COORDINATES FOR SEVERAL VARIABLES

With $k = p + iq$, we have for the classical case

$$[p, H] = \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \tag{A1}$$

$$[q, H] = \frac{dq}{dt} = \frac{\partial H}{\partial p}, \tag{A2}$$

and

$$[k, H] = -\frac{\partial H}{\partial q} + i\frac{\partial H}{\partial p} = 2i\frac{\partial H}{\partial k^*} = \frac{dk}{dt}. \tag{A3}$$

The second equality in (A3) is obtained with

$$p = \tfrac{1}{2}(k + k^*), \quad q = -\tfrac{1}{2}i(k - k^*), \tag{A4}$$

and

$$2\frac{\partial}{\partial k^*} = 2\frac{dp}{dk^*}\frac{\partial}{\partial p} + 2\frac{dq}{dk^*}\frac{\partial}{\partial q}. \tag{A5}$$

Using the fundamental quantum conditions and $h = 1$, we see that the rhs of (A3) becomes just $\sigma_k \partial H/\partial k^* = dk/dt$, where σ_k is a constant.

Now consider H as a function of $E = \omega + i\gamma$. Then

$$[\omega, H] = \frac{d\omega}{dt} = -\frac{\partial H}{\partial \gamma}, \tag{A6}$$

$$[\gamma, H] = \frac{d\gamma}{dt} = \frac{\partial H}{\partial \omega}, \tag{A7}$$

and

$$[E, H] = 2i\frac{\partial H}{\partial E^*} = \frac{dE}{dt}, \tag{A8}$$

and, again using the quantum conditions, we see that the rhs becomes $\sigma_E \partial H/\partial E^* = dE/dt$, where σ_E is a constant.

With

$$\frac{d\omega}{dt} = \frac{d\omega}{dp}\frac{dp}{dt} + \frac{d\omega}{dq}\frac{dq}{dt} = \frac{d\omega}{dp}\frac{\partial H}{\partial q} - \frac{d\omega}{dq}\frac{\partial H}{\partial q}, \tag{A9}$$

we find the operator canonical to ω is given by

$$\frac{\partial}{\partial \gamma} = \frac{d\omega}{dq}\frac{\partial}{\partial p} - \frac{d\omega}{dp}\frac{\partial}{\partial q} \tag{A10}$$

and, with an expansion for $d\gamma/dt$ similar to (A9), we find

$$\frac{\partial}{\partial \omega} = \frac{d\gamma}{dp}\frac{\partial}{\partial q} - \frac{d\gamma}{dq}\frac{\partial}{\partial p}. \tag{A11}$$

In general, for any variables $z(p, q) = z_1(p, q) + iz_2(p, q)$, the operators canonical to z_2 and z_1 are given by

$$\frac{\partial}{\partial z_1} = \frac{\partial z_2}{\partial p}\frac{\partial}{\partial q} - \frac{\partial z_2}{\partial q}\frac{\partial}{\partial p} \to i[q, z_2]\frac{\partial}{\partial q} + i[p, z_2]\frac{\partial}{\partial p} \tag{A12}$$

and

$$\frac{\partial}{\partial z_2} = \frac{\partial z_1}{\partial q}\frac{\partial}{\partial p} - \frac{\partial z_1}{\partial p}\frac{\partial}{\partial q} \to -i[p, z_1]\frac{\partial}{\partial p} - i[q, z_1]\frac{\partial}{\partial q}, \tag{A13}$$

where the second lines of (A12) and (A13) are obtained from the fundamental quantum conditions applied to the classical brackets.

[1] J. T. Anderson, J. Math. Phys. **8**, 998 (1967); Nuovo Cimento **52**, 375 (1967).
[2] J. T. Anderson, J. Math. Phys. **11**, 117 (1970).
[3] J. T. Anderson, Nuovo Cimento (in press).
[4] K. Huang, Phys. Rev. **115**, 765 (1959); **119**, 1129 (1960).
[5] T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958).
[6] W. Parry and D. ter Haar, Ann. Phys. (N.Y.) **19**, 496 (1962).
[7] K. Huang, in *Fundamental Problems in Statistical Mechanics*, edited by E. G. D. Cohen (North-Holland, Amsterdam, 1962), p. 62.
[8] K. Larsson and K. Otnes, Arkiv Fysik **15**, 49 (1959).

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Correlation Inequalities for Heisenberg Ferromagnets

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First, for a classical discrete approximation to the Heisenberg ferromagnet, in a Euclidean space of dimension 2^k where k is a positive integer, the correlation is nonnegative and a monotonic increasing function of interactions. Second, for the quantum mechanical Heisenberg ferromagnet itself, the correlation is nonnegative but *not* necessarily a monotonic increasing function of interaction. Both results allow for long-range interactions. Third, a family of inequalities on the number of connected components in graphs is deduced.

1. INTRODUCTION

Griffiths[1-3] has shown that, for Ising ferromagnets of arbitrary spin, the correlation is nonnegative and a monotonic increasing function of the interactions. It is natural to enquire whether the corresponding assertion is correct for the Heisenberg ferromagnet and its various approximations.

One such approximation is the classical discrete Heisenberg model in which the spin vector can take only the directions $\pm\mathbf{x}_i$, $i = 1, \cdots, d$, where the $\mathbf{x}_i$ are mutually orthogonal unit vectors in a d-dimensional space. In Sec. 2 of this paper, the monotonicity of correlations is proved for the cases $d = 2^k$ by replacing the problem by an equivalent ferromagnetic Ising model and using the results of Ref. 4. In Sec. 3, this result is obtained by using a combinatorial formulation. A further extension to the case where an external magnetic field is present is given, using both approaches, for $d = 2$. The question of the monotonicity of correlations for the case where the spin is 2 dimensional and is approximated by eight equispaced unit vectors remains open, as is the case with all extensions which replace $2d$ directions of spin by a larger but finite number.

For the case of the quantum mechanical Heisenberg ferromagnet, the correlation is shown to be nonnegative and, by means of an example, *not necessarily* a monotonic increasing function of the interaction. These questions, which are dealt with in Sec. 4, were raised by Dyson[5] simultaneously but independently of the current investigation. It may be that, for interesting subclasses of quantum mechanical Heisenberg ferromagnets, the monotonicity holds, but that question is not settled here.[6]

2. THE CLASSICAL DISCRETE HEISENBERG MODEL

Let $N = \{1, 2, \cdots, n\}$ be a collection of spin locations. At this stage, there is no assumption of dimensionality. Now choose a real Euclidean space of dimension d and fix a complete orthonormal set $\{\mathbf{x}_1, \cdots, \mathbf{x}_d\}$ in this space. Let $D = \{\mathbf{x}_1, \cdots, \mathbf{x}_d, -\mathbf{x}_1, \cdots, -\mathbf{x}_d\}$. The spin $\boldsymbol{\sigma}$ is a function from N to D and, therefore, for $j \in N$, $\boldsymbol{\sigma}_j \in D$. Let the Hamiltonian of the system be

$$H = -\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,$$

with $J_{ij} \geq 0$, because we are considering ferromagnets. If $A = \{i, j\}$, then let $\sigma^A = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, so that

$$H = -\sum_{\#A=2} J_A \sigma^A,$$

with $J_A \geq 0$. In the rest of this section, A, B, and C (with or without subscript) stand for 2-element subsets of N. We wish to establish

$$\langle \sigma^A \rangle \geq 0,$$
$$\frac{\partial \langle \sigma^A \rangle}{\partial J_B} \geq 0.$$

First proceed as in KS, utilizing its notation without additional comment. The partition function of the system is

$$Z = \sum_{\sigma} \cdots \sum_{\sigma_n \in D} \exp \sum_A J_A \sigma^A,$$
$$= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{A_1} \cdots \sum_{A_k} \sum_{\sigma_1 \in D} \cdots \sum_{\sigma_n \in D} J_{A_1} \cdots J_{A_k}^{\sigma^{A_1} \cdots \sigma^{A_k}}.$$

Consider

$$\sum_{\sigma_1 \in D} \cdots \sum_{\sigma_n \in D} \sigma^{A_1} \cdots \sigma^{A_k}. \tag{2.1}$$

If $A_r = \{i, j\}$ and, for spin configuration σ, $\sigma^{A_r} = \sigma_i \cdot \sigma_j = 0$, then the summand $\sigma^{A_1} \cdots \sigma^{A_k}$ with σ^{A_r} as a factor vanishes.

From this, it follows that a spin configuration which yields a nonvanishing contribution to (2.1) must be such that, if the A are considered as edges of a graph, then on each connected component (henceforth, just component), which may be an isolated vertex, the spins are all in the same or directly opposite direction, e.g., on one component the spins are all horizontal while on another component all the spins are vertical.

Let μ be a multiplicity function on the A in the sense of KS. Let $\gamma(\mu)$ be the number of components of the graph formed by taking the complete graph on the vertex set N and deleting those edges A such that $\mu(A) = 0$. Note that the isolated vertices in the resulting graph contribute to the count of components. From the above considerations, we obtain

$$Z = 2^n \sum_{\Delta\mu=\phi} \frac{J_\mu}{\mu!} d^{\gamma(\mu)}$$

and

$$Z\frac{\langle\sigma^R\rangle}{2^n} = \sum_{\Delta\mu=R} \frac{J_\mu}{\mu!} d^{\gamma(\mu+1\{R\})}.$$

Since $J_{ij} \geq 0$, we have $J_\mu \geq 0$, $Z \geq 0$, and $\langle\sigma^R\rangle \geq 0$. Thus, in a classical discrete Heisenberg ferromagnet where the spins are d dimensional, the correlation is nonnegative. It should also be noted that, when $d = 1$, the expansion for Z, etc., corresponds to the classical Ising-model results as given in KS.

Just as in KS, the monotonic increasing character of $\langle\sigma^R\rangle$ as a function of J_S is equivalent to

$$\langle\sigma^R\sigma^S\rangle \geq \langle\sigma^R\rangle\langle\sigma^S\rangle.$$

If one normalizes by multiplying both sides by Z^2, one can investigate whether, for each μ such that $\Delta\mu = R\Delta S$, the coefficient of J_μ on the left-hand side dominates the coefficient of J_μ on the right-hand side, as in KS. This reduces to

$$\sum_{\substack{\nu\leq\mu \\ \Delta\nu=\phi}} \frac{d^{\gamma(\nu)+\gamma(\mu-\nu+1\{R\}+1\{S\})}}{\nu!\,(\mu-\nu)!} \geq \sum_{\substack{\nu\leq\mu \\ \Delta\nu=R}} \frac{d^{\gamma(\nu+1\{R\})+\gamma(\mu-\nu+1\{S\})}}{\nu!\,(\mu-\nu)!}. \tag{2.2}$$

As in KS, it is sufficient to establish (2.2) for the case $\mu \leq 1$. If both sides of (2.2) are multiplied by $\mu!$, the factors $\mu!/\nu!\,(\mu-\nu)!$ represent the number of ways the choices of ν could be made if each unlabeled edge A were replaced by $\mu(A)$ labeled edges, so that in the configuration with labeled edges the multiplicity is at most one. For this case, (2.2) becomes

$$\sum_{\substack{\nu\leq\mu \\ \Delta\nu=\phi}} d^{\gamma(\nu)+\gamma(\mu-\nu+1\{R\}+1\{S\})} \geq \sum_{\substack{\nu\leq\mu \\ \Delta\nu=R}} d^{\gamma(\nu+1\{R\})+\gamma(\mu-\nu+1\{S\})}. \tag{2.3}$$

A direct proof of (2.3) for the case $d = 2^k$, $\mu(R) = \mu(S) = 0$ is given in Sec. 3. By departing from the previous convention on μ, this case can be formulated: $\mu \leq 1$, $\Delta\mu = \phi$, and $\mu(R) = \mu(S) = 1$ imply

$$\sum_{\substack{\nu\leq\mu,\,\Delta\nu=\phi \\ \nu(R)=\nu(S)=0}} d^{\gamma(\nu)+\gamma(\mu-\nu)} \geq \sum_{\substack{\nu\leq\mu,\Delta\nu=\phi \\ \nu(R)=1,\nu(S)=0}} d^{\gamma(\nu)+\gamma(\mu-\nu)}. \tag{2.4}$$

An indirect proof of (2.2) can be given for $d = 2$. However, this involves first proving the monotonicity of correlations as functions of the interactions. The proof required here uses an idea from Mills' thesis, which ultimately derives from Potts.[7,8] Consider an Ising model with the set $N^1 = \{1, 2, \cdots, 2n\}$ of spin locations, with interactions K_{ij} such that

$$1 \leq i \leq j \leq n \Rightarrow K_{ij} = K_{n+i,n+j} = \tfrac{1}{2}J_{ij},$$
$$i \leq n < j \quad \text{or} \quad j \leq n < i \Rightarrow K_{ij} = 0.$$

Of course, the Hamiltonian is

$$H = -\sum_{i<j} K_{ij}\sigma_i\sigma_j.$$

This Ising model consists of two classical Ising models which are replicas, have internal interactions $\frac{1}{2}$ that in the classical discrete Heisenberg model we have been studying, and do not interact with each other. With each $\sigma: N^1 \to \{-1, 1\}$ associate a $\boldsymbol{\sigma}: N \to D$ as follows:

$$\boldsymbol{\sigma}_i = (\tfrac{1}{2}(\sigma_i + \sigma_{n+i}), \tfrac{1}{2}(\sigma_i - \sigma_{n+i})), \qquad i \in N.$$

Note that this assignment yields

$$\begin{aligned}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j &= \tfrac{1}{4}[(\sigma_i + \sigma_{n+i})(\sigma_j + \sigma_{n+j}) \\ &\qquad + (\sigma_i - \sigma_{n+i})(\sigma_j - \sigma_{n+j})] \\ &= \tfrac{1}{2}(\sigma_i\sigma_j + \sigma_{n+i}\sigma_{n+j}).\end{aligned}$$

Thus, the Hamiltonian for a particular σ in the Ising model is equal to the Hamiltonian for the corresponding $\boldsymbol{\sigma}$ in the classical discrete Heisenberg model. Thus,

$$\langle\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\rangle = \tfrac{1}{2}(\langle\sigma_i\sigma_j\rangle + \langle\sigma_{n+i}\sigma_{n+j}\rangle).$$

Since both terms on the right-hand side are monotonically increasing functions of any K_{rs}, the term on the left is a monotonically increasing function of J_{rs}. This result also holds in the strong sense of KS, so that (2.2) and, in particular, (2.3) follow for the case $d = 2$.

For the case $d = 2^k$, we note that there are 2^{k+1} different spin states at each spin location. Accordingly,

we consider an Ising model with the set $N^k = \{1, 2, \cdots, (k+1)n\}$ of spin locations. We define projection operators

$$P_{Li} = 2^{-k} \prod_{l=1}^{k} (1 + (-1)^{L_l} \sigma_{ln+i}),$$

where $L = \{L_1, \cdots, L_k\}$ and $L_l = 0, 1$. There will be a unique operator P_{Li} corresponding to each of the directions $\mathbf{x}_1, \cdots, \mathbf{x}_d$ for $d = 2^k$. The equivalent Ising Hamiltonian is defined as

$$H = -\sum_{1 \le i < j \le n} J_{ij} \sum_{L} \sigma_i \sigma_j P_{Li} P_{Lj}, \tag{2.5}$$

which, when expanded, is a ferromagnetic Hamiltonian of the type considered by KS. In particular,

$$\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j = \sigma_i \sigma_j \sum_{L} P_{Li} P_{Lj}$$

is a sum of terms of the form $\sigma^{A_i} \sigma^{A_j}$ considered in KS, where $A_i = i + S$, S is a subset of $\{0, n, 2n, \cdots, kn\}$, $A_j = j + S$, and all terms have coefficient 1 or 0. Hence, the results of KS may be used immediately to demonstrate the monotonicity of correlations and, hence, the inequality (2.3). For the case $k = 1$, we have

$$\begin{aligned} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j &= \tfrac{1}{4} \sigma_i \sigma_j [(1 + \sigma_{n+i})(1 + \sigma_{n+j}) \\ &\qquad + (1 - \sigma_{n+i})(1 - \sigma_{n+j})], \\ &= \tfrac{1}{2} (\sigma_i \sigma_j + \sigma_i \sigma_{n+i} \sigma_j \sigma_{n+j}), \end{aligned}$$

and, if we redefine $\sigma_i \sigma_{n+i}$ as σ_{n+i}, we recover the expression already employed for $d = 2$.

The effect of an external magnetic field can be easily incorporated. If we add to (2.5) a term

$$-\sum_i H_i \sigma_i P_{L0i}, \quad H_i \ge 0,$$

where $L_0 = \{0, 0, \cdots, 0\}$, we can include the effect of the external field. This additional term is also of the type considered by KS, because all coefficients are ferromagnetic. Hence, Griffiths' theorems apply to this case also.

3. COMBINATORIAL APPROACH TO THE CLASSICAL DISCRETE HEISENBERG MODEL

The quantity $\gamma(\mu)$ introduced in Sec. 2 is a familiar quantity in topology, and is, in fact, the simplest Betti number[9] R_2^0. There exists a well-known relation between R_2^0 and R_2^1, which is what is usually known as the *cyclomatic number* $m(\mu)$ for a graph μ. The relation, which is a particular case of the Euler–Poincaré relation, is stated as follows. Let α^0 be the number of vertices of a graph and α^1 the number of edges. Then,

$$\alpha^0 - \alpha^1 = R_2^0 - R_2^1, \tag{3.1}$$

or, in the notation usually used in graph theory,

$$\gamma(\mu) = \alpha^0 - \alpha^1 + m(\mu). \tag{3.2}$$

In particular, for the graphs ν and $\mu - \nu$ considered in Sec. 2, we have

$$\gamma(\nu) = n - \alpha^1(\nu) + m(\nu),$$
$$\gamma(\mu - \nu) = n - \alpha^1(\mu - \nu) + m(\mu - \nu);$$

thus

$$\begin{aligned} \gamma(\nu) + \gamma(\mu - \nu) = m(\nu) + m(\mu - \nu) \\ + 2n - \#\{A : \mu(A) > 0\}. \end{aligned}$$

If we multiply both sides of (2.4) by $d^{-2n+\#\{A:\mu(A)>0\}}$, we obtain the equivalent relation

$$\sum_{\substack{\nu \le \mu, \Delta\nu = \phi \\ \nu(R) = \nu(S) = 0}} d^{m(\nu)+m(\mu-\nu)} \ge \sum_{\substack{\nu \le \mu, \Delta\nu = \phi \\ \nu(R) = 1, \nu(S) = 0}} d^{m(\nu)+m(\mu-\nu)}. \tag{2.4'}$$

Theorem A: $2^{m(\nu)+m(\mu-\nu)}$ is a positive definite function of ν.

Proof: Let $G \overset{\text{DEF}}{=} \{\nu \le \mu : \Delta\nu = \phi\}$ be the group of cycles of μ:

$$G_\alpha \overset{\text{DEF}}{=} \{\rho : \Delta\rho = \phi, \Delta(\rho \cap \alpha) = \phi\}, \quad \forall\, \alpha \in G;$$

then

$$\sum_{\alpha \in G} \chi_{G_\alpha}(\nu) = \#\{\alpha : \nu \in G_\alpha\} = 2^{m(\nu)+m(\mu-\nu)}, \tag{3.3}$$

where χ_A is the characteristic function of A. Since the characteristic function of a closed subgroup is always positive definite, Theorem 1 follows.

Corollary A_1: For any positive integer k, $2^{k[m(\nu)+m(\mu-\nu)]}$ is a positive definite function of ν.

The application of Corollary 1 yields (2.4') for the case $d = 2^k$.

In order to extend this type of argument to the case where an external magnetic field is present, we introduce a ghost state $\boldsymbol{\sigma}_0 = \mathbf{x}_1$, and let the index set N be augmented to

$$\bar{N} \overset{\text{DEF}}{=} N \cup \{0\}.$$

The quantity $\gamma(\mu)$ is now defined by first considering the graph with the vertex set $\bar{N}$ and the edge set $\{A : \mu(A) > 0\} \cup \{R\}$ and then by counting the number of connected components *not touching* 0, where isolated vertices other than 0 are counted as connected components. This is because any connected component which touches 0 is counted only once, instead of d times, because all spins in this component must be parallel to $\mathbf{x}_1$. Griffiths'[1] Theorem 1 is trivial, as before. For Griffiths' Theorem 2, it is necessary to establish

the desired inequality (2.4). We use the relative homology theory and the Euler–Poincaré relation for $K - L$, where K = graph (complex) with edges $\{R\} \cup \{A:\gamma(A) > 0\}$ and vertices $\bar{N}$ and $L = \{0\}$, the complex consisting of the single vertex $\{0\}$. In this language, we replace $\gamma(\nu) + \gamma(\mu - \nu)$ by $R_2^1(\nu, L) + R_2^1(\mu - \nu, L)$ and then, following Lefschetz,[9] replace this by $R_2^1(\nu) + R_2^1(\mu - \nu)$. The argument then follows as before.

In this section and the preceding one, we have been concerned with establishing (2.3), or its equivalent, (2.4), for the case $\mu(R) = \mu(S) = 0$. As an example, we now consider another case, where $\Delta\mu = R\Delta S$ and $\mu \leq 1$. In particular consider the case $\mu(R) = 1$ and $\mu(S) = 0$. The analog to Eq. (2.4) is that

$$\Delta\mu = \phi, \quad \mu(R) = 2, \quad \mu(S) = 1, \quad \mu(A) \leq 1, \quad \forall\, A \neq R,$$

imply

$$\sum_{\substack{\nu \leq \mu \\ \Delta\nu = \phi \\ \nu(R) \leq 1 \\ \nu(S) = 0}} d^{\gamma(\nu)+\gamma(\mu-\nu)} \geq \sum_{\substack{\nu \leq \mu \\ \Delta\nu = \phi \\ \nu(R) \geq 1 \\ \nu(S) = 0}} d^{\gamma(\mu)+\gamma(\mu-\nu)}. \qquad (3.4)$$

This can be reduced to the previous case as follows. Introduce symbols R_1 and R_2 to replace R, thus replacing an unlabeled edge by two labeled edges. The appropriate multiplicity function μ is now less than or equal to 1.

Define $\bar{\mu} \mid (\{A:A \subset N\} \setminus \{R\}) \cup \{R_1\} \cup \{R_2\}$ by

$$\bar{\mu} \mid (\{A:A \subset N\} \setminus \{R, S\}) = \mu \mid (\{A:A \subset N\} \setminus \{R\}) \cup \{R_1\} \cup \{R_2\}$$

and $\bar{\mu}(R_1) = \bar{\mu}(R_2) = \bar{\mu}(S) = 1$. For all $\nu \leq \bar{\mu}$, let $\Delta\nu$ be a subset of N defined by the action of Δ as a boundary so that $\Delta R_j = R$, $j = 1, 2$, and

$$\{i:\nu(R_i) = 1\} \text{ odd} \Rightarrow \Delta\nu = R\Delta(\Delta(\nu \mid (\{A:A \subset N\} \setminus \{R\})),$$

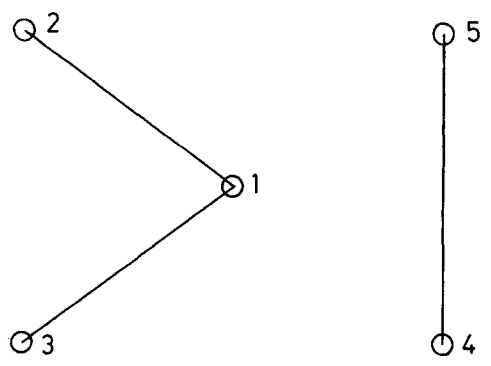

FIG. 1. μ of (2.3).

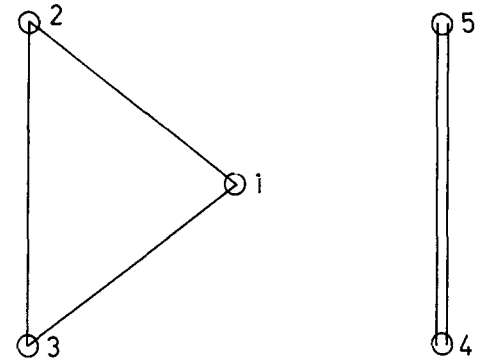

FIG. 2. μ of (3.4).

while

$$\{i:\nu(R_i) = 1\} \text{ even} \Rightarrow \Delta\nu = \Delta(\nu \mid (\{A:A \subset N\} \setminus \{R\})).$$

Note that $\Delta\bar{\mu} = \phi$, since $\Delta\mu = R\Delta S$. Now the validity of (2.3) in the case where $\Delta\mu = R\Delta S$, $\mu(R) = 1$, and $\mu(S) = 0$ is implied by the validity of

$$\sum_{\substack{\nu \leq \mu \\ \Delta\nu = \phi \\ (\bar{\mu}-\nu)(R_2) = 1 \\ (\bar{\mu}-\nu)(S) = 1}} d^{\gamma(\nu)+\gamma(\bar{\mu}-\nu)} \geq \sum_{\substack{\nu \leq \mu \\ \Delta\nu = \phi \\ \nu(R_2) - 1 \\ (\bar{\mu}-\nu)(S) = 1}} d^{\gamma(\nu)+\gamma(\bar{\mu}-\nu)}. \qquad (3.4')$$

This last follows from (2.4).

Example 1: $N = \{1, 2, 3, 4, 5\}$, $R = \{4, 5\}$, and $S = \{2, 3\}$. μ [of (2.3)] takes the value 1 on $\{1, 2\}$, $\{1, 3\}$, $\{4, 5\}$, and the value 0 on all other subsets of N. $\Delta\mu = R\Delta S$, $\mu \leq 1$, $\mu(R) = 1$, and $\mu(S) = 0$. Let $d = 2$. (See Fig. 1.) μ [of (2.4); see Fig. 2] takes value 1 on $\{1, 2\}$, $\{1, 3\}$, $\{2, 3\}$, but it takes value 2 on $\{4, 5\}$ and value 0 on all other subsets of N:

$$\Delta\mu = \phi, \quad \mu(R) = 2, \quad \mu(S) = 1.$$

$\bar{\mu}$ [of (3.4'); see Fig. 3] takes value 1 on $\{1, 2\}$, $\{1, 3\}$, $\{2, 3\}$, $\{4, 5\}_1$, and $\{4, 5\}_2$, but value 0 on all other subsets of N:

$$\Delta\bar{\mu} = \phi, \quad \bar{\mu}(R_1) = \bar{\mu}(R_2) = \bar{\mu}(S) = 1.$$

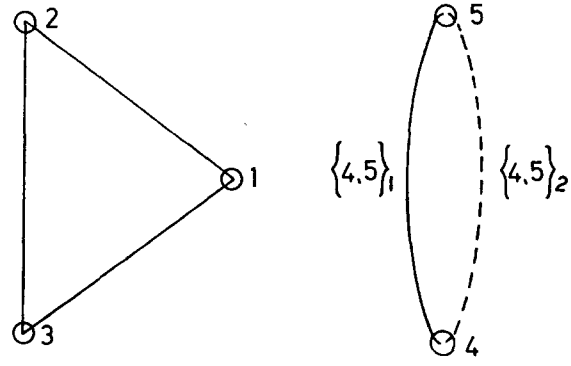

FIG. 3. μ of (3.4).

On the left-hand side of (3.4), there is only one ν: $\nu_{\text{lhs}} = \phi$. Thus,

$$\text{lhs} = 2^{\gamma(\phi)+\gamma(\mu)} = 2^{5+2} = 2^7.$$

On the right-hand side of (3.4), there is only one ν: $\nu_{\text{rhs}} = 2(1_{\{R\}})$ and

$$\text{rhs} = 2^{\gamma(2(1_{\{R\}}))+\gamma(\mu-2(1_{\{R\}}))},$$
$$= 2^{4+3} = 2^7.$$

Since $2^7 \geq 2^7$, Eq. (3.4) is satisfied.

On the left-hand side of (3.4'), there is only one ν: ν_{rhs} vanishes for all "subsets" of N,

$$\text{lhs} = 2^{\gamma(\phi)+\gamma(\bar{\mu})} = 2^{5+2} = 2^7.$$

On the right-hand side of (3.4'), there is only one ν:

$$D_{\text{rhs}}(\{4, 5\}_1) = \nu_{\text{rhs}}(\{4, 5\}_2) = 1,$$

but ν_{rhs} vanishes for all other "subsets" of N:

$$\text{rhs} = 2^{\gamma(\nu_{\text{rhs}})+\gamma(\bar{\mu}-\nu_{\text{rhs}})} = 2^{4+3} = 2^7.$$

Since $2^7 \geq 2^7$, Eq. (3.4') follows.

While only the case $\mu \leq 1$, $\Delta\mu = R\Delta S$, $\mu(R) = 1$, and $\mu(S) = 0$ has been analyzed, similar considerations apply to the remaining two subcases of $\mu \leq 1$ and $\Delta\mu = R\Delta S$ as well as to the general case where $\mu \leq 1$ is relaxed.

4. FERROMAGNETIC HEISENBERG MODEL

In this section, we are concerned with the question of whether Griffiths' Theorems 1 and 2[1-3] can be extended to the quantum mechanical ferromagnetic Heisenberg model. It is shown that Theorem 1 can be extended if we restrict ourselves to binary interactions even when an external magnetic field is present, but that Theorem 2 is not true in general.

For this model, the appropriate expressions for the partition function in the absence of an external field is

$$Z = \text{Tr}\left(\exp\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right), \tag{4.1}$$

where the $\boldsymbol{\sigma}_i$, $i \in N$, are a collection of Pauli spin matrices satisfying the usual commutation and anticommutation relations:

$$[\sigma_{ip}, \sigma_{jq}]_- = 2i\delta_{ij}\epsilon_{pqr}\sigma_{jr},$$
$$[\sigma_{ip}, \sigma_{iq}]_+ = 2\delta_{pq}. \tag{4.2}$$

The correlation functions $\langle \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \rangle$ are defined, as usual, by

$$\langle \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \rangle = Z^{-1}\,\text{Tr}\left(\boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \exp\sum_{i<j} J_{ij}(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\right)$$
$$= Z^{-1}\frac{\partial Z}{\partial J_{kl}} = \frac{\partial(\log Z)}{\partial J_{kl}}. \tag{4.3}$$

It is convenient to add a constant to the exponent in (3.1) which will not alter $\langle \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \rangle$, so that (4.3) may be replaced by

$$\langle \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \rangle = Z^{*-1}\,\text{Tr}\left(\boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \exp\sum_{i<j} J_{ij}(1 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\right), \tag{4.4}$$

where

$$Z^* = \text{Tr}\left(\exp\sum_{i<j} J_{ij}(1 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\right). \tag{4.5}$$

In the presence of an external field, (4.1) is replaced by

$$Z = \text{Tr}\left(\exp\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i H_i\sigma_{iz}\right), \tag{4.6}$$

and we have

$$\langle \boldsymbol{\sigma}_k \rangle = Z^{-1}\,\text{Tr}\left[\boldsymbol{\sigma}_k \exp\left(\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i H_i\sigma_{iz}\right)\right]. \tag{4.7}$$

We immediately find that

$$\langle \sigma_{kx} \rangle = \langle \sigma_{ky} \rangle = 0,$$

because

$$\langle \sigma_{kx,y} \rangle$$
$$= Z^{-1}\,\text{Tr}\left[\prod_{l=1}^{n} \sigma_{lz}\sigma_{kx,y} \times \exp\left(\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i H_i\sigma_{iz}\right)\prod_{l=1}^{n}\sigma_{lz}\right]$$
$$= -Z^{-1}\,\text{Tr}\left[\sigma_{kx,y}\exp\left(\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i H_i\sigma_{iz}\right)\right],$$
$$= -\langle \sigma_{kx,y} \rangle.$$

On the other hand,

$$\langle \sigma_{kz} \rangle_{H_i} = Z^{-1}\,\text{Tr}\left[\prod_{l=1}^{n}\sigma_{ly}\sigma_{kz} \times \exp\left(\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i H_i\sigma_{iz}\right)\prod_{l=1}^{n}\sigma_{ly}\right]$$
$$= -Z^{-1}\,\text{Tr}\left[\sigma_{kz}\exp\left(\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - \sum_i H_i\sigma_{iz}\right)\right]$$
$$= -\langle \sigma_{kz} \rangle_{-H_i}. \tag{4.8}$$

If we introduce a ghost spin $\boldsymbol{\sigma}_0$ with corresponding state $|s_0\rangle$ and use the preceding results, we can write (4.8) as

$$\langle \sigma_{kz} \rangle_{H_i} = \tfrac{1}{2}Z^{-1}\,\text{Tr}\left[(\sigma_{kx}\sigma_{0x} + \sigma_{ky}\sigma_{0y} + \sigma_{kz}\sigma_{0z}) \times \exp\left(\sum_{i<j} J_{ij}\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + \sum_i H_i\sigma_{iz}\sigma_{0z}\right)\right], \tag{4.9}$$

where Tr $(\cdots)$ is taken over $|s_0\rangle$ as well. A further convenient change is to replace $\sigma_{iz}\sigma_{0z}$ in the exponents of

the numerator and denominator by $(1 + \sigma_{iz}\sigma_{0z})$. We can now assert that Griffiths' Theorem 1 is

Theorem 1:

$$\langle \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l \rangle \underset{\text{ghost}}{\geq} 0, \quad 0 \leq k, \quad l \leq n, \tag{4.10}$$

where the average is taken with respect to Z^*_{ghost}, which is given by

$$Z^*_{\text{ghost}} = \operatorname{Tr}\left[\exp\left(\sum_{i<j} J_{ij}(1 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) + \sum_i J_{0i}(1 + \sigma_{iz}\sigma_{0z})\right)\right], \tag{4.11}$$

where $J_{0i} = H_i$. Equation (4.10) states that the *correlations and mean spin are nonnegative.*

The second theorem refers to the sign of the derivative of the correlations with respect to the bond energies. We have

$$\frac{\partial^2(\log Z)}{\partial J_{kl}\partial J_{rs}} = Z^{-1}\frac{\partial^2 Z}{\partial J_{kl}\partial J_{rs}} - Z^{-2}\frac{\partial Z}{\partial J_{kl}}\frac{\partial Z}{\partial J_{rs}} = \frac{\partial^2(\log Z^*_{\text{ghost}})}{\partial J_{kl}\partial J_{rs}}. \tag{4.12}$$

For the case of the Ising model and the classical discrete Heisenberg model, it has been shown that the expression (4.12) is positive and that this implies the *monotonicity of the correlations.* This result has the important consequence that a simple proof of the existence of a phase transition can be constructed for models with long-range bonds in an arbitrary number of dimensions, once it is known that a phase transition exists in a sufficiently simple case. Unfortunately, for the Heisenberg model, it is not known rigorously whether a phase transition exists even for very simple cases, nor, as will be seen from the content of the next theorem, even if a simple case with a transition is known, that a transition exists for more complicated cases. We show the following result.

Theorem 2:

$$\frac{\partial^2(\log Z^*_{\text{ghost}})}{\partial J_{kl}\partial J_{rs}} \not\geq 0$$

in general, even when all $J_{kl} \geq 0$.

Proof of Theorem 1: If we define

$$P_{kl} = \tfrac{1}{2}(1 + \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_l), \tag{4.13}$$

it is well known from Dirac's work[10] that the P_{kl} have the same algebraic properties as the set of transpositions of S_{n+1}, the symmetric group on $n + 1$ objects. Hence, a representation of $\boldsymbol{\sigma}_i$ is also a representation of transpositions. With the interpretation of $\boldsymbol{\sigma}_i$ as spin operators, this representation is 2^{n+1} dimensional. A typical basis vector in this representation can be written as $|s_0 s_1 s_2 \cdots s_N\rangle$, where the $s_i = \pm 1$ are the eigenvalues of the operators σ_{iz}, $i \in N + 1$. Such vectors form a complete orthonormal system with the usual unitary metric. In this basis, we have

$$P_{kl}\,|s_0 \cdots s_k \cdots s_l \cdots s_n\rangle = |s_0 \cdots s_l \cdots s_k \cdots s_n\rangle, \tag{4.14}$$

so that the matrix element of P_{kl} will be 1 or 0 only, and in each row and column of this matrix there will be only one nonzero entry.

We also define the projection operators

$$Q_k = \tfrac{1}{2}(1 + \sigma_{kz}\sigma_{0z}), \quad k \neq 0, \tag{4.15}$$

which have the following properties:

$$Q_k\,|s_0 \cdots s_k \cdots\rangle = |s_0 \cdots s_k \cdots\rangle, \quad \text{if} \quad s_0 = s_k,$$
$$= 0, \quad \text{if} \quad s_0 \neq s_k,$$

and

$$P_{kl}Q_k = Q_l P_{kl}, \quad k, l \neq 0,$$
$$P_{k0}Q_k = Q_k P_{k0}, \quad l = 0. \tag{4.16}$$

Q_k has the effect of locking s_k to s_0, and is diagonal in the basis chosen.

If we expand the exponential in (4.11) as a power series and use (4.16) to move any factors Q_k to the right, we obtain

$$Z^*_{\text{ghost}} = \sum C_{\mu+\nu} \operatorname{Tr}\left(\prod_\nu Q_a \prod_\mu P_{bc} \prod_\nu Q\right), \tag{4.17}$$

where the $C_{\mu+\nu}$ are positive coefficients and the products $\prod_\mu$ and $\prod_\nu$ are taken over μ and ν terms, respectively. We have also used the properties of the trace to insert a factor $\prod_\nu Q_a$ on the left-hand side. Because the operators P_{bc} are noncommuting, the product $\prod_\mu P_{bc}$ is some permutation operator whose form depends on the order of the factors. It is clear from the preceding remarks that $\operatorname{Tr}(\cdots) \geq 0$ and, hence, that

$$Z^*_{\text{ghost}} > 0. \tag{4.18}$$

Therefore, Theorem 1 will be proved if we can show that

$$\operatorname{Tr}(Q_\nu(2P_{kl} - 1)P_\mu Q_\nu) \geq 0, \tag{4.19}$$

where

$$Q_\nu = \prod_\nu Q_a, \quad P_\mu = \prod_\mu P_{bc},$$

and

$$0 \leq k, \quad l \leq n.$$

A cyclic permutation $(m \cdots m' \cdots m'')$ *is said to be tied to* 0 if, for at least one index in the cycle, say m', the projection operator $Q_{m'}$ appears in Q_ν.

Lemma: If $P_\mu \in S_{n+1}$, then, in the 2^{n+1}-dimensional spin representation,

$$\mathrm{Tr}\,(Q_\nu P_\mu Q_\nu) = 2^{m_1+m_2+\cdots+m_n+1},$$

where m_p is the number of cycles in P_μ of length p which are not tied to 0.

Proof: Let the decomposition of P_μ into cycles be

$$P_\mu = \prod_{r_1=1}^{m_1}(i_{r_1}) \prod_{r_2=1}^{m_2}(i_{r_2}i_{r_2'}) \prod_{r_3=1}^{m_3}(i_{r_3}i_{r_3'}i_{r_3''})\cdots,$$

and then

$$\langle s_0 s_1 \cdots s_n|\, Q_\nu P_\mu Q_\nu \,|s_0 s_1 \cdots s_n\rangle = 0,$$

unless $s = s' = s'' = \cdots = s^{(p)}$ for all spin locations in a given cycle of length p and if $s_0 = t' = \cdots$ for spins which are locked to s_0. Since s_0 and s can take two values, only the result follows.

In order to prove (4.19), we consider the two possibilities for the cyclic decomposition of P_μ:

$$\text{(i)}\quad P_\mu = (k\cdots k'l\cdots l')(\cdots)(\cdots)\cdots,$$

where the first cycle has length $p = p' + p''$ and $(\cdots)\cdots$ denotes the remaining cycles, and

$$\text{(ii)}\quad P_\mu = (k\cdots k')(l\cdots l')(\cdots)(\cdots)\cdots,$$

where the first cycle has length p' and the second has length p'', with $p = p' + p''$.

We also need a further subdivision into the cases where $(k\cdots k')$ and $(l\cdots l')$ are tied to 0 or are not.

For case (i), we have

$$\begin{aligned} P_{kl}P_\mu &= (kl)(k\cdots k'l\cdots l')(\cdots)\cdots \\ &= (k\cdots k')(l\cdots l')(\cdots)\cdots. \end{aligned}$$

Then we have the following cases:

(a) $(k\cdots k')$, $(l\cdots l')$ both tied [and so $(k\cdots k'l\cdots l')$ is tied]:

$$\mathrm{Tr}\,(P_{kl}P_\mu) = 2^{1+m_1+m_2+\cdots},$$
$$\mathrm{Tr}\,((2P_{kl}-1)P_\mu) = 2^{2+m_1+m_2+\cdots} - 2^{1+m_1+m_2+\cdots} > 0;$$

(b) $(k\cdots k')$ tied, $(l\cdots l')$ not tied [and so $(k\cdots k'l\cdots l')$ is tied]:

$$\mathrm{Tr}\,(P_{kl}P_\mu) = 2^{1+\cdots+m_{p''}+1+\cdots},$$
$$\mathrm{Tr}\,((2P_{kl}-1)P_\mu) = 2^{3+\cdots+m_{p''}+\cdots} - 2^{1+\cdots+m_{p''}+\cdots} > 0;$$

(c) is the same as (b), but with p' replacing p''.

(d) $(k\cdots k')\cdots(l\cdots l')$ both not tied [so $(k\cdots k'l\cdots l')$ is not tied]:

$$\mathrm{Tr}\,(P_{kl}P_\mu) = 2^{\cdots m_p-1+m_{p'}+1+m_{p''}+1+1},$$
$$\mathrm{Tr}\,((2P_{kl}-1)P_\mu) = 2^{3+m_p+m_{p'}+m_{p''}\cdots} - 2^{1+m_p+m_{p'}+m_{p''}} > 0.$$

For case (ii), we have

$$\begin{aligned} P_{kl}P_\mu &= (kl)(k\cdots k')(l\cdots l')(\cdots) \\ &= (k\cdots k'l\cdots l')(\cdots)\cdots. \end{aligned}$$

(a) $$\mathrm{Tr}\,(P_{kl}P_\mu) = 2^{1+m_1+\cdots},$$
$$\mathrm{Tr}\,((2P_{kl}-1)P_\mu) = 2^{2+m_1+\cdots} - 2^{1+m_1+\cdots} > 0.$$

(b) $$\mathrm{Tr}\,(P_{kl}P_\mu) = 2^{1+\cdots+m_{p''}-1+\cdots},$$
$$\mathrm{Tr}\,((2P_{kl}-1)P_\mu) = 2^{1+m_{p''}+\cdots} - 2^{1+m_{p''}+\cdots} = 0.$$

(c) is the same as (b).

(d) $$\mathrm{Tr}\,(P_{kl}P_\mu) = 2^{1+m_p+1+m_{p'}-1+m_{p''}-1+\cdots},$$
$$\mathrm{Tr}\,((2P_{kl}-1)P_\mu) = 2^{1+m_p+m_{p'}+m_{p''}\cdots} - 2^{1+m_p+m_{p'}+m_{p''}\cdots} = 0.$$

Hence, we have proved (4.19) and, consequently, Theorem 1.

Proof of Theorem 2[12]*:* In order to prove Theorem 2, we exhibit a simple counterexample to the contradictory assertion. Consider the case of a Heisenberg lattice with three spin locations, and put

$$Z^* = \mathrm{Tr}\,[\exp 2(J_{12}P_{12} + J_{23}P_{23})]. \tag{4.20}$$

The operators P_{12} and P_{23} are represented by a $2^3 = 8$-dimensional representation of S_3, and this reducible representation decomposes into four 1-dimensional and two 2-dimensional irreducible representations according to

$$8 = \{3\}^4 + \{2,1\}^2. \tag{4.21}$$

For these representations, we have

$$\begin{aligned} &\{3\}: P_{12} = P_{23} = (1), \\ &\{2,1\}: P_{12} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad P_{23} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}, \end{aligned} \tag{4.22}$$

and the eigenvalues of $J_{12}P_{12} + J_{23}P_{23}$ are therefore

$$\begin{aligned} &\{3\}: J_{12} + J_{23}, \\ &\{2,1\}: \pm(J_{12}^2 - J_{12}J_{23} + J_{23}^2)^{\frac{1}{2}}. \end{aligned} \tag{4.23}$$

Hence, we have

$$Z^* = 4(e^{2(J_{12}+J_{23})} + \cosh 2(J_{12}^2 + J_{23}^2 - J_{12}J_{23})^{\frac{1}{2}}) \tag{4.24}$$

and, if we expand $\log Z^*$ for small J_{12} and J_{23}, we find that

$$\begin{aligned} \log Z^* = \log 8 &+ (J_{12} + J_{23}) \\ &+ \tfrac{3}{2}(J_{12}^2 + J_{23}^2) - (J_{12}^3 + J_{23}^3) \\ &- \tfrac{1}{4}(J_{12}^4 + J_{23}^4) - J_{12}^2 J_{23}^2 + \cdots. \end{aligned} \tag{4.25}$$

Hence,

$$\frac{\partial^2(\log Z^*)}{\partial J_{12}\partial J_{23}} = -4J_{12}J_{23} + \cdots < 0, \quad (4.26)$$

for J_{12} and J_{23} sufficiently small and positive. Hence, Griffiths' Theorem 2 cannot be true when posed in its most general form. It is not known whether additional conditions can be imposed to restore this theorem.

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[1] R. B. Griffiths, J. Math. Phys. **8**, 478 (1967).
[2] R. B. Griffiths, J. Math. Phys. **8**, 484 (1967).
[3] R. B. Griffiths, J. Math. Phys. **10**, 1559 (1969).
[4] D. G. Kelly and S. Sherman, J. Math. Phys. **9**, 466 (1968). This reference will be referred to as KS.
[5] F. J. Dyson, Commun. Math. Phys. **12**, 91 (1969).
[6] The nonnegativity of correlations for the Heisenberg ferromagnet also follows by extending some results of J. Ginibre, Commun. Math. Phys. **10**, 140 (1968). We are grateful to Professor Ginibre for telling us of this possibility.
[7] R. B. Potts, Proc. Cambridge Phil. Soc. **48**, 106 (1952).
[8] R. G. J. Mills, Ph.D. thesis, University of Adelaide, 1966.
[9] S. Lefschetz, *Introduction to Topology* (Princeton U.P., Princeton, N.J., 1949).
[10] P. A. M. Dirac, *Quantum Mechanics* (Oxford U.P., Oxford, 1947), 3rd ed., Sec. 58.
[11] C. A. Hurst and S. Sherman, Phys. Rev. Letters **22**, 1357 (1969).

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When Is an Ising Magnet a Ferromagnet?

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A subcollection of the correlation inequalities recently obtained by Ginibre for Ising ferromagnets is shown to be enough to guarantee that an Ising magnet in an external magnetic field with only 2-body interactions is a ferromagnet. Thus, one has a necessary and sufficient set of correlation inequalities to guarantee that an Ising magnet in a nonnegative external magnetic field with only 2-body interactions is a ferromagnet.

Ever since Griffiths[1] obtained inequalities for the correlation functions of Ising ferromagnets with 2-body interactions it has been a natural question[2] to obtain enough inequalities on the correlation function of an Ising *magnet* with 2-body interactions that guarantee that it is the correlation function of an Ising ferromagnet. Recently, Ginibre[3] has given inequalities generalizing those of Griffiths,[1] Kelly and Sherman,[2] and Sherman.[4] This paper shows that a subcollection of Ginibre's inequalities resolves the aforementioned natural question. Ginibre's results and notations will be followed so that:

"We consider a finite set Λ of N sites. Each site carries a spin $\frac{1}{2}$, that is a finite set with two elements called up and down. A configuration of the system is defined by the set of down spins, which is a subset of Λ. Configurations are denoted by capital letters A, B, R, S, etc. The set of configurations Γ is a finite set with 2^N elements. The product RS of two configurations is defined as their symmetric difference $R\Delta S = R \cup S - R \cap S$. With this product, Γ is a commutative finite group. The unit element is the empty set $\varnothing$ and every element is of order 2: $R^2 = \varnothing$. With spin r is associated a function σ_r which is 1 for up and -1 for down. The spin products

$$\sigma_R = \prod_{r\in R} \sigma_r$$

are functions on Γ. In fact, they are the characters of the group Γ. They satisfy

$$\sigma_R\sigma_S = \sigma_{RS}, \quad (1)$$

$$\sigma_R(A)\sigma_R(B) = \sigma_R(AB), \quad (2)$$

$$\sigma_R(A) = \sigma_A(R) = (-1)^{n(A\cap R)}, \quad (3)$$

where $n(R)$ denotes the number of sites in R. A physical system is defined by a potential J, which is a real function on Γ, and with which are associated, respectively, a Hamiltonian, a probability density, a partition function, and correlation functions by the formulas

$$H = -\sum_{P\in\Gamma} J(P)\sigma_p, \quad (4)$$

$$W = Z^{-1}\exp(-H), \quad (5)$$

$$Z = \sum_{P\in\Gamma} \exp[-H(P)], \quad (6)$$

$$\langle\sigma_R\rangle = \sum_{A\in\Gamma} \sigma_R(A)W(A). \quad (7)"$$

Hence,

$$\frac{\partial^2(\log Z^*)}{\partial J_{12}\partial J_{23}} = -4J_{12}J_{23} + \cdots < 0, \quad (4.26)$$

for J_{12} and J_{23} sufficiently small and positive. Hence, Griffiths' Theorem 2 cannot be true when posed in its most general form. It is not known whether additional conditions can be imposed to restore this theorem.

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$$\langle\sigma_R\rangle = \sum_{A\in\Gamma} \sigma_R(A)W(A). \quad (7)"$$

By a ferromagnetic system we mean that $J(R) \geq 0$ for all $R \in \Gamma$.

Theorem: If, for an Ising magnet in an external magnetic field and with only binary interactions, $\rho_P(B) = \langle \sigma_B \rangle \langle \sigma_{BP} \rangle$ is a positive-definite function of B for each $P \in \Gamma$ such that $n(P) = 2$, then the magnet is a ferromagnet.

Proof: By hypothesis following Ginibre, Eq. (20): If $n(P) = 2$, then

$$0 \leq \hat{\rho}_P(T) = 2^N Z^{-2} \sum_A \sigma_P(A) \exp\left(\sum_Q J(Q)[1 + \sigma_Q(T)]\sigma_Q(A)\right)$$

so that, up to a positive normalization factor, $\hat{\rho}_P(T)$ is proportional to $\langle \sigma_P \rangle_T$, the average of σ in a new ferromagnetic system associated with the potential J_T defined by

$$J_T(Q) = 2J(Q), \quad \text{if} \quad n(Q \cap T) \quad \text{is even},$$
$$= 0, \quad \text{if} \quad n(Q \cap T) \quad \text{is odd}.$$

Suppose $n(T) = 2$. Then $J_T(T) = 2J(T)$, but, for $Q \neq T$ and $n(Q) \in \{1, 2\}$,

$$J(Q) = 0, \quad \text{if} \quad Q \cap T \neq \varnothing,$$
$$= 2J(Q), \quad \text{if} \quad Q \cap T = \varnothing.$$

In the new system, spins in T do not interact with spins outside of T. Moreover, spins in T have no external magnetic field acting on them. From this,

$$\langle \sigma_T \rangle_T = \tanh 2J(T)$$

and

$$\operatorname{sgn} \hat{\rho}_T(T) = \operatorname{sgn} \tanh 2J(T) = \operatorname{sgn} J(T).$$

Thus, if $n(T) = 2$, then $J(T) \geq 0$, and the system is ferromagnetic.

Corollary 1: If for an Ising magnet in an external magnetic field, with only binary interactions, $\hat{\rho}_P(P) \geq 0$ for each $P \in \Gamma$ such that $n(P) = 2$, then the magnet is a ferromagnet.

Corollary 2: Consider an Ising magnet in a nonnegative external magnetic with only binary interactions. The magnet is a ferromagnet if and only if $\rho_P(B) = \langle \sigma_B \rangle \langle \sigma_{BP} \rangle$ is a positive-definite function of B for each $P \in \Gamma$ such that $n(P) = 2$.

Incidentally, by the use of Sec. 3 in Ref. 4, expression (21) of Ref. 3 can be strengthened to read "any mixed derivative of any order of $Z^2 \hat{\omega}_{R,S}$ with respect to any collection of interactions $J(Q_1), \cdots, J(Q_k)$ is nonnegative."

Ginibre's result that for an Ising ferromagnet $\langle \sigma_B \rangle \times \langle \sigma_{BP} \rangle$ is a positive-definite function of $B \in \Gamma$ can be extended by methods of Ref. 2 (Proposition 1, Sec. 9) to show that the function is a nonnegative linear combination of indicator functions of subgroups of Γ. Such linear combinations are positive definite, but not all positive-definite functions on Γ are such linear combinations.

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[1] R. B. Griffiths, J. Math. Phys. **8**, 478, 484 (1967).
[2] D. G. Kelly and S. Sherman, J. Math. Phys. **9**, 466 (1968).
[3] J. Ginibre, Phys. Rev. Letters **23**, 828 (1969).
[4] S. Sherman, Commun. Math. Phys. **14**, 1 (1969).

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Quantum Statistical Mechanical Derivation of Generalized Hydrodynamic Equations

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Differential conservation equations are derived for the mass-, momentum-, and energy-density operators for a 1-component simple fluid of Bose or Fermi particles with arbitrary pairwise interactions. These equations are used in a statistical mechanical derivation of exact equations of motion for the expectations of these operators. The equations of motion are coupled to equations relating these expectations to the local temperature, chemical potential, and fluid velocity. The coupled equations are closed in the sense that the expectations and their thermodynamic conjugates listed above are the only unknowns, although some of the dependence in the equations on the conjugates is expressed only implicitly. The equations of motion are memory-retaining nonlocal generalizations of the classical hydrodynamic equations and apply to a normal fluid arbitrarily far from equilibrium. The formalism is not carried as far as has the corresponding classical formalism because the local equilibrium expectation of the momentum density here does not equal the fluid velocity times the expectation of the mass density as is true in classical statistical mechanics.

1. INTRODUCTION

In this paper generalized hydrodynamic equations valid for fluids far from equilibrium are derived from quantum statistical mechanics. The equations are closed since the currents are expressed as functionals of the local thermodynamic conjugate variables, which themselves are functionals of the mass, momentum, and energy densities. The system considered is a 1-component simple fluid of Bose or Fermi particles with arbitrary pairwise interactions. This system is often taken as a model for liquid ^{4}He or ^{3}He. However, except for a brief comment on superfluids, this paper is concerned only with normal fluids and hence not with ^{4}He below 2.17 *K*.

Although some of the material in this paper has appeared previously in a general formalism,[1,2] a self-contained derivation applicable to quantum fluids is presented here for greater clarity. The generalized hydrodynamic equations to be derived are identical in form to the corresponding equations derived from classical statistical mechanics. The latter equations may be transformed into those outlined without derivation by Richardson[3] and derived in detail by Piccirelli[4] for a fluid of interacting classical particles. However, the present formalism is not carried as far as Piccirelli's because the local equilibrium expectation of the momentum density is not as simple in quantum theory as in classical theory. As far as the present paper goes, it gives an efficient, exact, quantum statistical derivation of closed equations, previously widely believed to be impossible to derive exactly.

There are not many papers devoted to the derivation of hydrodynamic equations from quantum statistical mechanics. Born and Green[5] used a density-matrix hierarchy to obtain equations similar in form to hydrodynamic equations. Irving and Zwanzig[6] used the Wigner density to transform Irving and Kirkwood's[7] classical derivation into a quantum derivation. Fröhlich[8] used an expansion about total equilibrium, but did not give expressions for the coefficients in this expansion. Without attempting to derive hydrodynamic equations, Kadanoff and Martin[9] used them to determine the space and time dependence of correlation functions. Hohenberg and Martin[10] discussed superfluids by making assumptions in order to close their hydrodynamic equations. None of these authors used statistical mechanics to derive closed equations valid for fluids far from equilibrium.

Mori[11] derived hydrodynamic equations by expanding the statistical density operator about local equilibrium. He obtained expressions for the transport coefficients as time integrals of correlation functions,[12–14] but only after removing the thermodynamic forces from the integrals.[15] This can be done only when there is a wide separation in time scales. His formalism is closely related to an approximation of the one to be presented.

The remainder of this paper in outline is as follows. The Hamiltonian and the operators corresponding to the observed densities are defined in Sec. 2. Then exact operator equations, in the form of the classical hydrodynamic equations, are written down in Sec. 2, with their derivation given in Appendix A. Local thermodynamic variables such as temperature and chemical potential are defined in Sec. 3 using the local equilibrium statistical density operator. Then exact closed generalized hydrodynamic equations, which are the expectations of the above-mentioned operator equations, are written down in Sec. 3, with their derivation given in Appendix B. Further steps, omitted in this paper, are discussed in Sec. 4, along with a brief comment on extending the formalism to include superfluids.

2. OPERATOR EQUATIONS

The Hamiltonian of the 1-component simple fluid to be considered here is

$$\mathcal{H} \equiv \int d^3r \psi^+(\mathbf{r})\Big(-\frac{\hbar^2}{2m}\nabla^2 + V_1(\mathbf{r}) + \tfrac{1}{2}\int d^3r' \psi^+(\mathbf{r}')V_2(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\Big)\psi(\mathbf{r}), \quad (2.1)$$

where ψ^+ and ψ are Bose or Fermi particle creation and annihilation operators. Each particle has the external potential energy V_1, and each pair of particles has the interaction potential energy V_2, which may be any given functions.

The operators usually assumed to describe this fluid are the mass-, momentum-, and energy-density operators

$$\rho_m(\mathbf{r}) \equiv \psi^+(\mathbf{r})m\psi(\mathbf{r}), \quad (2.2)$$

$$\rho_\mathbf{p}(\mathbf{r}) \equiv \psi^+(\mathbf{r})\mathbf{p}\psi(\mathbf{r}), \quad (2.3)$$

and

$$\rho_e(\mathbf{r}) \equiv \psi^+(\mathbf{r})\mathcal{H}\psi(\mathbf{r}), \quad (2.4)$$

respectively. Here

$$\mathbf{p} \equiv (\hbar/2i)(\overrightarrow{\nabla} - \overleftarrow{\nabla}), \quad (2.5)$$

where the arrows over the gradient operators indicate in which direction they operate: to the right on $\psi(\mathbf{r})$ or to the left on $\psi^+(\mathbf{r})$. Also

$$\mathcal{H} \equiv \frac{p^2}{2m} + V_1(\mathbf{r}) + \tfrac{1}{2}\int d^3r' \psi^+(\mathbf{r}')V_2(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}'), \quad (2.6)$$

where the p^2 again operates to the right and left. This definition of $\rho_e(\mathbf{r})$ with the operator p^2 is used because it is Hermitian, because its integral over all space equals the Hamiltonian (2.1), and because it simplifies some equations later on.

In classical hydrodynamics, the time derivatives of the mass, momentum, and energy densities equal the divergences of the corresponding currents plus an external force term in the momentum equation. These are called differential conservation laws. Now the commutator of $i\mathcal{H}/\hbar$ with an operator corresponds to a time derivative. This commutator with the operators (2.2)–(2.4) can be expressed as divergences because total mass, momentum, and energy are conserved (except for the effect of the external force).

These commutators are calculated in Appendix A, and the resulting operator equations are

$$(i/\hbar)[\mathcal{H}, \rho_m(\mathbf{r})] = -\nabla \cdot \rho_\mathbf{p}(\mathbf{r}), \quad (2.7)$$

$$(i/\hbar)[\mathcal{H}, \rho_\mathbf{p}(\mathbf{r})] = \rho_m(\mathbf{r})\mathbf{F}_1(\mathbf{r})/m - \boldsymbol{\Delta} \cdot \mathbf{j}_\mathbf{p}(\mathbf{r}), \quad (2.8)$$

and

$$(i/\hbar)[\mathcal{H}, \rho_e(\mathbf{r})] = -\nabla \cdot \mathbf{j}_e(\mathbf{r}), \quad (2.9)$$

where the momentum current is given by

$$\mathbf{j}_\mathbf{p}(\mathbf{r}) \equiv \psi^+(\mathbf{r})(\mathbf{pp}/m)\psi(\mathbf{r}) + \tfrac{1}{2}\int d^3r' \int d^3r'' \int_{\mathbf{r}'}^{\mathbf{r}''} d\mathbf{r}''' \times \delta(\mathbf{r}-\mathbf{r}''')\mathbf{F}_2(\mathbf{r}'-\mathbf{r}'')\psi^+(\mathbf{r}'')\psi^+(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}''), \quad (2.10)$$

and the energy current is given by

$$\mathbf{j}_e(\mathbf{r}) \equiv \psi^+(\mathbf{r})\tfrac{1}{2}[\mathbf{p}/m, \mathcal{H}]_+\psi(\mathbf{r}) + \frac{1}{4m}\int d^3r' \int d^3r'' \int_{\mathbf{r}'}^{\mathbf{r}''} d\mathbf{r}''' \delta(\mathbf{r}-\mathbf{r}''')\mathbf{F}_2(\mathbf{r}'-\mathbf{r}'') \cdot \psi^+(\mathbf{r}'')\psi(\mathbf{r}')(\mathbf{p}'+\mathbf{p}'')\psi(\mathbf{r}')\psi(\mathbf{r}''). \quad (2.11)$$

Here,

$$\mathbf{F}_1(\mathbf{r}) \equiv -\nabla V_1(\mathbf{r}) \quad (2.12)$$

is the external force on a particle, and

$$\mathbf{F}_2(\mathbf{r}'-\mathbf{r}'') \equiv -\nabla V_2(\mathbf{r}'-\mathbf{r}'') \quad (2.13)$$

is the force on a particle at $\mathbf{r}'$ exerted by another particle at $\mathbf{r}''$.

The line integral in Eqs. (2.10) and (2.11) may be taken along any curve between the points $\mathbf{r}'$ and $\mathbf{r}''$, except as restricted by the following. The expectation of the currents must always be zero for all $\mathbf{r}$ for which the expectation of the mass density $\rho_m(\mathbf{r})$ is zero. Consistent with this restriction, one way of removing the above ambiguity[16] is to use the shortest curve between $\mathbf{r}'$ and $\mathbf{r}''$ that remains inside the region where the expectation of $\rho_m(\mathbf{r})$ is nonzero. For most $\mathbf{r}'$ and $\mathbf{r}''$, the curve is a straight line, and the currents (2.10) and (2.11) are then analogous to Richardson's[3,17] for classical statistical mechanics.

Infinite-series expressions for the currents $\mathbf{j}_\mathbf{p}$ and $\mathbf{j}_e$ have been given by Irving and Kirkwood[7] for classical statistical mechanics, and by Grossmann[18] for quantum statistical mechanics. Higher-order terms in these expressions can be dropped only if the interparticle force $\mathbf{F}_2$ is short range. Richardson's currents, as well as the currents (2.10) and (2.11), both agree with these series expansions. Kugler's currents,[19] however, do not agree with the series expansions even in the short-range limit, and their expectations are not zero where the expectation of $\rho_m(\mathbf{r})$ is zero.

3. CLOSED EQUATIONS

The expectations of Eqs. (2.7)–(2.9) are differential conservation laws similar in form to the equations of classical hydrodynamics. However, the expectations of the currents $\mathbf{j}_\mathbf{p}$ and $\mathbf{j}_e$ on the right are as yet unknowns, and there are more unknowns than equations. In order to obtain the hydrodynamic equations, it is necessary to express these currents in terms of the temperature and other thermodynamic variables,

which themselves must be expressed in terms of the expectations of the mass-, momentum-, and energy-density operators (2.2)–(2.4). Then the equations will be closed.

The expectations of the mass-, momentum-, and energy-density operators are given by

$$\langle \rho_m(\mathbf{r})\rangle_t \equiv \mathrm{Tr}\,[\rho_m(\mathbf{r})\rho(t)], \tag{3.1}$$

$$\langle \rho_{\mathfrak{p}}(\mathbf{r})\rangle_t \equiv \mathrm{Tr}\,[\rho_{\mathfrak{p}}(\mathbf{r})\rho(t)], \tag{3.2}$$

and

$$\langle \rho_e(\mathbf{r})\rangle_t \equiv \mathrm{Tr}\,[\rho_e(\mathbf{r})\rho(t)], \tag{3.3}$$

where $\rho(t)$ is the statistical density operator satisfying the Liouville equation. These expectations are the unknowns whose values are to be found by deriving the closed equations of motion they satisfy and then integrating these equations of motion.

In order to derive these equations, we introduce new variables $\beta(\mathbf{r}, t)$, $\mu(\mathbf{r}, t)$, and $v(\mathbf{r}, t)$, which are defined to be functionals of the expectations (3.1)–(3.3) as follows. Introduce the local equilibrium statistical density operator

$$\sigma(t) \equiv \frac{1}{Z(t)} \exp\left[-\int d^3r\beta(\mathbf{r}, t) \times \left(\rho_e(\mathbf{r}) - \frac{\mu(\mathbf{r}, t)}{m}\rho_m(\mathbf{r}) - \mathbf{v}(\mathbf{r}, t)\cdot\rho_{\mathfrak{p}}(\mathbf{r})\right)\right], \tag{3.4}$$

where for normalization

$$Z(t) \equiv \mathrm{Tr}\left\{\exp\left[-\int d^3r\beta(\mathbf{r}, t) \times \left(\rho_e(\mathbf{r}) - \frac{\mu(\mathbf{r}, t)}{m}\rho_m(\mathbf{r}) - \mathbf{v}(\mathbf{r}, t)\cdot\rho_{\mathfrak{p}}(\mathbf{r})\right)\right]\right\}. \tag{3.5}$$

The $\beta(\mathbf{r}, t)$, $\mu(\mathbf{r}, t)$, and $\mathbf{v}(\mathbf{r}, t)$ are to be chosen to satisfy

$$\mathrm{Tr}\,[\rho_m(\mathbf{r})\sigma(t)] = \langle \rho_m(\mathbf{r})\rangle_t, \tag{3.6}$$

$$\mathrm{Tr}\,[\rho_{\mathfrak{p}}(\mathbf{r})\sigma(t)] = \langle \rho_{\mathfrak{p}}(\mathbf{r})\rangle_t, \tag{3.7}$$

and

$$\mathrm{Tr}\,[\rho_e(\mathbf{r})\sigma(t)] = \langle \rho_e(\mathbf{r})\rangle_t, \tag{3.8}$$

where the functions on the right are already defined in Eqs. (3.1)–(3.3). Equations (3.4)–(3.8) are not to be considered here as expressions for $\langle\rho_m\rangle$, $\langle\rho_{\mathfrak{p}}\rangle$, and $\langle\rho_e\rangle$, but are coupled nonlinear integral equations for β, μ, and $\mathbf{v}$ as unknowns. The functional dependence of β, μ, and $\mathbf{v}$ on $\langle\rho_m\rangle$, $\langle\rho_{\mathfrak{p}}\rangle$, and $\langle\rho_e\rangle$ just defined is a time-independent one; β, μ, and $\mathbf{v}$ depend upon t only because they depend upon $\langle\rho_m\rangle$, $\langle\rho_{\mathfrak{p}}\rangle$, and $\langle\rho_e\rangle$, which themselves depend upon t. The multipliers $\beta\mu$, $\beta\mathbf{v}$, and β are called the thermodynamic conjugates of the expectations $\langle\rho_m\rangle$, $\langle\rho_{\mathfrak{p}}\rangle$, and $\langle\rho_e\rangle$. Here $\beta(\mathbf{r}, t)$ is the local temperature, $\mu(\mathbf{r}, t) + \frac{1}{2}mv(\mathbf{r}, t)^2$ is the local chemical potential, and $\mathbf{v}(\mathbf{r}, t)$ is the local fluid velocity.[20,21]

Equations (3.4)–(3.9) are just definitions and are to be used even for large deviations from equilibrium, as in a shock wave, for example. No assumption is made here that the fluid remains in any sense close to equilibrium. The statistical density operator $\rho(t)$ is assumed to equal the local equilibrium statistical density operator $\sigma(t)$ only at the initial time $t = 0$. This initial condition is reasonable for a fluid initially constrained away from equilibrium.[21] The fluid would be initially in equilibrium only if β and μ were constants and $\mathbf{v}$ were zero.

All of the traces to be calculated in the following will involve $\sigma(t)$ rather than $\rho(t)$. So, for convenience, let angular brackets have the definition

$$\langle A\rangle_t \equiv \mathrm{Tr}\,[A\sigma(t)], \tag{3.9}$$

where A may be any quantum-mechanical operator. Because of the definition of β, μ, and $\mathbf{v}$, this definition is consistent with Eqs. (3.6)–(3.8). Of course, the local equilibrium statistical density operator $\sigma(t)$ does not satisfy the Liouville equation. As a result, the expectation of an arbitrary operator A is not given by Eq. (3.9), but must be calculated as a trace of A times $\rho(t)$, which does satisfy the Liouville equation.

The expectations of Eqs. (2.7)–(2.9), including the currents $\mathbf{j}_{\mathfrak{p}}$ and $\mathbf{j}_e$, are calculated exactly in Appendix B, and the resulting closed equations of motion are

$$\frac{\partial\langle\rho_m(\mathbf{r})\rangle_t}{\partial t} = -\nabla\cdot\langle\rho_{\mathfrak{r}}(\mathbf{r})\rangle_t, \tag{3.10}$$

$$\frac{\partial\langle\rho_{\mathfrak{p}}(\mathbf{r})\rangle_t}{\partial t} = \frac{\mathbf{F}_1(\mathbf{r})\langle\rho_m(\mathbf{r})\rangle_t}{m} - \nabla\cdot\langle\mathbf{j}_{\mathfrak{p}}(\mathbf{r})\rangle_t + \nabla\cdot\int_0^t dt'\int d^3r'[\mathsf{K}_{\mathfrak{p}\mathfrak{p}}(\mathbf{r}, t, \mathbf{r}', t'):\nabla'\beta(\mathbf{r}', t')\mathbf{v}(\mathbf{r}', t') - \mathsf{K}_{\mathfrak{p}e}(\mathbf{r}, t, \mathbf{r}', t')\cdot\nabla'\beta(\mathbf{r}', t')], \tag{3.11}$$

and

$$\frac{\partial\langle\rho_e(\mathbf{r})\rangle_t}{\partial t} = -\nabla\cdot\langle\mathbf{j}_e(\mathbf{r})\rangle_t + \nabla\cdot\int_0^t dt'\int d^3r'[\mathsf{K}_{e\mathfrak{p}}(\mathbf{r}, t, \mathbf{r}', t'):\nabla'\beta(\mathbf{r}', t')\mathbf{v}(\mathbf{r}', t') - \mathsf{K}_{ee}(\mathbf{r}, t, \mathbf{r}', t')\cdot\nabla'\beta(\mathbf{r}', t')], \tag{3.12}$$

where the kernels are correlation functions given by

$$\mathsf{K}_{\mathfrak{p}\mathfrak{p}}(\mathbf{r}, t, \mathbf{r}', t') \equiv \langle\mathbf{j}_{\mathfrak{p}}(\mathbf{r})T(t, t')(1 - P)\bar{\mathbf{j}}_{\mathfrak{p}}(\mathbf{r}')\rangle_{t'}, \tag{3.13}$$

$$\mathsf{K}_{\mathfrak{p}e}(\mathbf{r}, t, \mathbf{r}', t') \equiv \langle\mathbf{j}_{\mathfrak{p}}(\mathbf{r})T(t, t')(1 - P)\bar{\mathbf{j}}_e(\mathbf{r}')\rangle_{t'}, \tag{3.14}$$

$$\mathsf{K}_{e\mathfrak{p}}(\mathbf{r}, t, \mathbf{r}', t') \equiv \langle\mathbf{j}_e(\mathbf{r})T(t, t')(1 - P)\bar{\mathbf{j}}_{\mathfrak{p}}(\mathbf{r}')\rangle_{t'}, \tag{3.15}$$

and

$$\mathsf{K}_{ee}(\mathbf{r}, t, \mathbf{r}', t') \equiv \langle \mathbf{j}_e(\mathbf{r}) T(t, t')(1 - P)\mathbf{j}_e(\mathbf{r}')\rangle_{t'} . \quad (3.16)$$

Here, the operator P is related to a projection operator with respect to the weight σ.[22] It automatically subtracts out an average of the current $\mathbf{j}$ to its right, so that the correlation functions can approach zero for large $t - t'$. The operator T gives the unitary[23] transformation on the operator to its right, advancing it in time, but with the hydrodynamic motion projected out at each instant by the operator P. This dependence of T on P, given by Eq. (B5), is essential if the correlation functions are to become zero and remain zero after a time that is short compared with hydrodynamic times.[24] More generally, the correlation functions may decay in about the same time as the expectations (3.1)–(3.3), and P is still essential.

Equations (3.10)–(3.12) are memory-retaining nonlocal generalizations of the classical hydrodynamic equations. In a near-equilibrium approximation, the correlation functions (3.13)–(3.15) satisfy reciprocity relations.[25] However, no approximations are made in the present paper. The first terms on the right of Eqs. (3.10)–(3.12) are called reversible terms since they do not directly change the entropy.[26] The time integral terms are called irreversible terms since they do change the entropy. The reversible terms describe only the macroscopic flow, while the irreversible terms describe the microscopic dissipative effects due to the interaction V_2.

Equations (3.4)–(3.16) are the desired closed equations of motion for $\langle \rho_m(\mathbf{r})\rangle_t$, $\langle \rho_{\mathrm{p}}(\mathbf{r})\rangle_t$, $\langle \rho_e(\mathbf{r})\rangle_t$, $\beta(\mathbf{r}, t)$, $\mu(\mathbf{r}, t)$, and $\mathbf{v}(\mathbf{r}, t)$. These are the only unknowns in the equations. However, the dependence of the kernels on β, μ; and $\mathbf{v}$ is stated only implicitly in the definition of P and T given in Appendix B. A method for extracting this dependence approximately is discussed in Sec. 4.

4. DISCUSSION

Equations (3.10)–(3.12) are memory-retaining nonlocal generalizations of the classical hydrodynamic equations. The advantages of this formalism are: (1) The equations of motion are closed since the correlation functions (3.13)–(3.16) are functionals of the local temperature, local chemical potential, and local fluid velocity, which themselves are given in Eqs. (3.4)–(3.8) as functionals of the mass, momentum, and energy densities. (2) All traces are to be calculated using the local equilibrium statistical density operator $\sigma(t)$ as in Eq. (3.9). This is physically desirable and is easier than calculating traces using $\rho(t)$, which, as a solution to the Liouville equation, is linear in the initial condition and thus contains the initial condition explicitly. In the present formalism, the initial condition is contained only implicitly through the initial values of the macroscopic unknowns. (3) The equations of motion are exact and apply to systems arbitrarily far from equilibrium. They apply even when the classical hydrodynamic equations do not, e.g., near a critical point where a memory-retaining nonlocal theory is necessary. (4) The equations reduce to the classical hydrodynamic equations in the appropriate limits, and the resulting expressions for the transport coefficients are independent of the order of taking these limits, as is discussed below.

Equations (3.4)–(3.16) are identical in form to generalized hydrodynamic equations derived from classical statistical mechanics, except that expressions in them involve traces over operators rather than integrals over functions of phase. However, as will be discussed, the dependence of these expressions on the local velocity $\mathbf{v}(\mathbf{r}, t)$ is more complicated in quantum theory than it is in classical theory. Hence, approximations appear to be necessary here, although they are not necessary at this step in the classical derivation.

In the classical derivation,[4] the reversible currents $\langle \rho_{\mathrm{p}}\rangle$, $\langle \mathbf{j}_{\mathrm{p}}\rangle$, and $\langle \mathbf{j}_e\rangle$ become $\langle \rho_m\rangle\mathbf{v}$, $\langle \rho_m\rangle\mathbf{v}\mathbf{v} + \langle \mathbf{j}_{\mathrm{p}}\rangle^{+}$, and $\langle \rho_e\rangle\mathbf{v} + \langle \mathbf{j}_{\mathrm{p}}\rangle^{+} \cdot \mathbf{v}$, respectively. Here the plus indicates that, in the local equilibrium density σ, the $\mathbf{v}$ term is dropped and μ is replaced by $\mu + \frac{1}{2}mv^2$. These results can be proved[4] by translating one of the momentum integrals by $m\mathbf{v}$. When this is done on the irreversible terms, the thermodynamic forces $\nabla\beta\mathbf{v}$ and $\nabla\beta$ become $\nabla\mathbf{v}$ and $\nabla\beta$. Thus the equations take a form closely paralleling the classical hydrodynamic equations.

In the quantum derivation, the reversible currents have additional terms,[27] which are much too complicated to write here, but which vanish in the limit of small $\hbar^2\beta$ or in the limit of small $\nabla \times \mathbf{v}$. Also, except in one of these limits, the $\mathbf{v}\nabla\beta$ term cannot be removed from the thermodynamic force $\nabla\beta\mathbf{v}$. Thus, it appears to be necessary, at this point, to take the approximation in which terms containing $\hbar^2\beta$ and $\nabla \times \mathbf{v}$ are dropped.

In the short-memory local limit, the correlation functions become sharp like δ functions, so that the thermodynamic forces $\nabla\mathbf{v}$ and $\nabla\beta$ can be removed from the integrals, which then become transport coefficients.[28] These correlation functions must still contain the operator P both explicitly and through the dependence given by Eq. (B5), so that they will become zero and remain zero after a time that is short compared with hydrodynamic times.[24] This operator P does not appear in the Green–Kubo[12–14] expressions for transport coefficients. As a result, in their expressions the integral over an *infinite* volume must be

performed before the integral over the infinite-time interval in order to obtain a nonzero result for the transport coefficients.[29] However, because in the present formalism the operator P projects out the hydrodynamic motion at each instant in the time development of the correlation functions, the order of integration here is not important, and the space integral here need not be infinite.

The final step in deriving the equations of motion is to obtain explicit expressions for the kernels in terms of quantities that can be calculated. For linear deviations from equilibrium, this can be done with a continued fraction expansion.[30] A simple method of truncating this kind of expansion has been used to predict a nuclear magnetic resonance lineshape in excellent agreement with experiments.[31] The application of this technique to fluids is limited at the present by the difficulty of calculating the moments, which involve traces over σ.

For superfluids, additional variables and additional equations of motion coupled to Eqs. (3.10)–(3.12) appear to be necessary. A derivation of these exact closed equations has not yet been accomplished except for zero interaction V_2. If V_2 is zero, the extra variables are the expectations of $\psi^+(\mathbf{r})$ and $\psi(\mathbf{r})$, and Eqs. (A2) and (A3) are used along with Eqs. (2.7)–(2.9). Terms linear in $\psi^+(\mathbf{r})$ and $\psi(\mathbf{r})$ must be added onto the exponent in Eqs. (3.4) and (3.5), where the multipliers in these terms are determined by Eqs. (3.6)–(3.8) plus two new equations involving the expectations of $\psi^+(\mathbf{r})$ and $\psi(\mathbf{r})$. The result is that extra terms are added to Eqs. (3.10)–(3.12) coupling these equations to two new equations of motion that are the expectations of Eqs. (A2) and (A3). By use of a canonical transformation whose exponent is linear in $\psi^+(\mathbf{r})$ and $\psi(\mathbf{r})$, the particle-nonconserving terms added to the exponent in Eqs. (3.4) and (3.5) can be transformed away and the reversible terms in Eqs. (3.10)–(3.12) become the usual sum of super and normal terms appearing in the phenomenological theory.[32] This is a beautifully simple derivation of 2-fluid generalized hydrodynamic equations for the noninteracting Bose fluid. However, the irreversible terms here are not zero and cannot be approximated in a short-memory local limit. If V_2 is not zero, the problem with the irreversible terms is removed, but expressions containing V_2 become unpleasant when the above canonical transformation is performed. At the present it is not known how to correct this.

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APPENDIX A

In this appendix, Eqs. (2.7)–(2.11) are derived using

$$[\psi(\mathbf{r}), \psi(\mathbf{r}')]_\mp = 0, \quad [\psi(\mathbf{r}), \psi^+(\mathbf{r}')]_\mp = \delta(\mathbf{r}-\mathbf{r}'), \quad [\psi^+(\mathbf{r}), \psi^+(\mathbf{r}')]_\mp = 0, \tag{A1}$$

where the minus sign denotes commutator for bosons and the plus sign denotes anticommutator for fermions.

For either bosons or fermions, Eqs. (2.1) and (A1) give

$$[\mathcal{H}, \psi(\mathbf{r})] = -\Big(-\frac{\hbar^2}{2m}\nabla^2 + V_1(\mathbf{r}) + \int d^3r'\,\psi^+(\mathbf{r}')V_2(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\Big)\psi(\mathbf{r}) \tag{A2}$$

and

$$[\mathcal{H}, \psi^+(\mathbf{r})] = \psi^+(\mathbf{r})\Big(-\frac{\hbar^2}{2m}\overleftarrow{\nabla}^2 + V_1(\mathbf{r}) + \int d^3r'\,\psi^+(\mathbf{r}')V_2(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\Big), \tag{A3}$$

where the upper (lower) equation is most easily derived by expanding the commutator on the left into two terms and using Eqs. (A1) on the second (first) term only. No integration by parts is necessary.

Equations (A2) and (A3) along with the identities

$$[\mathcal{H}, \psi^+A\psi] = [\mathcal{H}, \psi^+]A\psi + \psi^+[\mathcal{H}, A]\psi + \psi^+A[\mathcal{H}, \psi], \tag{A4}$$

$$\overleftarrow{\nabla}^2 - \vec{\nabla}^2 = -(\overleftarrow{\nabla} + \vec{\nabla})\cdot(\vec{} - \overleftarrow{\nabla}), \tag{A5}$$

and

$$[\mathbf{p}, A] = -i\hbar(\nabla A) \tag{A6}$$

give

$$[\mathcal{H}, \psi^+(\mathbf{r})A\psi(\mathbf{r})] = i\hbar\nabla\cdot\{\psi^+(\mathbf{r})\tfrac{1}{2}[\mathbf{p}/m, A]_+\psi(\mathbf{r})\} + \psi^+(\mathbf{r})\Big(\mathcal{H} + \frac{p^2}{2m} + V_1(\mathbf{r}) + \int d^3r'\,\psi^+(\mathbf{r}')V_2(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}'), A\Big)\psi(\mathbf{r}), \tag{A7}$$

where A may be any linear operator. Notice that the ∇ in $[\mathbf{p}, A]_+$ does not operate on A.

Equation (A7) is used as follows. Let $A = im/\hbar$ to get Eq. (2.7). Let $A = i\mathbf{p}/\hbar$ and use Eq. (A6) to get

$$(i/\hbar)[\mathcal{H}, \rho_{\mathbf{p}}(\mathbf{r})] = \rho_m(\mathbf{r})\mathbf{F}_1(\mathbf{r})/m - \nabla\cdot[\psi^+(\mathbf{r})(\mathbf{pp}/m)\psi(\mathbf{r})] - \int d^3r'\,\mathbf{F}_2(\mathbf{r}'-\mathbf{r})\psi^+(\mathbf{r})\psi^+(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}), \tag{A8}$$

where $\mathbf{F}_1(\mathbf{r})$ and $\mathbf{F}_2(\mathbf{r})$ are defined by Eqs. (2.12) and (2.13). Finally, let $A = i\hbar/\hbar$ and use Eqs. (2.5) and

(A6) to get

$$(i/\hbar)[\mathcal{H}, \rho_e(\mathbf{r})] = -\nabla \cdot \{\psi^+(\mathbf{r})\tfrac{1}{2}[\mathbf{p}/m, \hat{\pi}]_+\psi(\mathbf{r})\} - \frac{1}{2m}\int d^3r' \mathbf{F}_2(\mathbf{r}' - \mathbf{r}) \cdot \psi^+(\mathbf{r})\psi^+(\mathbf{r}')(\mathbf{p} + \mathbf{p}')\psi(\mathbf{r}')\psi(\mathbf{r}), \tag{A9}$$

where the $\mathbf{p}'$ term comes from the $[\mathcal{H}, \hat{\pi}]$ term in Eq. (A7).

The last terms in Eqs. (A8) and (A9) are of the form

$$\int d^3r' f(\mathbf{r}, \mathbf{r}'), \tag{A10}$$

where

$$f(\mathbf{r}', \mathbf{r}) = -f(\mathbf{r}, \mathbf{r}'). \tag{A11}$$

As a result, the integral of these terms over all $\mathbf{r}$ is zero, and the terms can be written as divergences

$$\int d^3r' f(\mathbf{r}, \mathbf{r}') = \nabla \cdot \int d^3r' \int d^3r'' \int_{\mathbf{r}'}^{\mathbf{r}''} d\mathbf{r}''' \tfrac{1}{2}\delta(\mathbf{r} - \mathbf{r}''') f(\mathbf{r}', \mathbf{r}''). \tag{A12}$$

This is easily proved by letting the ∇ operate on the δ to become $-\nabla'''$, thus permitting the $\mathbf{r}'''$ line integral to be performed.

When Eq. (A12) is applied to Eqs. (A8) and (A9), Eqs. (2.8) and (2.9) result, where the currents are defined by Eqs. (2.10) and (2.11).

APPENDIX B

In this appendix, Eqs. (3.10)–(3.16) are derived from the Liouville equation. Although this derivation is a special case of a previously published general formalism,[1,2] it is presented here in a self-contained form for convenience in the present application.

The Liouville equation is

$$\frac{\partial \rho(t)}{\partial t} = -iL\rho(t), \tag{B1}$$

where the Liouville operator is defined by

$$LA \equiv [\mathcal{H}, A]/\hbar \tag{B2}$$

for any quantum-mechanical operator A. Here $\mathcal{H}$ is the Hamiltonian (2.1). The initial condition for $\rho(t)$ is assumed to be

$$\rho(0) = \sigma(0). \tag{B3}$$

In order to express the expectations of the operators $\mathbf{j}_p$ and $\mathbf{j}_e$ in terms of just the desired unknowns, it is convenient to introduce an operator $P(t)$ defined by

$$P(t)A \equiv \sum_{i=m,p,e} \int d^3r \frac{\delta\sigma(t)}{\delta\langle\rho_i(\mathbf{r})\rangle} \operatorname{Tr}[\rho_i(\mathbf{r})A], \tag{B4}$$

where A may be any quantum-mechanical operator. Also, it is convenient to introduce another operator $T(t, t')$ defined by

$$\frac{\partial T(t, t')}{\partial t'} = T(t, t')[1 - P(t')]iL \tag{B5}$$

with the initial condition

$$T(t, t) = 1. \tag{B6}$$

The operators $P(t)$ and $T(t, t')$, like L, operate to their right on quantum-mechanical operators. Both P and T are functionals of β, μ, and $\mathbf{v}$.

Equations (B5), (B1), and (B4), and the chain rule for calculating the total derivative of $\sigma(t')$ give

$$\partial\{T(t, t')[\rho(t') - \sigma(t')]\}/\partial t' = -T(t, t')[1 - P(t')]iL\sigma(t').$$

Integrate this over t' from 0 to t and use Eqs. (B6) and (B3) to get

$$\rho(t) = \sigma(t) - \int_0^t dt' T(t, t')[1 - P(t')]iL\sigma(t'). \tag{B7}$$

This expresses the nonequilibrium statistical density operator satisfying Eqs. (B1)–(B3) as a functional of β, μ, and $\mathbf{v}$.

A different expression for the nonequilibrium statistical density operator $\rho(t)$ as a function of $\sigma(t)$ has been given by Zubarev.[33] His expression, although exact, is not in a form that is convenient for obtaining exact equations of motion formally similar to hydrodynamic equations. His resulting approximate expressions for the currents do not involve the operator $P(t)$ and, hence, do not have the advantages listed following Eq. (3.16) above.

The application of Eq. (B7) is aided by the identity

$$LA = \int_0^1 dx A^x (L \log A) A^{1-x}, \tag{B8}$$

which may be proved for an arbitrary quantum-mechanical A by integrating $dA^x\mathcal{H}A^{1-x}/dx$ over x from 0 to 1. Equations (B8), (3.4), and (2.7)–(2.9) give

$$iL\sigma = \int d^3r\beta\left[\nabla \cdot \mathbf{j}_e - \frac{\mu\nabla \cdot \bar{\rho}_p}{m} + \frac{\mathbf{v} \cdot \bar{\rho}_m\mathbf{F}_1}{m} - \mathbf{v}\nabla : \bar{\mathbf{j}}_p\right]\sigma, \tag{B9}$$

where the bar over an operator is defined by

$$\bar{A} \equiv \int_0^1 \sigma(t)^x A\sigma(t)^{-x}\, dx - \langle A\rangle_t \tag{B10}$$

for any quantum-mechanical operator A. The last term in Eq. (B10) drops out of Eq. (B9) because

Tr $(\sigma L \log \sigma)$ is zero for any statistical density operator σ and any Hamiltonian $\mathcal{H}$ in Eq. (B2).

When Eq. (B9) is used in Eq. (B7), the terms in ρ_m and ρ_p drop out. This is proved as follows. The well-known[34] rule for differentiating an operator gives

$$\frac{\delta\sigma(t)}{\delta\beta(\mathbf{r}, t)\mu(\mathbf{r}, t)} = \frac{\bar{\rho}_m(\mathbf{r})\sigma(t)}{m} \tag{B11}$$

and

$$\frac{\delta\sigma(t)}{\delta\beta(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)} = \bar{\rho}_p(\mathbf{r})\sigma(t), \tag{B12}$$

where the bar is defined in Eq. (B10) and σ is given in Eq. (3.4). Equations (B4), (B11), and (B12) and the chain rule for calculating a total derivative give

$$P(t)\bar{\rho}_m(\mathbf{r})\sigma(t) = \bar{\rho}_m(\mathbf{r})\sigma(t) \tag{B13}$$

and

$$P(t)\bar{\rho}_p(\mathbf{r})\sigma(t) = \bar{\rho}_p(\mathbf{r})\sigma(t). \tag{B14}$$

Because of Eqs. (B13) and (B14), the ρ_m and ρ_p terms drop out of $[1 - P(t)]iL\sigma(t)$, where $iL\sigma$ is given by Eq. (B9).

When this result is used along with Eq. (B7) to calculate the expectations of $\mathbf{j}_p$ and $\mathbf{j}_e$ in Eqs. (2.7)–(2.9) and when Eqs. (3.1)–(3.3) and (B1) are used on the other terms, Eqs. (3.10)–(3.16) follow after an integration by parts in the space integral on the right. In this integration the surface term vanishes because the current operators, by definition, vanish outside the volume containing the fluid.

[1] B. Robertson, Phys. Rev. **144**, 151 (1966).

[2] B. Robertson, Phys. Rev. **160**, 175 (1967); **166**, 206 (1968), Erratum.

[3] J. M. Richardson, J. Math. Anal. Appl. **1**, 12 (1960).

[4] R. A. Piccirelli, Phys. Rev. **175**, 77 (1968).

[5] M. Born and H. S. Green, Proc. Roy. Soc. (London) **A191**, 168 (1947).

[6] J. H. Irving and R. W. Zwanzig, J. Chem. Phys. **19**, 1173 (1951).

[7] J. H. Irving and J. G. Kirkwood, J. Chem. Phys. **18**, 817 (1950).

[8] H. Fröhlich, Physica **37**, 215 (1967).

[9] L. P. Kadanoff and P. C. Martin, Ann. Phys. (N.Y.) **24**, 419 (1963).

[10] P. C. Hohenberg and P. C. Martin, Ann. Phys. (N.Y.) **34**, 291 (1965).

[11] H. Mori, J. Phys. Soc. Japan **11**, 1029 (1956); Phys. Rev. **112**, 1829 (1958); **115**, 298 (1959).

[12] M. S. Green, J. Chem. Phys. **20**, 1281 (1952); **22**, 398 (1954).

[13] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957); R. Kubo, M. Yokota, and S. Nakajima, J. Phys. Soc. Japan **12**, 1203 (1957).

[14] R. W. Zwanzig, Ann. Rev. Phys. Chem. **16**, 67 (1965).

[15] G. V. Chester, Rept. Progr. Phys. **26**, 452 (1963).

[16] A similar ambiguity results from the possibility of adding to the currents the curl of an arbitrary operator that vanishes wherever the expectation of the mass density vanishes. These ambiguities suggest that only the divergences of the currents (rather than the currents themselves) should be used. The currents themselves are used here in order to retain the formal similarity with classical hydrodynamics. Even so, the currents always have $\nabla \cdot$ operating on them in the formalism to follow.

[17] This formal similarity is most apparent with Eqs. (28) and (29) of Ref. 4.

[18] S. Grossmann, Z. Physik **191**, 103 (1966). The results of interest above are given in Eqs. (24) and (35), where S is defined in Eq. (4a). Most of this paper concerns systems with nonlocal interactions, for which the continuity equation (2.7) above is not valid. No examples of such a system are given. Also, Grossmann states that any density can be made to satisfy a differential conservation law (with the source term zero), provided only that a suitable current is used. He states that this is always possible even if the total volume integral of the density is not conserved. However, for densities for which the source term is not naturally zero, this requires a current whose contribution to a surface integral exactly equals the volume integral of the source. Such a current is not physical. For example, the density ρ_p in Eq. (2.8) above has the source $\mathbf{F}_1\rho_m/m$, which is not a natural divergence. The author thanks Dr. Grossmann for bringing this paper to his attention.

[19] A. Kugler, Z. Physik **198**, 236 (1967).

[20] See the discussion following Eq. (17) of Ref. 1.

[21] See the references given in the left column of p. 176 of Ref. 2.

[22] Appendix B of Ref. 2.

[23] Equation (B4) of Ref. 1.

[24] The author thanks Dr. R. A. Piccirelli and Dr. W. C. Mitchell for pointing out this important advantage of the present formalism.

[25] Appendix C of Ref. 1.

[26] Footnote 18 of Ref. 2.

[27] The explicit form of these terms is, of course, a consequence of the Definitions (2.3) and (2.4) assumed for the form of the momentum- and energy-density operators. It is not known whether a different definition would make the additional terms vanish. However, with the present definitions, it is just the additional term in the reversible current $\langle \rho_p \rangle$ that gives a nontrivial result in the quantum theory of the equilibrium diamagnetism of a charged fluid, where $\mathbf{v}$ is replaced by the vector potential $\mathbf{A}$ and $\frac{1}{2}A^2$ is subtracted from μ.

[28] This is discussed in detail on p. 181 of Ref. 2. Notice that the correlation functions are not completely determined because any solenoidal current operator that vanishes outside the volume containing the fluid can be added to $\mathbf{j}_p$ or $\mathbf{j}_e$ without violating the definition of these currents. The equations of motion (3.11) and (3.12) do not have this ambiguity because of the ∇ operators, which can be made to operate on $\mathbf{j}_p$ and $\mathbf{j}_e$ after an integration by parts. In order to eliminate the ambiguity from the transport coefficient [e.g., Eq. (30) of Ref. 2], the $\mathbf{r}$ dependence must be averaged over the volume containing the fluid as in Eqs. (38) on p. 405 of Ref. 12. Then, only the volume integrals of the currents appear, and these depend only on the divergences of the currents and on the currents being zero outside, as can be seen by integrating $\mathbf{r}\nabla \cdot \mathbf{j}$ by parts.

[29] See, e.g., R. W. Zwanzig, J. Chem. Phys. **40**, 2527 (1964).

[30] H. Mori, Progr. Theoret. Phys. (Kyoto) **34**, 399 (1965).

[31] B. Robertson, Bull. Am. Phys. Soc. **12**, 1141 (1967).

[32] I. M. Khalatnikov, *Introduction to the Theory of Superfluidity* (Benjamin, New York, 1965).

[33] D. N. Zubarev, Dokl. Akad. Nauk SSSR **164**, 537 (1965) [Sov. Phys. Dokl. **10**, 850 (1966)]. See also T. N. Khazanovich, Mol. Phys. **17**, 281 (1969), Eqs. (3.1)–(3.3).

[34] See, e.g., Appendix A of Ref. 1.

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Equal-Time Commutation Relations and Divergence Conditions*

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The connection between divergence conditions for currents or generalized currents and equal-time commutation relations is investigated in terms of the response of physical systems to external fields. We give a simple method of constructing physical amplitudes and of obtaining generalized Ward identities and equal-time commutation relations for currents. In order to set up this scheme, we have to make an assumption about the response of the physical system to a change of the external parameters and also consider the gradient terms. In this way, we try to reproduce the current algebra formalism. It is hoped that, when this has been done, we will have made it plausible that a certain representation of the algebra exist. However, we do not discuss the formal reconstruction of the field theory of strong interactions in terms of electromagnetic, weak, and gravitational scattering data. The discussion in this paper is mostly restricted to finite-dimensional algebras, but a generalization of the method to infinite-dimensional situations is briefly outlined.

1. INTRODUCTION

In this paper, an attempt is made to put together various phenomenological concepts and statements from current algebra into a unifying framework. It is hoped that this may give some insight into the dynamical foundations of current algebra. The aim is to give a simple and direct way to construct physical amplitudes and to obtain the equal-time commutation rules for the currents together with the basic identities from which low-energy theorems can be deduced. This is realized by working in terms of current operators (or the matrix elements of the currents) and "external fields." A basic assumption concerning the response of the physical system to a perturbation of the "external" parameters is made. This assumption is the simplest possible one, namely, the existence of a linear response between the current operator and the external parameter. Functional methods are used, and we further assume that the "external field" can be treated as a c number in the formalism used, such that functional differentiation with respect to the "external field" is a well-defined mathematical operation.

In the usual approach to current algebra, the equal-time commutation rules for the currents are postulated. There is, however, an alternative way to obtain many of the results in current algebra by using another method. As Veltman[1] has shown, by studying the modified divergence conditions for vector and axial-vector currents when first-order electromagnetic and weak interactions are taken into account, many of the current algebra results can be derived without using directly the postulated equal-time commutation rules for the currents. Using standard field-theoretical methods and the usual canonical commutation rules, together with the field equations for the field operators, Nauenberg[2] has derived the equal-time commutation rules for the currents from the modified divergence conditions.

The application of equal-time commutation rules also implies the manipulation of Schwinger (or gradient) terms. As is shown by Schwinger,[3] these terms can be handled in quantum electrodynamics in a very natural way by using a variational principle. The electromagnetic current is defined through the response of the physical system to an external c-number electromagnetic field. The method gives, however, a general foundation for equal-time commutation rules for quantities that satisfy a divergence condition or conservation law. It is important, when this method is used, that a possible explicit dependence of the operator quantities upon the "external fields" also be considered.

In the first part of the paper, some well-known formulas from ordinary field theory are listed, and we shall see how the basic quantities of the S-matrix elements, the vacuum expectation values of chronologically ordered products of the field operators, can be generated with the help of a variational principle. This is done by using external sources and investigating the response of the physical system to a small variation of the external source functions. At the end of the analysis, we let the sources vanish. Details of this formalism will be discussed at length in a later publication,[4] although we try to make this paper as self-contained as possible.

As will be shown in Ref. 4, the same results can also be obtained by working in terms of c-number background fields or asymptotic fields, related in a definite way to the source functions. This last method gives us some ideas of how physical amplitudes can be constructed, when ordinary field operators, satisfying equations of motion, cannot in advance be expected to exist, for example, in strong interaction

physics. In this case, however, we assume that we may work with electromagnetic and weak-current operators, and also an energy–momentum tensor operator. The matrix elements of these quantities are supposed to be measurable, in principle, by interactions with external electromagnetic or gravitational fields, or with lepton pairs.[5] Henceforth, in all these cases, the term "external field" is used to denote the c-number parameter that will be used to test the response of the system. As mentioned before, it is assumed that a simple effective coupling between the currents or their matrix elements and the external fields exists. It will be seen that the gradient terms can be treated consistently, if an explicit dependence of the currents upon the external fields is assumed to exist.

A more detailed investigation of the response $\delta\mathbf{R}$ is done in one of the sections of the paper. We also make an explicit assumption about how the divergence condition is modified in the presence of an external perturbation. Using this information, we shall see how an algebraic structure emerges. As an application of this result, we consider a physical system with conserved vector currents and derive the commutation relations discussed by Nauenberg. The derivation is, however, made without the use of a field equation for the electromagnetic potential and without the use of canonical commutation rules.

Some of the results from quantum electrodynamics are also collected for completeness. These topics are discussed in detail in the papers of Schwinger[3] and Johnson.[6]

Finally, as an interesting example, we study a matter field in interaction with an external gravitational field. In this case, it is assumed that the response $\delta\mathbf{R}$ is given by $\delta\mathbf{S}$, where $\mathbf{S}$ is the action for the system. The full dynamical effect of the gravitational field is not discussed. This kind of treatment is justified because of the weak coupling this field has to a matter field. The gravitational field is described in vierbein formalism, and introduced as a compensating field, by requiring invariance under the wider group of Lorentz transformations, where the parameters depend on the coordinates of space–time. In this case, we obtain a commutation relation for a quantity of current character, and, also, gradient terms appear here. The more interesting problem of obtaining the equal-time commutation relations for the energy–momentum tensor will be discussed in Ref. 7.

2. THE S MATRIX IN THE FRAMEWORK OF STANDARD FIELD THEORY

In this and the following section, a condensed notation is used.[8] (Let u^i_A be a complete set of functions which satisfy the equation ${}^0\vec{S}_{,ij'}u^{j'}_A = 0$. Here, the index "$i$" stands for a discrete index as well as a continuous one. A "comma" means functional differentiation. Thus, ${}^0S_{,ij'}$ means the differential operator

$$\frac{\delta}{\delta\varphi^i(x)}\frac{\delta}{\delta\varphi^j(x')}\,{}^0S.$$

The repeated index "j'" means summation over the discrete variable and integration over the continuous variable.) The discussion is carried through for boson operators only. In order to generate the physical amplitudes, external sources are used. We define two vacuum states as follows:

$$\mathbf{a}^{\pm}_A\,|0, \pm\infty\rangle = 0, \quad [\mathbf{a}_A; \mathbf{a}^{\dagger}_B] = \delta_{AB},$$

and

$$[\mathbf{a}_A; \mathbf{a}_B] = 0, \tag{1}$$

where $\mathbf{a}^{\pm}_A$ are annihilation operators. In the absence of an external perturbation, the two vacuums $|0, \pm\infty\rangle$ become identical. The asymptotic field operator $\boldsymbol{\varphi}^{i\pm}$ can be written as

$$\boldsymbol{\varphi}^{i\pm} = \mathbf{a}^{\pm}_A u^i_A + (\mathbf{a}^{\pm}_A)^{\dagger} u^{i*}_A, \tag{2}$$

where u^i_A are a complete set of functions satisfying

$${}^0\vec{S}_{,ij'}u^{j'}_A = 0. \tag{3}$$

${}^0S_{,ij'}$ is assumed to be a nonsingular differential operator, derived from the functional ${}^0S$, describing free particles. The following orthonormality conditions hold:

$$-i\int_{\Sigma} u^{i'}_A S^{\mu}_{i'j''} u^{j''}_B\, d\Sigma_{\mu} = 0,$$

$$-i\int_{\Sigma} u^{i'*}_A S^{\mu}_{i'j''} u^{j''}_B\, d\Sigma_{\mu} = \delta_{AB}. \tag{4}$$

In a local field theory, ${}^0\vec{S}_{,ij'}$ can be written as[8]

$${}^0S_{,ij'} = A_{ij}\delta^{(4)}(x; x') + B_{ij}{}^{\mu}\delta^{(4)}_{,\mu}(x; x') + C^{\mu\nu'}_{ij}\delta^{(4)}_{,\mu\nu}(x; x') \tag{5}$$

and the relation between ${}^0S_{,ij'}$ and $S^{\mu}_{i'j''}$ is

$$S^{\mu}_{i'j''} = \tfrac{1}{2}(B^{\mu}_{ij} - B^{\mu}_{ji})\delta^{(4)}(x; x')\delta^{(4)}(x; x'') + C^{\mu\nu}_{ij}[\delta^{(4)}(x; x')\delta^{(4)}_{,\nu}(x; x'') - \delta^{(4)}_{,\nu}(x; x')\delta^{(4)}(x; x'')] \tag{6}$$

with

$$S^{\mu}_{i'j''} = -S^{\mu}_{j''i'}.$$

Using Eq. (4) gives the result

$$\mathbf{a}^{\pm}_A = -i\int_{\pm\infty} u^{i'*}_A S^{\mu}_{i'j''}\boldsymbol{\varphi}^{j''}\, d\Sigma_{\mu}. \tag{7}$$

When the vacuums $|0, \pm\rangle$ have been defined, the elements of the S matrix (assuming that no stable-bound systems exist) are defined in the following way:

$$\langle A_1' \cdots A_n'; +\infty \mid A_1 \cdots A_m; -\infty\rangle,$$

where

$$|A_1 \cdots A_n; \pm\infty\rangle = \mathbf{a}_{A_1}^{\pm\dagger} \cdots \mathbf{a}_{A_n}^{\pm\dagger} |0\pm\rangle. \tag{8}$$

Using the LSZ-reduction method, we can show that[8]

$$\begin{aligned}\langle A_1' \cdots A_n'; +\infty \mid A_1 \cdots A_m; -\infty\rangle &= \sum_{i=0}^{\infty} P(m, n; i)\delta_{A_1'A_1} \cdots \delta_{A_i'A_i} \\ &\times \langle A_{i+1}', \cdots A_n', +\infty \mid A_{i+1} \cdots A_m; -\infty\rangle_s. \end{aligned} \tag{9}$$

This is the decomposition law for the S matrix. P indicates that the sum is taken over all distinct permutations of the A's and the A''s. The number of permutations in each case is given by the formula

$$(m, n; i) = m!\, n!/(m - i)!\, (n - i)!\,. \tag{10}$$

The elements $\langle A_1' \cdots +\infty \mid A_1 \cdots -\infty\rangle$ are given in terms of the vacuum expectation values

$$\langle 0^+| T(\boldsymbol{\varphi}^i \cdots \boldsymbol{\varphi}^n) |0^-\rangle$$

as follows:

$$\begin{aligned}\langle A_1' \cdots A_n'; +\infty \mid A_1 \cdots A_m; -\infty\rangle_s &= (-i)^{m+n} u_{A_1'}^{j_1 *} \cdots u_{A_n'}^{j_n *}\, {}^0\vec{S}_{,j_1 l_1} \cdots {}^0\vec{S}_{,j_n l_n} \\ &\times \langle 0^+| T(\boldsymbol{\varphi}^{l_1} \cdots \boldsymbol{\varphi}^{l_n} \varphi^{k_1} \cdots \varphi^{k_m}) |0^-\rangle \\ &\times {}^0\overleftarrow{S}_{,k_1 i_1} \cdots {}^0\overleftarrow{S}_{,k_m i_m} u_{A_1}^{i_1} \cdots u_{A_m}^{i_m}. \end{aligned} \tag{11}$$

3. CONSTRUCTION OF THE VACUUM EXPECTATION VALUES $\langle 0^+| T(\boldsymbol{\varphi}^i \cdots \boldsymbol{\varphi}^n) |0^-\rangle$

As we have seen, if the expectation values of the chronologically ordered products of the field operators are known, it is possible to write down the S-matrix elements $\langle A_1' \cdots; +\infty \mid A_1 \cdots; -\infty\rangle$. These vacuum expectation values can be generated with the help of a variational principle. We shall use it in the form developed by Schwinger. The following equation is the starting point:

$$\delta\langle \alpha \mid \beta\rangle = i\, \langle \alpha|\, \delta\mathbf{S}\, |\beta\rangle. \tag{12}$$

It tells us how the amplitude $\langle \alpha \mid \beta\rangle$ changes under an infinitesimal change $\delta\mathbf{S}$ of the action $\mathbf{S}$. It is to be observed that $\delta\langle \alpha \mid \beta\rangle = 0$ when $\delta\mathbf{S}$ lies outside the time interval bracketed by α and β.

If external sources are introduced to test the linear response of the physical system, the change in the action operator is

$$\delta\mathbf{S} = \int d^4x \boldsymbol{\varphi}^i \delta\mathfrak{J}_i \equiv \boldsymbol{\varphi}^i \delta\mathfrak{J}_i. \tag{13}$$

Taking for $\langle \alpha \mid \beta\rangle$ the vacuum amplitude $\langle 0^+ \mid 0^-\rangle$, we conclude from (12) that

$$\frac{1}{i}\frac{\delta}{\delta\mathfrak{J}_k}\langle 0^+ \mid 0^-\rangle = \langle 0^+|\, \boldsymbol{\varphi}^k\, |0^-\rangle. \tag{14}$$

Remember that $\langle 0^+ \mid 0^-\rangle$ was a functional of the classical background. If a second variation is performed, the result is

$$\frac{1}{i}\frac{\delta}{\delta\mathfrak{J}_i}\frac{1}{i}\frac{\delta}{\delta\mathfrak{J}_k}\langle 0^+ \mid 0^-\rangle = \langle 0^+|\, T(\boldsymbol{\varphi}^i\boldsymbol{\varphi}^k)\, |0^-\rangle, \tag{15}$$

where

$$T(\boldsymbol{\varphi}^i\boldsymbol{\varphi}^k) = \theta(i; k)\boldsymbol{\varphi}^i\boldsymbol{\varphi}^k + \theta(k; i)\boldsymbol{\varphi}^k\boldsymbol{\varphi}^i. \tag{16}$$

Thus, from the knowledge of the amplitude $\langle 0^+ \mid 0^-\rangle$, one can construct the vacuum expectation values $\langle 0^+|\, T(\boldsymbol{\varphi}^i \cdots)\, |0^-\rangle$ by repeated functional differentiation with respect to the external source $\mathfrak{J}_i$. Setting

$$\langle 0^+ \mid 0^-\rangle = e^{iW}, \tag{17}$$

we easily derive the following relations (see Ref. 8):

$$\begin{aligned}\frac{\langle 0^+|\, \boldsymbol{\varphi}^i\, |0^-\rangle}{\langle 0^+ \mid 0^-\rangle} &= \frac{\delta W}{\delta\mathfrak{J}_i} \overset{\text{def}}{=} \varphi^i, \\ \frac{\langle 0^+|\, T(\boldsymbol{\varphi}^i\boldsymbol{\varphi}^k)\, |0^-\rangle}{\langle 0^+ \mid 0^-\rangle} &= \varphi^i\varphi^k - iG^{ik}, \\ \frac{\langle 0^+|\, T(\boldsymbol{\varphi}^i\boldsymbol{\varphi}^j\boldsymbol{\varphi}^k)\, |0^-\rangle}{\langle 0^+ \mid 0^-\rangle} &= \varphi^i\varphi^j\varphi^k - iP\varphi^i G^{jk} + (-i)^2 R^{ijk}, \end{aligned} \tag{18}$$

and so on. Here

$$G^{i_1 \cdots i_n} = \frac{\delta}{\delta\mathfrak{J}_{i_1}} \cdots \frac{\delta}{\delta\mathfrak{J}_{i_n}} W \tag{19}$$

and P means summation over distinctly permuted indices.

In the relations (18), only the last terms are important when the external sources are absent; all other terms to the right can be related to background effects.

4. CONSTRUCTION OF A COVARIANT PHYSICAL AMPLITUDE WITHOUT THE EXPLICIT USE OF FIELD OPERATORS $\boldsymbol{\varphi}^i$

In standard field theory the Lagrangian density $\mathfrak{L}$ is expressed as a simple function of a number of local fields $\boldsymbol{\varphi}^i$, satisfying field equations. However, it is doubtful whether such a description is adequate for strong interactions. In any case, field operators such as the electromagnetic current, the energy–momentum tensor, the weak current of baryons and mesons, etc., should be well defined. The matrix elements of the operators mentioned above should also be measurable by interactions with external fields or leptons.

Equation (12), which was used to generate the vacuum expectation values of the field operators φ^i, cannot be used directly now, because we are not assuming the existence of an action operator S. However, it is assumed that the response of the system to an external perturbation in the c-number field is given by an expression closely related to (13), namely,

$$\delta\langle\alpha \mid \beta\rangle = i\int d^4x\, \langle\alpha|\, \mathbf{j}_i\, |\beta\rangle\, \delta\phi^i. \tag{12'}$$

It is clear that the physical amplitudes cannot be given only in terms of the chronologically ordered products of the currents. When the variation in (12') is performed, a possible explicit dependence of the currents upon the external fields must also be considered. This has been discussed by Schwinger.[3] A second variation yields the expression

$$\delta\langle\alpha|\, \mathbf{j}_i\, |\beta\rangle = \int d^4x' \left(\langle\alpha|\, \frac{\delta'\mathbf{j}_i(x)}{\delta\phi^k(x')} + iT(\mathbf{j}_i(x)\mathbf{j}_k(x'))\, |\beta\rangle\right)\delta\phi^k(x'), \tag{20}$$

where $\delta'\mathbf{j}_i(x)/\delta\phi^k(x')$ gives the explicit dependence on ϕ_k. Equations (12') and (20) give

$$\delta^{(2)}\delta^{(1)}\langle\alpha \mid \beta\rangle = (i)^2\int d^4x \int d^4x' \delta\phi^i(x)\delta\phi^k(x') \times \left(\langle\alpha|\, -i\,\frac{\delta'\mathbf{j}_i(x)}{\delta\phi^k(x')} + T(\mathbf{j}_i(x)\mathbf{j}_k(x'))\, |\beta\rangle\right). \tag{21}$$

Let $\langle\alpha|$ and $|\beta\rangle$ be out- and in-states respectively; if we consider the amplitude $\langle\alpha \mid \beta\rangle$ as a functional of the classical background field, then it follows that

$$\frac{1}{i}\frac{\delta}{\delta\phi^i}\frac{1}{i}\frac{\delta}{\delta\phi^k}\langle\alpha \mid \beta\rangle = \langle\alpha|\, T(\mathbf{j}_i(x)\mathbf{j}_k(x')) - i\,\frac{\delta'\mathbf{j}_i(x)}{\delta\phi^k(x')}\, |\beta\rangle. \tag{22}$$

Certain integrability conditions must be satisfied. From the symmetry condition on the second variation of $\langle\alpha \mid \beta\rangle$, it follows that

$$\frac{\delta'\mathbf{j}_i(x)}{\delta\phi^k(x')} = \frac{\delta'\mathbf{j}_k(x')}{\delta\phi^i(x)}, \tag{23}$$

where it is assumed that $\phi^i(x)$ denotes a boson field.

We define the amplitude M_{ik} as

$$M_{ik} = \frac{1}{i}\frac{\delta}{\delta\phi^i}\frac{1}{i}\frac{\delta}{\delta\phi^k}\langle\alpha \mid \beta\rangle. \tag{24}$$

If we assume that $\mathbf{j}_k$ is a 4-vector in space–time, we can write (24) more completely:

$$M_{ik}^{\mu\nu'} = \frac{1}{i}\frac{\delta}{\delta\phi_\mu^i(x)}\frac{1}{i}\frac{\delta}{\delta\phi_\nu^k(x')}\langle\alpha \mid \beta\rangle = \langle\alpha|\, T(\mathbf{j}_i^\mu(x)\mathbf{j}_k^\nu(x')) - i\,\frac{\delta'\mathbf{j}_i^\mu(x)}{\delta\phi_\nu^k(x')}\, |\beta\rangle. \tag{24'}$$

The divergence of (24') is

$$\partial_\mu M_{ik}^{\mu\nu'} = \langle\alpha|\, T(\partial_\mu\mathbf{j}_i^\mu(x)\mathbf{j}_k^\nu(x')) + \delta(x_0; x_0')[\mathbf{j}_i^0(x); \mathbf{j}_k^\nu(x')] - i\partial_\mu\,\frac{\delta'\mathbf{j}_i^\mu(x)}{\delta\phi_\nu^k(x')}\, |\beta\rangle. \tag{25}$$

Let us assume that the divergence of the current $\mathbf{j}_k^\mu(x)$ is known:

$$\partial_\mu\mathbf{j}_i^\mu(x) = \mathbf{D}_i(x)$$

and that this relation is maintained under variation:

$$0 = \delta\langle\alpha|\, (\partial_\mu\mathbf{j}_i^\mu - \mathbf{D}_i)\, |\beta\rangle = \delta\langle\alpha|\, \partial_\mu\mathbf{j}_i^\mu\, |\beta\rangle - \delta\langle\alpha|\, \mathbf{D}_i\, |\beta\rangle.$$

The first term here is, according to (20), equal to

$$\partial_\mu\delta\langle\alpha|\, \mathbf{j}_i^\mu\, |\beta\rangle = \langle\alpha|\, \partial_\mu\left(\delta'\mathbf{j}_i^\mu + i\int d^4x' T(\mathbf{j}_i^\mu(x)\mathbf{j}_k^\nu(x'))\delta\phi_\nu^k(x')\right)|\beta\rangle.$$

For the other term, a variation similar to that leading to Eq. (20) gives

$$\delta\langle\alpha|\, \mathbf{D}_i\, |\beta\rangle = \langle\alpha|\, \left\{\delta'\mathbf{D}_i + i\int d^4x' T(\mathbf{D}_i(x)\mathbf{j}_k^\nu(x'))\delta\phi_\nu^k(x')\right\}|\beta\rangle.$$

Since the equalities hold for arbitrary states $|\alpha\rangle$ and $|\beta\rangle$, it follows that

$$\partial_\mu\left\{\delta'\mathbf{j}_i^\mu + i\int d^4x' T(\mathbf{j}_i^\mu(x)\mathbf{j}_k^\nu(x'))\delta\phi_\nu^k(x')\right\} = \delta'\mathbf{D}_i + i\int d^4x' T(\mathbf{D}_i(x)\mathbf{j}_k^\nu(x'))\delta\phi_\nu^k(x').$$

Using the formula

$$\partial_\mu T(\mathbf{j}_i^\mu(x)\mathbf{j}_k^\nu(x')) = T(\partial_\mu\mathbf{j}_i^\mu(x)\mathbf{j}_k^\nu(x')) + \delta(x_0; x_0')[\mathbf{j}_i^0(x); \mathbf{j}_k^\nu(x')],$$

we then have (see Ref. 3)

$$-i\int d^4x'\delta(x_0; x_0')[\mathbf{j}_i^0(x); \mathbf{j}_k^\nu(x')]\delta\phi_\nu^k(x') = \partial_\mu\delta'\mathbf{j}_i^\mu(x) - \delta'\mathbf{D}_i(x). \tag{26}$$

From (26), we get the equal-time commutator

$$\delta(x_0; x_0')[\mathbf{j}^0(x); \mathbf{j}_k^\nu(x')] = i\partial_\mu\,\frac{\delta'\mathbf{j}_i^\mu(x)}{\delta\phi_\nu^k(x')} - i\,\frac{\delta'\mathbf{D}_i(x)}{\delta\phi_\nu^k(x')}. \tag{27}$$

The divergence of the amplitude $M_{ik}^{\mu\nu}$ then takes the form

$$\partial_\mu M_{ik}^{\mu\nu'} = \langle\alpha|\, T(\mathbf{D}_i(x)\mathbf{j}_k^{\nu}(x')) + \frac{1}{i}\frac{\delta'\mathbf{D}_i(x)}{\delta\phi_\nu^k(x')}\,|\beta\rangle. \quad (28)$$

Low-energy theorems can be obtained from Eq. (28). It is seen that, in order to derive such theorems, only a knowledge of the divergence of the current $\mathbf{j}_k^\mu$ is necessary.

Now we go a step further and take divergence of (28) with respect to x':

$$\begin{aligned}\partial_\mu\partial_{\nu'}M_{ik}^{\mu\nu'} &= \langle\alpha|\, T(\mathbf{D}_i(x)\mathbf{D}_k(x')) \\ &\quad + \delta(x_0; x_0')[\mathbf{j}_k^0(x'); \mathbf{D}_i(x)] \\ &\quad + \frac{1}{i}\partial_{\nu'}\frac{\delta'\mathbf{D}_i(x)}{\delta\phi_\nu^k(x')}\,|\beta\rangle\end{aligned}$$

or

$$\begin{aligned}\langle\alpha|\, T(\mathbf{D}_i\mathbf{D}_{k'})\,|\beta\rangle &= \partial_\mu\partial_{\nu'}M_{ik}^{\mu\nu'} \\ &\quad - \langle\alpha|\,[\mathbf{j}_{k'}^0; \mathbf{D}_i]\,|\beta\rangle\,\delta(x_0; x_0') \\ &\quad - \frac{1}{i}\langle\alpha|\,\partial_{\nu'}\frac{\delta'\mathbf{D}_i}{\delta\phi_{\nu'}^k}\,|\beta\rangle. \quad (29)\end{aligned}$$

This equation is the starting point for the calculation of scattering lengths, for example (see Ref. 9).

Let us consider Eq. (28):

$$\partial_\mu M_{ik'}^{\mu\nu} = \langle\alpha|\, T(\mathbf{D}_i(x)\mathbf{j}_k^{\nu}(x')) + \frac{1}{i}\frac{\delta'\mathbf{D}_i(x)}{\delta\phi_\nu^k(x')}\,|\beta\rangle. \quad (30)$$

If the following form,

$$\frac{\delta'\mathbf{D}_i(x)}{\delta\phi_\mu^j(x')} = f_{ijk}\mathbf{j}^{\mu k}(x)\delta^{(4)}(x; x'),$$

of the change of $\mathbf{D}_i$ is assumed (see Sec. 5), it follows that

$$\begin{aligned}\partial_\mu M_{ik'}^{\mu\nu} &= \langle\alpha|\, T(\partial_\mu\mathbf{j}_i^\mu(x)\mathbf{j}_k^{\nu}(x'))\,|\beta\rangle \\ &\quad + \frac{1}{i}\delta^{(4)}(x; x')f_{ikl}\langle\alpha|\,\mathbf{j}^{l\nu}(x)\,|\beta\rangle. \quad (31)\end{aligned}$$

See Ref. 9, p. 220.

Feynman has conjectured that, for low-energy theorems, one gets the correct answer if one consistently neglects "seagulls" and Schwinger terms and Eq. (31) is then simply postulated. In our approach, it is seen that the form of Eq. (31) depends on the fact that the term

$$\delta(x_0; x_0')[\mathbf{j}_i^0(x); \mathbf{j}_k^{\nu}(x')] - i\partial_\mu\left(\frac{\delta'\mathbf{j}_i^\mu(x)}{\delta\phi_\nu^k(x')}\right)$$

in (25) can be eliminated, and only a knowledge of the divergence $\mathbf{D}_i$ is necessary to obtain (31).

The following is to be noted in connection with Eq. (29). From (20), it is seen that the amplitude $M_{ik}^{\mu\nu'}$ can be obtained from the matrix element $\langle\alpha|\,\mathbf{j}_i^\mu\,|\beta\rangle$ as follows:

$$M_{ik}^{\mu\nu'} = \langle\alpha|\, T(\mathbf{j}_i^\mu\mathbf{j}_k^{\nu'}) + \frac{1}{i}\frac{\delta'\mathbf{j}_i^\mu}{\delta\phi_{\nu'}^k}\,|\beta\rangle = \frac{1}{i}\frac{\delta}{\delta\phi_{\nu'}^k}\langle\alpha|\,\mathbf{j}_i^\mu\,|\beta\rangle.$$

5. DIVERGENCE CONDITIONS AND ASSOCIATED LIE ALGEBRAS

Let us look at a physical system with which we associate the currents $\mathfrak{J}^{\mu i}(x)$. In the absence of an external perturbation, they are supposed to have well-defined transformation properties in space–time, as well as in an internal space V_N of N dimensions, not specified in detail for the moment. For simplicity, we have assumed that $\mathfrak{J}^{\mu i}(x)$ transform as 4-vectors in space–time. The index i is associated with V_N, which is also equipped with a symmetrical quantity g_{ij} which can be used to construct invariants in V_N.

(i) First let us write, for the divergence of the currents,

$$\partial_\mu\mathfrak{J}^{\mu i}(x) = \mathbf{D}^i(x), \quad \mu = 0, 1, 2, 3, \quad i = 1, 2, \cdots, N.$$

(ii) Then we assume that, in the presence of an external field, A_μ^i, $\mathbf{D}_i$ is modified as follows:

$$\delta'\mathbf{D}^i = f_{jk}^i\delta A_\mu^j\mathfrak{J}^{\mu k}, \quad (32)$$

where f_{jk}^i is supposed to be constant.

As in the discussion leading to (26), we have

$$\begin{aligned}\partial_\mu\Big(\delta'\mathfrak{J}^{\mu k}(x) + i\int d^4x'\,T(\mathfrak{J}^{\mu k}(x)\delta\mathbf{R}(x'))\Big) \\ = \delta'\mathbf{D}^k(x) + i\int d^4x'\,T(\mathbf{D}^k(x)\delta\mathbf{R}(x')),\end{aligned}$$

from which it follows that

$$\begin{aligned}-i\int d^4x'[\mathfrak{J}^{0k}(x); \delta\mathbf{R}(x')]\delta(x_0; x_0') \\ = \partial_0\delta'\mathfrak{J}^{0k}(x) + \partial_{(i)}\delta'\mathfrak{J}^{(i)k} - f_{jl}^k\delta A^j{}_\mu(x)\mathfrak{J}^{\mu l}(x), \\ (i) = 1, 2, 3, \quad (33)\end{aligned}$$

where $\delta\mathbf{R}$ is a measure of the response of the physical system to a change of the c-number field A_μ^i. Thus, $\delta\mathbf{R}$ must be an invariant in space–time and in V_N. The simple choice is then

$$\delta\mathbf{R} = g_{ij}\delta A^i{}_\mu\mathfrak{J}^{\mu j}. \quad (34)$$

Accordingly,

$$\begin{aligned}-ig_{ij}[\mathfrak{J}^{0k}(x); \mathfrak{J}^{\rho j}(x')]\delta(x_0; x_0') \\ = \partial_\mu\left(\frac{\delta'\mathfrak{J}^{\mu k}(x)}{\delta A^i{}_\rho(x')}\right) - f_{jl}^k\delta_i^j\delta_\mu^\rho\mathfrak{J}^{l\mu}(x)\delta^{(4)}(x; x'). \quad (33')\end{aligned}$$

Now let A^i_μ vanish, and consider a class of physical systems for which

$$\frac{\delta'_{(3)}\mathfrak{J}^{0k}(x)}{\delta A^i_\rho(x')} = 0,$$

where

$$\frac{\delta'\mathfrak{J}^{0k}(x)}{\delta A^i_\rho(x')} = \delta(x_0; x'_0)\frac{\delta'_{(3)}\mathfrak{J}^{0k}(x)}{\delta A^i_\rho(x')}.$$

Thus, in the absence of an external field, we have

$$i[\mathfrak{J}^{0k}(x); \mathfrak{J}^\rho_i(x')]_{x_0=x_0'} = f^k_{il}\mathfrak{J}^{l\rho}(x)\delta^{(3)}(x; x') - \partial_{(i)}\left(\frac{\delta'_{(3)}\mathfrak{J}^{(i)k}(x)}{\delta A^i_\rho(x')}\right). \quad (35)$$

We assume that it is possible to define the charges $Q^l(x_0)$ as

$$\mathbf{Q}^l(x_0) = \int d^3x \mathfrak{J}^{0l}(x).$$

Equation (35) then gives the equal-time commutator

$$i[\mathbf{Q}^k(x_0); \mathbf{Q}_i(x_0)] = f^k_{il}\mathbf{Q}^l(x_0). \quad (36)$$

From the Jacobi identity for Q^l follows

$$(f^k_{ij}f^j_{lm} + f^k_{mj}f^j_{il} + f^k_{lj}f^j_{mi})\mathbf{Q}^l = 0$$

or

$$f^k_{ij}f^j_{lm} + f^k_{mj}f^j_{il} + f^k_{lj}f^j_{mi} = 0. \quad (36')$$

From Eqs. (36), it follows that f^i_{jk} can be interpreted as structure constants of a Lie algebra, and we can take

$$g_{ij} = \text{const}\, f^k_{il}f^l_{jk}. \quad (37)$$

If the symmetric matrix g_{ij} is nonsingular, the generated Lie algebra is semisimple. For a compact simple Lie algebra, $g_{ij} = \delta_{ij}$. Mathematically, the constant is of no importance. However, we shall see in the Appendix that it can be convenient to give it a physical meaning. Equation (32) can be written

$$\delta'\mathbf{D}^i = (\delta\vec{A}_\mu \times \vec{\mathfrak{J}}^\mu)^i,$$

where $\times$ means the cross product for the Lie algebra. Thus, in V_N, a scalar product and a cross product are defined.

A system for which the currents are conserved can be treated in the following way, and the same conclusions can be drawn. We discard the renormalization effects due to the presence of the A field; that is, we suppose that these effects are of second order.

(i) The currents $\mathfrak{J}^{\mu i}_{(x)}$ are conserved:

$$\partial_\mu\mathfrak{J}^{\mu i}(x) = 0, \quad \mu = 0, 1, 2, 3, \quad i = 1, 2, \cdots, N.$$

(ii) In the presence of an external field A^i_μ, the divergence of $\mathfrak{J}^{\mu i}$ is modified as follows:

$$\partial_\mu\mathfrak{J}^{i\mu} = f^i_{jk}A^j_\mu\mathfrak{J}^{\mu k}.$$

Equation (33′) now has the form

$$-ig_{ij}[\mathfrak{J}^{0k}(x); \mathfrak{J}^{\rho j}(x')]\delta(x_0; x'_0) = \partial_\mu\left(\frac{\delta'\mathfrak{J}^{\mu k}(x)}{\delta A^i_\rho(x')}\right) - f^k_{jl}\delta^j_i\delta^\rho_\mu\mathfrak{J}^{l\mu}(x)\delta^{(4)}(x; x') - f^k_{jl}A^j_\mu(x)\frac{\delta'\mathfrak{J}^{\mu l}(x)}{\delta A^i_\rho(x')}. \quad (38)$$

If the external field A^i_μ vanishes, the last term goes to zero and, in this case, we also get a similar expression for the equal-time commutator of the currents.

6. COMMUTATION RULES DERIVED FROM DIVERGENCE CONDITIONS

As an example of how equal-time commutation rules can be derived from divergence conditions, consider the charged components of the *vector* current of hadrons. In the presence of an electromagnetic interaction, one no longer has the conservation rule[9]

$$\partial_\mu\mathbf{j}^{\mu(+)}(x) = 0.$$

Instead,

$$\nabla_\mu\mathbf{j}^{\mu(+)}(x) = 0, \quad \nabla_\mu \equiv \partial_\mu + ieA_\mu. \quad (39)$$

Here, it is assumed that A_μ is a given c-number field. The electromagnetic current vector of the system is defined through the response to an infinitesimal variation of the external potential A_μ. Thus,

$$-i\int d^4x'\delta(x_0; x'_0)[\mathbf{j}^{0(+)}(x); e\mathbf{j}^{(e)}_\mu\delta A^\mu(x')] = \partial_\mu\delta'\mathbf{j}^{\mu(+)}(x) - \delta'\mathbf{D}^{(+)}(x),$$

or

$$-i\delta(x_0; x'_0)[\mathbf{j}^{0(+)}(x); \mathbf{j}^{(e)}_\mu(x')]e = \partial_0\frac{\delta'\mathbf{j}^{0(+)}(x)}{\delta A_\mu(x')} + \partial_i\frac{\delta'\mathbf{j}^{i(+)}(x)}{\delta A_\mu(x')} - \frac{\delta'\mathbf{D}^{(+)}(x)}{\delta A_\mu(x')},$$

where

$$\mathbf{D}^{(+)}(x) = -ieA_\mu\mathbf{j}^{\mu(+)}(x), \quad i = 1, 2, 3.$$

We introduce 3-dimensional functional derivatives defined as

$$\frac{\delta'}{\delta A_\mu(x)} = \delta(x_0; x'_0)\frac{\delta'_{(3)}}{\delta A_\mu(x)}. \quad (40)$$

If a term proportional to $A_\mu(x)$ is neglected, we get

$$[\mathbf{j}^{(e)}_\mu(x'); \mathbf{j}^{0(+)}(x)]_{x_0=x_0'} = \mathbf{j}^{(+)}_\mu(x)\delta^{(3)}(x'; x) + \frac{1}{e}\partial_k\left(\frac{1}{i}\frac{\delta'_{(3)}\mathbf{j}^{k(+)}(x)}{\delta A_\mu(x')}\right), \quad k = 1, 2, 3. \quad (41)$$

This equation holds for a class of physical systems for which the following is true:

$$\frac{1}{i}\frac{\delta'_{(3)}\mathbf{j}^{0(+)}(x)}{\delta A_\mu(x')} = 0.$$

Let us compare this with the ordinary field-theoretical situation. Using ordinary canonical commutation relations and a field operator $\mathbf{A}_\mu$ satisfying the field equation

$$\Box \mathbf{A}_\mu(x) = \mathbf{j}^{(e)}_\mu(x),$$

we can show that,[2] to first-order electromagnetic effects,

$$[\mathbf{j}^{(e)}_\mu(x'); \mathbf{j}^{0(+)}(x)]_{x_0=x_0'} = \mathbf{j}^{(+)}_\mu(x)\delta^{(3)}(x; x') + \frac{1}{e}\partial_k\left[\frac{\partial \mathbf{A}_\mu}{\partial x^0}(x'); \mathbf{j}^{k(+)}(x)\right]_{x_0=x_0'}.$$

It is then clear that the condition

$$\frac{1}{i}\frac{\delta'_{(3)}\mathbf{j}^{0(+)}(x)}{\delta A_\mu(x')} = 0$$

corresponds to the following equal-time commutation relation in the ordinary field theoretical approach:

$$\left[\frac{\partial \mathbf{A}_\mu}{\partial x_0}(x'); \mathbf{j}^{0(+)}(x)\right]_{x_0=x_0'} = 0.$$

In the same way, we have for the $\mathbf{j}^{\mu(-)}$ component of the vector current

$$(\partial_\mu - ieA_\mu)\mathbf{j}^{\mu(-)}(x) = 0,$$
$$\partial_\mu \mathbf{j}^{\mu(-)} = ieA_\mu \mathbf{j}^{\mu(-)} \equiv \mathbf{D}^{(-)},$$

from which follows the commutation rule

$$[\mathbf{j}^{(e)}_\mu(x'); \mathbf{j}^{0(-)}(x)]_{x_0=x_0'} = -\mathbf{j}^{(-)}_\mu(x)\delta^{(3)}(x; x') + \frac{1}{e}\partial_k\left(\frac{1}{i}\frac{\delta'_{(3)}\mathbf{j}^{k(-)}(x)}{\delta A_\mu(x')}\right), \quad k = 1, 2, 3. \quad (42)$$

7. QUANTUM ELECTRODYNAMICS

As another illustration of a physical system with an associated conserved current, let us consider quantum electrodynamics. The current operator is $\mathbf{j}_\mu(x)$ and the external potential $A_\mu(x)$. We define the physical amplitude $M^{\mu\nu}$ as

$$M^{\mu\nu} = \frac{1}{i}\frac{\delta}{\delta A_\mu(x)}\frac{1}{i}\frac{\delta}{\delta A_\nu(x')}\langle\alpha|\,\beta\rangle = \langle\alpha|\, T(\mathbf{j}^\mu(x)\mathbf{j}^\nu(x')) + \frac{1}{i}\frac{\delta'\mathbf{j}^\mu(x)}{\delta A_\nu(x')}\,|\beta\rangle. \quad (43)$$

If we compute the divergence of $M^{\mu\nu}$ and use the current conservation law, we get

$$\partial_\mu M^{\mu\nu} = \langle\alpha|\,[\mathbf{j}^0(x); \mathbf{j}^\nu(x')]\,|\beta\rangle\,\delta(x_0; x_0') + \frac{1}{i}\partial_\mu\langle\alpha|\frac{\delta'\mathbf{j}^\mu(x)}{\delta A_\nu(x')}|\beta\rangle. \quad (44)$$

As before, we restrict ourselves to those physical systems for which the time component $\mathbf{j}^0(x)$ does not depend explicitly upon the external potential and those which satisfy the relation

$$\frac{\delta'\mathbf{j}^\rho(x)}{\delta A_\nu(x')} = \frac{\delta'\mathbf{j}^\nu(x')}{\delta A_\rho(x)}. \quad (23')$$

If 3-dimensional functional derivatives are introduced, Eq. (44) can be written as

$$\partial_\mu M^{\mu\nu} = \delta(x_0; x_0')\langle\alpha|\,[\mathbf{j}^0(x); \mathbf{j}^\nu(x')]\,|\beta\rangle + \frac{1}{i}\partial_\mu\left(\langle\alpha|\,\delta(x_0; x_0')\frac{\delta'_{(3)}\mathbf{j}^\mu(x)}{\delta A_\nu(x')}\,|\beta\rangle\right).$$

Because $M^{\mu\nu}$ is supposed to represent a physical amplitude, the divergence of $M^{\mu\nu}$ must be equal to zero and, thus,

$$\langle\alpha|\,[\mathbf{j}^0(x); \mathbf{j}^\nu(x')]_{x_0=x_0'}\,|\beta\rangle = -\frac{1}{i}\partial_i\langle\alpha|\frac{\delta'_{(3)}\mathbf{j}^i(x)}{\delta A_\nu(x')}|\beta\rangle, \quad i = 1, 2, 3. \quad (45)$$

Let the external potential vanish, and let $\langle\alpha|$ and $|\beta\rangle$ represent the vacuum state. Then

$$\langle 0|\,[\mathbf{j}^0(x); \mathbf{j}^\nu(x')]_{x_0=x_0'}\,|0\rangle = i\partial_i\langle 0|\frac{\delta'_{(3)}\mathbf{j}^i(x)}{\delta A_\nu(x')}|0\rangle, \quad i = 1, 2, 3. \quad (46)$$

The equal-time commutator of the electromagnetic current cannot be equal to zero, because that would lead to contradictions (see Ref. 3). Now when the external potential is set equal to zero, we can use Lorentz invariance and the vacuum expectation value of the equal-time commutator of the current can be written in a spectral representation as follows (see Ref. 6):

$$\langle 0|\,[\mathbf{j}_0(x); \mathbf{j}_k(x')]_{x_0=x_0'}\,|0\rangle = i\partial_k\left(\int_0^\infty dm m^2\rho(m)\delta^{(3)}(x; x')\right),$$

or

$$\langle 0|\,[\mathbf{j}_0(x); \mathbf{j}_k(x')]_{x_0=x_0'}\,|0\rangle = i\partial_k\delta^{(3)}(x; x')\int_0^\infty dm m^2\rho(m), \quad k = 1, 2, 3. \quad (47)$$

8. A SET OF FIELDS ψ^A IN INTERACTION WITH A WEAK EXTERNAL GRAVITATIONAL FIELD

Let S be the action operator for a set of free fields ψ^A,[10]

$$\mathbf{S} = \int d^4y \mathfrak{L}(\psi^A, \partial_k \psi^A),$$
$$A = 1, \cdots, n, \quad k = 1, 2, 3, 4, \tag{48}$$

where it is assumed that S is a scalar under Lorentz transformations. $\mathfrak{L}$ is the Lagrangian density. The fields ψ^A are defined with respect to some Lorentz frame, the y system. Besides this y system, a system of curvilinear coordinates x^μ, $\mu = 0, 1, 2, 3$, is also introduced. The following quantities can then be defined:

$$h^i{}_\mu(x) = \frac{\partial y^i}{\partial x^\mu}, \quad h_i{}^\mu(x) = \frac{\partial x^\mu}{\partial y^i}. \tag{49}$$

At every point x, there is thus a local Lorentz frame. The action integral can now be written in curvilinear coordinates:

$$\mathbf{S} = \int d^4x h \mathfrak{L}(\psi^A(x), h_i{}^\mu(x)\psi^A_{,\mu}(x)), \tag{50}$$

where

$$\sqrt{-g} = h \equiv \det(h^i{}_\mu).$$

The action S is now invariant under Lorentz transformations

$$\text{(i)} \quad \begin{aligned} y^{k'} &= y^k + \delta\xi^k{}_l y^l, \\ \delta h^i{}_\mu &= \delta\xi^i{}_l h^l{}_\mu, \\ \delta\psi^A &= \tfrac{1}{2}(G_{kl})^A{}_B \psi^B \delta\xi^{kl}, \quad \delta\xi^{kl} = -\delta\xi^{lk}, \\ & \qquad x^\mu \text{ const}, \end{aligned} \tag{51}$$

and transformations of the curvilinear coordinates x^μ,

$$\text{(ii)} \quad x^{\mu'} = x^\mu + f^\mu(x). \tag{52}$$

The fields ψ^A are defined to transform as scalars under (52). G_{kl} are $n \times n$ matrices and are representations of the generators of the Lorentz group. They satisfy the commutation relations

$$[G_{kl}; G_{mn}] = \tfrac{1}{2} C^{ij}{}_{klmn} G_{ij}, \quad G_{kl} = -G_{lk}. \tag{53}$$

$c^{ij}{}_{klmn}$ are the structure constants of the Lorentz group.

The gravitational field is introduced by requiring S to be invariant under the wider group of Lorentz transformations, where $\delta\xi^{kl}$ now are arbitrary functions of x. That is,

$$\begin{aligned} \delta h^i{}_\mu &= \delta\xi^i{}_l(x) h^l{}_\mu, \\ \delta\psi^A(x) &= \tfrac{1}{2}(G_{kl})^A{}_B \psi^B \delta\xi^{kl}(x). \end{aligned} \tag{54}$$

In this way, a new field is introduced—the compensating field $A^{kl}{}_\mu$ (see Ref. 10)—and the new action is given by

$$\mathbf{S} = \int d^4x h \mathfrak{L}(\psi^A, h_i{}^\mu \nabla_\mu \psi^A), \tag{55}$$

where

$$\nabla_\mu \psi = (\partial_\mu - \tfrac{1}{2} A^{kl}{}_\mu G_{kl})\psi. \tag{56}$$

It is now assumed that the $A^{kl}{}_\mu$ describes an external gravitational field and, thus, that the full dynamical effect is *not* taken into consideration.

If a small numerical variation in $A^{kl}{}_\mu$ is performed, we can define the quantities $\mathbf{J}_{kl}{}^\mu$ as

$$\begin{aligned} \delta\mathbf{S} &= \tfrac{1}{2}\int d^4x h \mathfrak{J}_{kl}{}^\mu \delta A^{kl}{}_\mu, \\ &= \tfrac{1}{2}\int d^4x \tilde{\mathfrak{J}}_{kl}{}^\mu \delta A^{kl}{}_\mu, \end{aligned} \tag{57}$$

where $\tilde{\mathfrak{J}}_{kl}{}^\mu = h\mathfrak{J}_{kl}{}^\mu$.

Let the vierbein field undergo the following transformation:

$$h'^i{}_\mu = h^i{}_\mu + \delta h^i{}_\mu,$$

with

$$\delta h^i{}_\mu = \delta\xi^i{}_k(x) h^k{}_\mu. \tag{58}$$

The change $\delta h^i{}_\mu$ induces a change $\delta A^{kl}{}_\mu$ in the compensating field

$$A'^{ij}{}_\mu = A^{ij}{}_\mu + \delta A^{ij}{}_\mu. \tag{59}$$

It is easy to see that the change $\delta A^{ij}{}_\mu$ is given by the expression

$$\delta A^{ij}{}_\mu = -\delta\xi^{ij}{}_{,\mu} + \delta\xi^i{}_k A^{kj}{}_\mu + \delta\xi_k{}^j A^{ik}{}_\mu. \tag{60}$$

An alternative form is

$$\delta A^{ij}{}_\mu = -\delta\xi^{ij}{}_{,\mu} + \tfrac{1}{4} C^{ij}{}_{klmn} A^{mn}{}_\mu \delta\xi^{kl}. \tag{61}$$

From (57) and (61), it follows that

$$\delta\mathbf{S} = \tfrac{1}{2}\int d^4x (\partial_\mu \tilde{\mathfrak{J}}_{ij}{}^\mu + \tfrac{1}{4}\tilde{\mathfrak{J}}_{kl}{}^\mu C^{kl}{}_{ijmn} A^{mn}{}_\mu)\delta\xi^{ij}. \tag{62}$$

The requirement of invariance of S under transformation (58) gives the "conservation" law

$$\partial_\mu \tilde{\mathfrak{J}}_{ij}{}^\mu + \tfrac{1}{4}\tilde{\mathfrak{J}}_{kl}{}^\mu C^{kl}{}_{ijmn} A^{mn}{}_\mu = 0. \tag{63}$$

For later use, this formula is written in the following way:

$$\begin{aligned} \partial_0 \tilde{\mathfrak{J}}^0_{ij} &= -\partial_{(a)} \tilde{\mathfrak{J}}^{(a)}_{ij} - \tfrac{1}{4}\tilde{\mathfrak{J}}_{kl}{}^\mu C^{kl}{}_{ijmn} A^{mn}{}_\mu \\ &\equiv \mathbf{B}_{ij}, \quad (a) = 1, 2, 3. \end{aligned} \tag{64}$$

Consider now the response $\delta\mathfrak{L}$ of the system to a change in $A^{ij}{}_\mu$:

$$\delta\mathfrak{L} = \tfrac{1}{2}\tilde{\mathfrak{J}}^\mu_{kl}\delta A^{kl}{}_\mu = \tfrac{1}{4}\tilde{\mathfrak{J}}^\mu_{kl}\delta A_{ij\mu}(g^{ik}g^{jl} - g^{il}g^{jk}),$$

where $\tilde{\mathfrak{J}}^\mu_{kl} = -\tilde{\mathfrak{J}}^\mu_{lk}$ and $\delta A_{kl\mu} = -\delta A_{lk\mu}$. g^{ik} is the flat space–time metric. It is not difficult to show that

$$g_{kr}g_{ls} - g_{ks}g_{lr} = -\tfrac{1}{16} C^{ij}{}_{klmn} C^{mn}{}_{rsij}.$$

Thus, in this case, also, we have a coupling of the form (37).

In order to use Schwinger's method in this case, an equation of the form

$$\partial_0 \mathbf{A}(x) = \mathbf{B}(x)$$

is needed. In our case, infinitesimal variations in the numerical external field $A^{kl}{}_{\mu}$ were used to define the quantities $\tilde{\mathfrak{J}}^{\mu}_{kl}$, and Eq. (64) is an expression that must hold for all values of the parameters. According to Ref. 3, the following equation must hold:

$$-i\int d^3x'[\mathbf{A}(x); \delta\mathfrak{L}(x')]_{x^0=x^{0\prime}} = \partial_0\delta'\mathbf{A}(x) - \delta'\mathbf{B}(x), \tag{65}$$

where δ' refers as usual to a possible explicit dependence of the operators $\mathbf{A}$ and $\mathbf{B}$ upon the numerical parameters.

In the present case, the formula can be applied if the following identifications are made:

$$\begin{aligned} \mathbf{A} &\equiv \tilde{\mathfrak{J}}^0_{ij}, \\ \mathbf{B} &\equiv -\partial_{(a)}\tilde{\mathfrak{J}}^{(a)}_{ij} - \tfrac{1}{4}\tilde{\mathfrak{J}}^{\mu}_{kl}C^{kl}{}_{ijmn}A^{mn}{}_{\mu}, \\ \delta\mathfrak{L} &= \tfrac{1}{2}\tilde{\mathfrak{J}}^{\mu}{}_{kl}\delta A^{kl}_{\mu}, \quad (a) = 1, 2, 3. \end{aligned} \tag{66}$$

Thus,

$$\begin{aligned} -\frac{i}{2}\int d^3x'[\tilde{\mathfrak{J}}^0_{ij}(x); \tilde{\mathfrak{J}}^{\nu}_{kl}(x')]_{x_0=x_0'}\delta A^{kl}_{\nu}(x') \\ = \partial_0\delta'\tilde{\mathfrak{J}}^0_{ij} + \partial_{(a)}\delta'\tilde{\mathfrak{J}}^{(a)}_{ij} + \tfrac{1}{4}\delta'\tilde{\mathfrak{J}}^{\mu}_{kl}C^{kl}{}_{ijmn}A_{\mu}{}^{mn} \\ + \tfrac{1}{4}\tilde{\mathfrak{J}}^{\mu}_{kl}C^{kl}{}_{ijmn}\delta' A_{\mu}{}^{mn}, \quad (a) = 1, 2, 3. \end{aligned} \tag{67}$$

From (67), we get

$$\begin{aligned} -\frac{i}{2}[\tilde{\mathfrak{J}}^0_{ij}(x); \tilde{\mathfrak{J}}^{\nu}_{kl}(x')]_{x_0=x_0'} \\ = \tfrac{1}{4}\tilde{\mathfrak{J}}^{\nu}_{rs}C^{rs}{}_{ijkl}\delta^{(3)}(x; x') + \partial_{(i)}\frac{\delta'_{(3)}\tilde{\mathfrak{J}}^{(i)}_{ij}(x)}{\delta A^{kl}{}_{\nu}(x')} \\ + \frac{1}{4}\frac{\delta'_{(3)}\tilde{\mathfrak{J}}^{\mu}_{rs}(x)}{\delta A^{kl}{}_{\nu}(x')}C^{rs}{}_{ijmn}A^{mn}{}_{\mu}. \end{aligned} \tag{68}$$

As before, we only consider physical systems for which

$$\frac{\delta'_{(3)}\tilde{\mathfrak{J}}^0_{ij}(x)}{\delta A^{kl}{}_{\nu}(x')} = 0.$$

Then, in the limit of flat space–time,

$$\begin{aligned} -i[\mathfrak{J}^0_{ij}(x); \mathfrak{J}^{\nu}_{kl}(x')]_{x_0=x_0'} \\ = \tfrac{1}{2}\mathfrak{J}^{\nu}_{rs}C^{rs}{}_{ijkl}\delta^{(3)}(x; x') + 2\partial_{(i)}\left(\frac{\delta'_{(3)}\tilde{\mathfrak{J}}^{(i)}_{ji}(x)}{\delta A^{kl}{}_{\nu}(x')}\right), \\ (i) = 1, 2, 3. \end{aligned} \tag{69}$$

The same result can be obtained in the following way, where now the infinite dimensional character of the vierbein group is emphasized[8]:

$$\mathbf{D}_{ij} = \partial_{\mu}\tilde{\mathfrak{J}}^{\mu}_{ij}.$$

From Eq. (63), it follows that

$$\mathbf{D}_{ij} = -\tfrac{1}{4}\tilde{\mathfrak{J}}^{\mu}_{kl}C^{kl}{}_{ijmn}A^{mn}{}_{\mu} \tag{70}$$

and

$$\frac{\delta'\mathbf{D}_{ij}(x)}{\delta A^{mn}{}_{\mu}(x')} = -\tfrac{1}{4}\int d^4x''C^{(kl)''}{}_{(ij)(mn)'}\tilde{\mathfrak{J}}^{\mu}_{kl}(x''). \tag{71}$$

$C^{(kl)''}{}_{(ij)(mn)'}$ are the "structure constants" of the vierbein group and are defined as follows:

$$C^{(kl)''}{}_{(ij)(mn)'} = C^{kl}{}_{ijmn}\delta^{(4)}(x; x')\delta^{(4)}(x; x''). \tag{72}$$

Thus, using (32) and (33), generalized to infinite-dimensional groups, we get (69).

We also see here the presence of a gradient term. Putting $\nu = 0$ in (69) and integrating over 3-dimensional x space, we obtain the commutation relations for the homogeneous Lorentz group. This was, of course, an expected result because we were studying vierbein rotations. In order to obtain an equal-time commutation relation for the energy–momentum tensor, from which the Poincaré algebra follows, we must study the general coordinate transformations given by (52). Schwinger has solved this problem for the energy density $\mathbf{T}_{00}(x)$ for a special class of physical systems. However, it is possible to give a closed expression for the equal-time commutator $[\mathbf{T}_{0\mu}(x'); \mathbf{T}_{\rho 0}(x'')]_{x_0''=x_0''}$ from general arguments and holding for arbitrary physical systems. This problem will be discussed in a separate paper.[7]

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APPENDIX

In order to evaluate (29), the equal-time commutator $[\mathfrak{J}^0_k(x); \mathbf{D}_i(x')]_{x_0=x_0'}$ must be known. In this appendix, some of the properties of this commutator are studied. Let us integrate the commutator (35) over 3-dimensional x space. Then

$$i[\mathbf{Q}^k(x_0); \mathfrak{J}^{\rho}_i(x')]_{x_0=x_0'} = f^k_{il}\mathfrak{J}^{l\rho}(x').$$

Let us assume that we have a compact simple Lie algebra, such that g_{ik} is diagonal and positive definite. The change of $[\mathfrak{J}^0_k(x); \mathbf{D}_i(x')]_{x_0=x_0'}$ is

$$\delta'\{i[\mathfrak{J}^0_k(x); \mathbf{D}_i(x')]_{x_0=x_0'}\} = i[\mathfrak{J}^0_k(x); \delta'\mathbf{D}_i(x')]_{x_0=x_0'},$$

if we restrict ourselves to physical systems which

satisfy

$$\frac{\delta'_{(3)}\mathfrak{J}^0_k(x)}{\delta A^i_\rho(x')} = 0.$$

But

$$\delta'\mathbf{D}_i(x') = f_{ilm}\delta A^l_\mu \mathfrak{J}^{\mu m}(x').$$

Therefore,

$$i[\mathfrak{J}^0_k(x);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = if_{ilm}\delta A^l_\mu(x')[\mathfrak{J}^0_k(x);\, \mathfrak{J}^{\mu m}(x')]_{x_0=x_0'},$$

$$i[\mathbf{Q}_k(x_0);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = if_{ilm}\delta A^l_\mu(x')[\mathbf{Q}_k(x);\, \mathfrak{J}^{\mu m}(x')]_{x_0=x_0'},$$

or

$$i[\mathbf{Q}_k(x_0);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = f_{ilm}\delta A^l_\mu(x') f_k{}^m{}_n \mathfrak{J}^{\mu n}(x').$$

Next, we compute

$$ig^{ik}[\mathbf{Q}_k(x_0);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = f^k{}_{lm} f_k{}^m{}_n \delta A^l_\mu \mathfrak{J}^{\mu n}(x') = \frac{1}{\text{const}}\,\delta\mathbf{R}(x').$$

Thus,

$$g^{ik}i[\mathbf{Q}_i(x_0);\, \delta'\mathbf{D}_k(x')]_{x_0=x_0'} = \frac{1}{\text{const}}\,\delta\mathbf{R}(x').$$

Also,

$$i[\mathbf{Q}_i(x_0);\, \delta\mathbf{R}(x')]_{x_0=x_0'} = \delta'\mathbf{D}_i(x'),$$

and

$$i[\mathbf{Q}_i(x_0);\, \mathfrak{J}^\rho{}_k(x')]_{x_0=x_0'} = f_{ikl}\mathfrak{J}^{\rho l}(x').$$

* Work supported in part by the Swedish Natural Science Research Council.

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[5] M. Gell-Mann, Phys. Rev. **125**, 1067 (1962).
[6] K. Johnson, Nucl. Phys. **25**, 431 (1961).
[7] K. Bergström, J. Math. Phys. **11**, 2498 (1970).
[8] B. S. De Witt, *Dynamical Theory of Groups and Fields* (Gordon and Breach, New York, 1965).
[9] S. L. Adler and R. F. Dashen, *Current Algebras* (Benjamin, New York, 1968).
[10] R. Utiyama, Phys. Rev. **101**, 1597 (1956).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 11, NUMBER 8 AUGUST 1970

Equal-Time Commutation Relation for the Energy–Momentum Tensor

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(Received 25 November 1969)

Using a method outlined in a previous paper, we derive an equal-time commutation relation for the energy–momentum tensor. We make no restrictions on the external gravitational field $g_{\mu\nu}$ that couples to the energy–momentum tensor. As a special case of the equal-time commutation relation derived, we obtain Schwinger's commutation relation for the energy density.

1. INTRODUCTION

In this paper, an equal-time commutation relation for the energy–momentum tensor associated with an arbitrary Lorentz-invariant physical system is derived. The energy–momentum tensor is defined through the response of the physical system to a change of an external gravitational field. This definition is used by Schwinger in Ref. 1, where an equal-time commutation relation for the energy density $T_{00}(x)$ is obtained. For a restricted class of physical systems, when the gravitational field vanishes, the commutator takes the form

$$-i[T_{00}(x');\, T_{00}(x'')]_{x_0'=x_0''} = \delta^{(3)}_{,i}(\mathbf{x}';\, \mathbf{x}'')[T^i_0(x') + T^i_0(x'')]. \quad (1)$$

The derivation in Ref. 1 was done with a special gravitational field, namely,

$$g_{kl} = \delta_{kl}, \quad g_{0k} = 0, \quad g_{00} \neq 1, \quad k, l = 1, 2, 3.$$

In this paper, an attempt is made to derive an equal-time commutation relation of the form $[T_{0\alpha}(x');\, T_{\beta\gamma}(x'')]_{x_0'=x_0''}$, under somewhat more general conditions. Thus, no restrictions on the gravitational field, except that it be a c-number field, will be made.

In the presence of an external gravitational field, the energy–momentum tensor $T_{\mu\nu}$ is not conserved. Let us introduce the density quantity $\tilde{T}_{\mu\nu}$ defined as

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

Then we can write

$$\partial^\mu \tilde{T}_{\mu\nu} = D_\nu. \quad (3)$$

In Ref. 2, a method to derive equal-time commutation relations from divergence conditions for currents associated with finite-dimensional Lie groups was outlined, and in the last section we also generalized the method to an infinite-dimensional continuous group,[3] the "vierbein group." "Infinite dimensional"

satisfy

$$\frac{\delta'_{(3)}\mathfrak{J}^0_k(x)}{\delta A^i_\rho(x')} = 0.$$

But

$$\delta'\mathbf{D}_i(x') = f_{ilm}\delta A^l_\mu \mathfrak{J}^{\mu m}(x').$$

Therefore,

$$i[\mathfrak{J}^0_k(x);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = if_{ilm}\delta A^l_\mu(x')[\mathfrak{J}^0_k(x);\, \mathfrak{J}^{\mu m}(x')]_{x_0=x_0'},$$

$$i[\mathbf{Q}_k(x_0);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = if_{ilm}\delta A^l_\mu(x')[\mathbf{Q}_k(x);\, \mathfrak{J}^{\mu m}(x')]_{x_0=x_0'},$$

or

$$i[\mathbf{Q}_k(x_0);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = f_{ilm}\delta A^l_\mu(x') f_k{}^m{}_n \mathfrak{J}^{\mu n}(x').$$

Next, we compute

$$ig^{ik}[\mathbf{Q}_k(x_0);\, \delta'\mathbf{D}_i(x')]_{x_0=x_0'} = f^k{}_{lm} f_k{}^m{}_n \delta A^l_\mu \mathfrak{J}^{\mu n}(x') = \frac{1}{\text{const}}\,\delta\mathbf{R}(x').$$

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[7] K. Bergström, J. Math. Phys. **11**, 2498 (1970).
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[9] S. L. Adler and R. F. Dashen, *Current Algebras* (Benjamin, New York, 1968).
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The derivation in Ref. 1 was done with a special gravitational field, namely,

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In this paper, an attempt is made to derive an equal-time commutation relation of the form $[T_{0\alpha}(x');\, T_{\beta\gamma}(x'')]_{x_0'=x_0''}$, under somewhat more general conditions. Thus, no restrictions on the gravitational field, except that it be a c-number field, will be made.

In the presence of an external gravitational field, the energy–momentum tensor $T_{\mu\nu}$ is not conserved. Let us introduce the density quantity $\tilde{T}_{\mu\nu}$ defined as

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implies in this case that the coordinate manifold of the group is infinite dimensional and that the coordinates are functions over a finite-dimensional manifold, in this case space–time. In the presence of the gravitational field, space–time is curved, and we have to consider general coordinate transformations in a 4-dimensional Riemannian space.

The energy–momentum tensor $T_{\mu\nu}$ can be regarded as a generalized current, and the relevant group now is the general coordinate transformation group. Some properties of this infinite-dimensional group will be listed in Sec. 2. In Sec. 3 the equal-time commutator for the energy–momentum tensor is derived and a consistency check of the compatibility of the commutator $[T_{0\alpha}(x'); T_{\beta 0}(x'')]_{x_0'=x_0''}$ with the Poincaré algebra, is performed in Sec. 4.

2. THE GENERAL COORDINATE TRANSFORMATION GROUP

Here, we shall collect some well-known properties of the general coordinate transformation group (see Ref. 3). We consider infinitesimal coordinate transformations in a 4-dimensional Riemannian space–time

$$x'^{\mu} = x^{\mu} + \delta\xi^{\mu}(x), \quad \mu = 0, 1, 2, 3, \tag{4}$$

where $\delta\xi^{\mu}(x)$ are functions of space–time. The Jacobian is required to exist and to be different from zero.

Let $Q_{\mu}(x)$ be the infinitesimal generators of the group. They satisfy the identity

$$[Q_{\mu}(x'); Q_{\nu}(x'')] = \int d^4x\, C^{\rho}_{\mu'\nu''} Q_{\rho}(x), \tag{5}$$

where $C^{\rho}_{\nu'\mu''}$ is given by

$$C^{\rho}_{\nu'\mu''} = \delta^{\rho}_{\nu}\delta_{,\mu}(x; x')\delta(x; x'') - \delta^{\rho}_{\mu}\delta_{,\nu}(x; x'')\delta(x; x'). \tag{6}$$

Here, the comma means partial differentiation with respect to x. Since we have an infinite-dimensional group, we have a 4-dimensional integration to the right, as well as a summation over the discrete indices. $C^{\rho}_{\nu'\mu''}$ is a 3-point function whose transformation properties are determined from the transformation properties of the 4-dimensional δ function $\delta^{(4)}(x; x')$. (The 4-dimensional δ function transforms like a density of zero weight at the first argument and like a density of unit weight at the second.) Thus, $C^{\rho}_{\nu'\mu''}$ transforms like a contravariant vector of zero weight at x, and like a covariant vector of unit weight at x' and x''. Note that (5) is a completely covariant expression. The infinitesimal generators $Q_{\mu}(x)$ are covariant vectors of unit weight.

Let us assume that φ transforms as a scalar, vector, tensor, etc., under the coordinate transformation (4). The change of φ under the transformation is given by

$$\begin{aligned}\delta\varphi &\equiv \varphi'(x) - \varphi(x) \\ &= -\varphi_{,\mu}\delta\xi^{\mu} + G^{\mu}_{\nu}\varphi \cdot \delta\xi^{\mu}_{,\nu}.\end{aligned} \tag{7}$$

Here, the G^{μ}_{ν} are the generators of the linear group. They satisfy the commutation relation

$$[G^{\nu}_{\mu}; G^{\alpha}_{\beta}] = \delta^{\nu}_{\mu}G^{\alpha}_{\beta} - \delta^{\alpha}_{\beta}G^{\nu}_{\mu}. \tag{8}$$

3. THE ENERGY-MOMENTUM TENSOR

Let us consider a physical system which interacts with an external gravitational field $g^{\nu\mu}(x)$. We define the energy-momentum tensor as

$$\begin{aligned}\delta R(x) &= (-g)^{\frac{1}{2}} T_{\mu\nu}\delta g^{\mu\nu} = \tilde{T}_{\mu\nu}\delta g^{\mu\nu}, \\ \delta S &= \int d^4x\, \delta R(x),\end{aligned} \tag{9}$$

where S is the action for the system. (Compare Ref. 2.) Then $T_{\mu\nu}(x)$ is, by definition, a symmetric quantity, and Eq. (3) holds in the presence of a nonvanishing gravitational field. Following Schwinger,[1] we must have, for arbitrary variations of $g^{\mu\nu}$, the relation

$$\begin{aligned}-i\int d^4x''[\tilde{T}_{0\mu}(x'); \delta R(x'')]\delta(x_0'; x_0'') \\ = \partial^{\rho'}\delta' T_{\rho\mu}(x') - \delta' D_{\mu}(x'),\end{aligned} \tag{10}$$

where δ' gives the explicit dependence of the operators $\tilde{T}_{0\mu}$ and D_{μ} upon the external gravitational field. In Ref. 2, we made an assumption about the explicit dependence of the divergence of a current upon the external field, for finite-dimensional algebraic structures [Eq. (32) of Ref. 2] and also generalized to an infinite-dimensional situation [Eq. (71) of Ref. 2]. The following expression for the functional derivative $\delta' D_{\nu}(x')/\delta g^{\mu\omega}(x'')$ is thus suggested, in analogy with Eq. (71) of Ref. 2:

$$\frac{\delta' D_{\nu}(x')}{\delta g^{\mu\omega}(x'')} = \int d^4x\, C^{\rho}_{\nu'\mu''}\tilde{T}_{\rho\omega}(x), \tag{11}$$

where $C^{\rho}_{\nu'\mu''}$ is given by (6). Finally, we get the following equal-time commutation relation for the energy–momentum tensor:

$$\begin{aligned}-i[\tilde{T}_{0\mu}(x'); \tilde{T}_{\nu\omega}(x'')]\delta(x_0'; x_0'') \\ = \partial^{\rho'}\frac{\delta'\tilde{T}_{\rho\mu}(x')}{\delta g^{\nu\omega}(x'')} - \int d^4x\, C^{\rho}_{\mu'\nu''}\tilde{T}_{\rho\omega}(x).\end{aligned} \tag{12}$$

This relation holds in the absence of an external perturbation, and because $(-g)^{\frac{1}{2}} = 1$ in flat space–time, we can write

$$\begin{aligned}-i[T_{0\mu}(x'); T_{\nu\omega}(x'')]\delta(x_0'; x_0'') \\ = \partial^{\rho'}\frac{\delta'\tilde{T}_{\rho\mu}(x')}{\delta g^{\nu\omega}(x'')} - \int d^4x\, C^{\rho}_{\mu'\nu''}T_{\rho\omega}(x).\end{aligned} \tag{13}$$

Note that for ν, $\omega = 1, 2, 3$ the right-hand side of Eq. (13) should be symmetrized.

4. THE POINCARÉ ALGEBRA

In order to see that the Poincaré algebra follows from the equal-time commutation relation for the energy–momentum tensor derived in Sec. 3, we define in flat space-time the operators

$$P_\mu(x_0) = \int d^3\mathbf{x}\, T_{0\mu}(x)$$

and

$$M_{\mu\nu}(x_0) = \int d^3\mathbf{x}\,(T_{\mu 0}(x)x_\nu - T_{\nu 0}(x)x_\mu). \quad (14)$$

We compute next the equal-time commutator between P_μ and $M_{\rho\nu}$:

$$\begin{aligned} i[P_\mu(x_0'); M_{\rho\nu}(x_0'')]_{x_0'=x_0''} &= i\int d^3\mathbf{x}''[P_\mu(x_0'); T_{\rho 0}(x'')]x_\nu'' \\ &\quad - i\int d^3\mathbf{x}''[P_\mu(x_0'); T_{\nu 0}(x'')]x_\rho'' \\ &= \int d^3\mathbf{x}''\int d^4x'\int d^4x\, C^\sigma_{\mu'\rho''}T_{\sigma 0}(x)x_\nu'' \\ &\quad - \int d^3\mathbf{x}''\int d^4x'\int d^4x\, C^\sigma_{\mu'\nu''}T_{\sigma 0}(x)x_\rho''. \end{aligned} \quad (15)$$

Let us first study the case where $\mu = i$, $\rho = k$, $\nu = l$, and $i, k, l = 1, 2, 3$. Then,

$$\begin{aligned} -i[P_i(x_0'); M_{kl}(x_0'')]_{x_0'=x_0''} &= \int d^3\mathbf{x}''\int d^4x'\int d^4x\, C^\sigma_{i'l''}T_{\sigma 0}(x)x_k'' \\ &\quad - \int d^3\mathbf{x}''\int d^4x'\int d^4x\, C^\sigma_{i'k''}T_{\sigma 0}(x)x_l'' \\ &= \int d^3\mathbf{x}' T_{l0}(\mathbf{x}'; x_0'')g_{ik} \\ &\quad - \int d^3\mathbf{x}'\, T_{k0}(\mathbf{x}'; x_0'')g_{il} \end{aligned} \quad (16)$$

or

$$-i[P_i(x_0'); M_{kl}(x_0'')]_{x_0'=x_0''} = P_l(x_0'')g_{ik} - P_k(x_0'')g_{il}, \quad \text{for } i, k, l = 1, 2, 3. \quad (17)$$

In order to establish that the operators M_{kl} are conserved, we consider the equal-time commutator between P_0 and M_{kl}:

$$\begin{aligned} -i[P_0(x_0'); M_{kl}(x_0'')]_{x_0'=x_0''} &= \int d^3\mathbf{x}''\int d^4x'\int d^4x\, C^\sigma_{0'l''}T_{\sigma 0}(x)x_k'' \\ &\quad - \int d^3\mathbf{x}''\int d^4x'\int d^4x\, C^\sigma_{0'k''}T_{\sigma 0}(x)x_l'' \\ &= \int d^3\mathbf{x}'\,\partial_0 T_{l0}(\mathbf{x}'; x_0'')x_k' \\ &\quad - \int d^3\mathbf{x}'\,\partial_0 T_{k0}(\mathbf{x}'; x_0'')x_l'. \end{aligned} \quad (18)$$

In the limit of flat space-time, $T_{\mu\nu}$ is conserved. Thus,

$$-i[P_0(x_0'); M_{kl}(x_0'')]_{x_0'=x_0''} = \int d^3\mathbf{x}(T_{lk} - T_{kl}) = 0. \quad (19)$$

In the same manner, we have

$$-i[P_0(x_0'); M_{0l}(x_0'')]_{x_0'=x_0''} = -P_l(x_0''), \quad \text{for } l = 1, 2, 3, \quad (20)$$

and

$$-i[P_k(x_0'); M_{0l}(x_0'')]_{x_0'=x_0''} = g_{kl}P_0(x_0''), \quad \text{for } l, k = 1, 2, 3. \quad (21)$$

Next, we consider the commutator

$$\begin{aligned} -i[M_{ij}(x_0); M_{kl}(x_0')]_{x_0=x_0'} &= -i\int d^3\mathbf{x}\int d^3\mathbf{x}'\{[T_{i0}(x); T_{k0}(x')]_{x_0=x_0'}x_jx_l' \\ &\quad - [T_{i0}(x); T_{l0}(x')]_{x_0=x_0'}x_jx_k' \\ &\quad - [T_{j0}(x); T_{k0}(x')]_{x_0=x_0'}x_ix_l' \\ &\quad + [T_{j0}(x); T_{l0}(x')]_{x_0=x_0'}x_ix_k'\}. \end{aligned} \quad (22)$$

Let us look at the *first* and *last* terms of this equation. From (12), we get

$$\begin{aligned} -i[T_{i0}(x); T_{k0}(x')]_{x_0=x_0'} &= \partial^m \frac{\delta'_{(3)}\tilde{T}_{mi}(x)}{\delta g^{k0}(x')} - \int dx_0\int d^4x''\, C^{\rho''}_{ik'}T_{\rho 0}(x''), \\ & \qquad m = 1, 2, 3, \end{aligned} \quad (23)$$

where

$$\frac{\delta'\tilde{T}_{\alpha\beta}(x)}{\delta g^{\mu\nu}(x')} = \delta(x_0; x_0')\frac{\delta'_{(3)}\tilde{T}_{\alpha\beta}(x)}{\delta g^{\mu\nu}(x')} \quad (24)$$

and

$$\begin{aligned} -i[T_{j0}(x); T_{l0}(x')]_{x_0=x_0'} &= \partial^m \frac{\delta'_{(3)}\tilde{T}_{mj}(x)}{\delta g^{l0}(x')} - \int dx_0\int d^4x''\, C^{\rho''}_{jl'}T_{\rho 0}(x''). \end{aligned} \quad (25)$$

If (23) and (25) are substituted into (22) and integrated over 3-dimensional x space and x' space, after a partial integration over $\mathbf{x}$, we get the following term, which is symmetrical in k and l:

$$\int d^3\mathbf{x}\int d^3\mathbf{x}'\left(\frac{\delta'_{(3)}\tilde{T}_{jl}(x)}{\delta g^{k0}(x')}x_l' + \frac{\delta'_{(3)}\tilde{T}_{lj}(x)}{\delta g^{l0}(x')}x_k'\right). \quad (26)$$

The second and third terms in (22) give rise to exactly the same expression with opposite sign. Thus, there is no contribution from the gradient terms in Eq. (22).

We also study the term

$$\begin{aligned} &\int d^4x\int d^4x''\int d^3\mathbf{x}'\, C^{\rho''}_{ik'}T_{\rho 0}(x'')x_jx_l' \\ &\quad = \int d^4x\int d^3\mathbf{x}'[\delta^{(4)}_{,k}(x'; x)T_{i0}(x')x_jx_l' \\ &\qquad - \delta^{(4)}_{,i}(x; x')T_{k0}(x)x_jx_l'] \\ &\quad = -g_{il}\int d^3\mathbf{x}\, T_{k0}(x)x_j + g_{kj}\int d^3\mathbf{x}\, T_{i0}(x)x_l. \end{aligned} \quad (27)$$

Thus,

$$
\begin{aligned}
&i[M_{ij}(x_0); M_{kl}(x_0')]_{x_0=x_0'} \\
&\quad = g_{il}\int d^3\mathbf{x}\, T_{k0}(x)x_j - g_{kj}\int d^3\mathbf{x}\, T_{i0}(x)x_l \\
&\qquad - g_{ik}\int d^3\mathbf{x}\, T_{l0}(x)x_j + g_{lj}\int d^3\mathbf{x}\, T_{i0}(x)x_k \\
&\qquad - g_{jl}\int d^3\mathbf{x}\, T_{k0}(x)x_i + g_{ki}\int d^3\mathbf{x}\, T_{j0}(x)x_l \\
&\qquad + g_{jk}\int d^3\mathbf{x}\, T_{l0}(x)x_i - g_{li}\int d^3\mathbf{x}\, T_{j0}(x)x_k \\
&\quad = g_{il}M_{kj}(x_0) - g_{kj}M_{il}(x_0) \\
&\qquad - g_{ik}M_{lj}(x_0) + g_{lj}M_{ik}(x_0). \qquad (28)
\end{aligned}
$$

In the same way, the commutator $-i[M_{0i}(x_0); M_{kl}(x_0')]_{x_0=x_0'}$ can be investigated. Then, we can conclude that the algebra of the inhomogeneous Lorentz group follows from the equal-time commutation relation for the energy–momentum tensor $T_{\mu\nu}$.

Finally, we consider the equal-time commutation relation for the energy density $T_{00}(x)$:

$$
\begin{aligned}
&-i[T_{00}(x'); T_{00}(x'')]\delta(x_0'; x_0'') \\
&\quad = \partial^\mu \frac{\delta'\tilde{T}_{0\mu}(x')}{\delta g^{00}(x'')} + \delta^{(4)}_{,0}(x'; x'')T_{00}(x') \\
&\qquad - \delta^{(4)}_{,0}(x''; x')T_{00}(x''). \qquad (29)
\end{aligned}
$$

But in flat space–time, $T_{\mu\nu}$ is conserved, and we can write

$$
\begin{aligned}
&-i[T_{00}(x'); T_{00}(x'')]\delta(x_0'; x_0'') \\
&\quad = \partial^\mu \frac{\delta'\tilde{T}_{0\mu}(x')}{\delta g^{00}(x'')} + \delta(x_0'; x_0'')\cdot\delta^{(3)}_{,i}(\mathbf{x}'; \mathbf{x}'') \\
&\qquad \times [T^i_0(x_0') + T^i_0(x'')]. \qquad (30)
\end{aligned}
$$

Here

$$
\partial^\mu \frac{\delta'\tilde{T}_{0\mu}(x')}{\delta g^{00}(x'')} = 0 \qquad (31)
$$

for a restricted class of physical systems. This has been verified by Schwinger.[1] For systems with higher spin, (31) is usually different from zero.[4,5]

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[1] J. Schwinger, Phys. Rev. **130**, 406 (1963).
[2] K. Bergström, J. Math. Phys. **11**, 2489 (1970). Preceding paper.
[3] B. S. De Witt, *Dynamical Theory of Groups and Fields* (Gordon and Breach, New York, 1965).
[4] J. Schwinger, Phys. Rev. **130**, 800 (1963).
[5] D. G. Boulware and S. Deser, J. Math. Phys. **8**, 7 (1967).

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Error Bounds for Asymptotic Approximations of Zeros of Hankel Functions Occurring in Diffraction Problems*

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Error bounds on the asymptotic approximation for large argument of the zeros of the Hankel function of the first kind as a function of its order are found. These zeros occur as residue poles in the problem of scalar diffraction of high-frequency plane waves by a totally reflecting sphere.

1. INTRODUCTION

Here, $H^1_\nu(\beta)$ is the Hankel function of the first kind and $\nu_n(\beta)$ is the nth complex zero in the first quadrant (ordered by increasing modulus) of $H^1_\nu(\beta)$ as a function of its order ν. The asymptotic approximation of $\nu_n(\beta)$ for large real β is

$$
\nu_n(\beta) = \beta + \left(\frac{\beta}{2}\right)^{\frac{1}{3}} a_n e^{-\frac{2}{3}\pi i} + \left(\frac{2}{\beta}\right)^{\frac{1}{3}} \frac{a_n^2 e^{-\frac{4}{3}\pi i}}{60} + \alpha_n(\beta), \qquad (1)
$$

where a_n is the nth negative zero of the Airy function Ai (u) and $\alpha_n(\beta) = O(\beta^{-1})$.

We give a general theorem showing how error bounds for the asymptotic approximation of complex zeros depend on error bounds for the asymptotic approximation of the functions. After finding error bounds on the asymptotic approximation of $H^1_\nu(\beta)$ in terms of the Airy function Ai (u), we use this general theorem to find a strict bound on $\alpha_n(\beta)$ in (1) in terms of several constants. In addition, these

Thus,

$$
\begin{aligned}
&i[M_{ij}(x_0); M_{kl}(x_0')]_{x_0=x_0'} \\
&\quad = g_{il}\int d^3\mathbf{x}\, T_{k0}(x)x_j - g_{kj}\int d^3\mathbf{x}\, T_{i0}(x)x_l \\
&\qquad - g_{ik}\int d^3\mathbf{x}\, T_{l0}(x)x_j + g_{lj}\int d^3\mathbf{x}\, T_{i0}(x)x_k \\
&\qquad - g_{jl}\int d^3\mathbf{x}\, T_{k0}(x)x_i + g_{ki}\int d^3\mathbf{x}\, T_{j0}(x)x_l \\
&\qquad + g_{jk}\int d^3\mathbf{x}\, T_{l0}(x)x_i - g_{li}\int d^3\mathbf{x}\, T_{j0}(x)x_k \\
&\quad = g_{il}M_{kj}(x_0) - g_{kj}M_{il}(x_0) \\
&\qquad - g_{ik}M_{lj}(x_0) + g_{lj}M_{ik}(x_0). \qquad (28)
\end{aligned}
$$

In the same way, the commutator $-i[M_{0i}(x_0); M_{kl}(x_0')]_{x_0=x_0'}$ can be investigated. Then, we can conclude that the algebra of the inhomogeneous Lorentz group follows from the equal-time commutation relation for the energy–momentum tensor $T_{\mu\nu}$.

Finally, we consider the equal-time commutation relation for the energy density $T_{00}(x)$:

$$
\begin{aligned}
&-i[T_{00}(x'); T_{00}(x'')]\delta(x_0'; x_0'') \\
&\quad = \partial^\mu \frac{\delta'\tilde{T}_{0\mu}(x')}{\delta g^{00}(x'')} + \delta^{(4)}_{,0}(x'; x'')T_{00}(x') \\
&\qquad - \delta^{(4)}_{,0}(x''; x')T_{00}(x''). \qquad (29)
\end{aligned}
$$

But in flat space–time, $T_{\mu\nu}$ is conserved, and we can write

$$
\begin{aligned}
&-i[T_{00}(x'); T_{00}(x'')]\delta(x_0'; x_0'') \\
&\quad = \partial^\mu \frac{\delta'\tilde{T}_{0\mu}(x')}{\delta g^{00}(x'')} + \delta(x_0'; x_0'')\cdot\delta^{(3)}_{,i}(\mathbf{x}'; \mathbf{x}'') \\
&\qquad \times [T^i_0(x_0') + T^i_0(x'')]. \qquad (30)
\end{aligned}
$$

Here

$$
\partial^\mu \frac{\delta'\tilde{T}_{0\mu}(x')}{\delta g^{00}(x'')} = 0 \qquad (31)
$$

for a restricted class of physical systems. This has been verified by Schwinger.[1] For systems with higher spin, (31) is usually different from zero.[4,5]

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[1] J. Schwinger, Phys. Rev. **130**, 406 (1963).
[2] K. Bergström, J. Math. Phys. **11**, 2489 (1970). Preceding paper.
[3] B. S. De Witt, *Dynamical Theory of Groups and Fields* (Gordon and Breach, New York, 1965).
[4] J. Schwinger, Phys. Rev. **130**, 800 (1963).
[5] D. G. Boulware and S. Deser, J. Math. Phys. **8**, 7 (1967).

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Error Bounds for Asymptotic Approximations of Zeros of Hankel Functions Occurring in Diffraction Problems*

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Error bounds on the asymptotic approximation for large argument of the zeros of the Hankel function of the first kind as a function of its order are found. These zeros occur as residue poles in the problem of scalar diffraction of high-frequency plane waves by a totally reflecting sphere.

1. INTRODUCTION

Here, $H^1_\nu(\beta)$ is the Hankel function of the first kind and $\nu_n(\beta)$ is the nth complex zero in the first quadrant (ordered by increasing modulus) of $H^1_\nu(\beta)$ as a function of its order ν. The asymptotic approximation of $\nu_n(\beta)$ for large real β is

$$
\nu_n(\beta) = \beta + \left(\frac{\beta}{2}\right)^{\frac{1}{3}} a_n e^{-\frac{2}{3}\pi i} + \left(\frac{2}{\beta}\right)^{\frac{1}{3}} \frac{a_n^2 e^{-\frac{4}{3}\pi i}}{60} + \alpha_n(\beta), \qquad (1)
$$

where a_n is the nth negative zero of the Airy function Ai (u) and $\alpha_n(\beta) = O(\beta^{-1})$.

We give a general theorem showing how error bounds for the asymptotic approximation of complex zeros depend on error bounds for the asymptotic approximation of the functions. After finding error bounds on the asymptotic approximation of $H^1_\nu(\beta)$ in terms of the Airy function Ai (u), we use this general theorem to find a strict bound on $\alpha_n(\beta)$ in (1) in terms of several constants. In addition, these

constants have been evaluated numerically to obtain results such as $|\alpha_1(\beta)| \leq 1.71/\beta^{\frac{2}{3}}$ for $\beta \geq 20$.

Interest in the zeros of the Hankel function as a function of its order arises from their importance in the problem of scalar diffraction of high-frequency plane waves by a totally reflecting sphere. We give a brief discussion of this problem here and refer the reader to the paper of Nussenzveig[1] for more information. If a is the radius of the sphere, K is the wavenumber which is 2π divided by the wavelength λ, and $\beta = Ka$; then that the waves are of high frequency relative to the size of the sphere is expressed by the conditions $\beta \gg 1$ and $\beta^{\frac{1}{3}} \gg 1$.

For high frequencies, a large number of terms of the partial-wave-series solution is needed to obtain a good approximation to the total field. In order to avoid this difficulty, Watson[2] transformed the partial-wave series into an integral and after modifying the contour, he changed the integral into a residue series whose residue poles are the zeros $\nu_n(\beta)$. The zeros $\nu_n(\beta)$ are symmetrically distributed with respect to the origin and lie in the first and fourth quadrants. In the first quadrant, there are an infinite number of zeros and they all lie close to the curve

$$\text{Re}\,[(\nu^2 + \beta^2)^{\frac{1}{2}} - \nu \operatorname{arc\,cosh}(\nu/\beta)] = 0.$$

The residue poles inside the contour are the zeros $\nu_n(\beta)$ in the upper half-plane.[1] We study the first zeros which are near the origin, since the first terms are the dominant terms of the residue series. These same poles have been used by Regge[3] and others in recent quantum mechanical studies.

Because of the importance of these poles in the residue series, numerous studies have been made concerning them. Perhaps the first asymptotic approximation of the zeros $\nu_n(\beta)$ was found by van der Pol and Bremmer[4] using the Debye expansion for the Bessel function. Franz[5] used the saddle-point method on the Sommerfeld integral representation for the Hankel function and obtained essentially the first two terms of (1). Next, Magnus and Kotin[6] did an extensive theoretical study of these zeros obtaining results such as the simplicity of the zeros, the existence of infinitely many zeros, and the asymptotic behavior of the zeros for large $|\nu|$. Later, Keller, Rubinow, and Goldstein[7] obtained asymptotic expansions of $\nu_n(\beta)$ for large and small values of β and also for large values of n. Their expansion for large β is equivalent to (1). In addition, they computed approximate values for certain zeros for specific values of β; however, neither they nor anyone else has obtained strict *a priori* error bounds for these approximations to the zeros. Recently, Cochran[8] gave a systematic theoretical treatment of these zeros, including a new derivation of (1).

It is desirable to determine *a priori* error bounds for the asymptotic expansion (1) in order to obtain error bounds on Watson's approximation to the total field in the scattering problem. In particular, $\nu_n(\beta)$ is approximated six times by various truncations of (1) in obtaining a shadow-region expansion for the total field.[1] Obtaining *a priori* bounds on these approximations would be an important first step in determining the accuracy of the shadow region approximation.

Many other physical problems require the investigation of zeros of specific transcendental functions. The method applied here to find precise error bounds on the asymptotic approximation (1) could be applied to study the zeros of other transcendental functions. For example, one could analyze the zeros as a function of the order ν of $dH_\nu^1(\beta)/d\beta$ and $dH_\nu^1(\beta)/d\beta + icH_\nu^1(\beta)$, which occur in diffraction problems with cylindrical and spherical symmetry.

2. AN APPROXIMATION THEOREM FOR COMPLEX ZEROS

From the definition of an asymptotic expansion, we know that the difference between a function and its truncated asymptotic expansion is of the order of magnitude of the first omitted term. Since the first omitted term is usually available as an error estimate, the problem of finding strict error bounds seems to have been somewhat neglected. However, strict error bounds are useful both theoretically and numerically. Here, we give an approximation theorem which is a rigorous statement of the intuitive idea that if two functions are close together, then their zeros are close together.

Theorem 1: Suppose $f(z) = g(z) + \epsilon(z)$, where $f(z)$ and $g(z)$ are holomorphic in the disk $|z - b| \leq \rho$ and $g(z)$ has exactly one zero b in the disk. Let

$$m = \min_\theta |g(b + \rho e^{i\theta})|, \quad E = \max_\theta |\epsilon(b + \rho e^{i\theta})|,$$

and

$$M = \max_\theta |g'(b + \rho e^{i\theta})|.$$

If $m > E$, then $f(z)$ has exactly one zero c in the disk and $|c - b| \leq E\rho^2 M/m(m - E)$.

The proof of this theorem and an application to the complex zeros $j_{\nu,n}$ of the Bessel function $J_\nu(z)$ were given in an earlier paper.[9]

3. APPROXIMATION OF THE HANKEL FUNCTION

If one applies Olver's asymptotic approximation theorem for complex variables[10] to his uniform asymptotic approximation of Bessel functions of large order,[11] one obtains[12] an asymptotic approximation with error bound for $H_\nu^1(\beta)$ for real positive β and complex ν such that $0 \le \arg \nu \le \frac{1}{2}\pi$ in terms of the Airy function Ai (u).

If

$$z = \frac{\beta}{\nu}, \quad \left(\frac{dz}{d\zeta}\right)^2 = \frac{\zeta z^2}{1 - z^2},$$

$$z(0) = 1, \quad u = \nu^{\frac{2}{3}}\zeta e^{\frac{2}{3}\pi i},$$

and

$$|\arg(-u)| < \tfrac{1}{3}\pi,$$

then

$$\frac{\nu^{\frac{1}{3}}e^{\frac{1}{3}\pi i}}{2^{\frac{2}{3}}}\left(\frac{1 - z^2}{\zeta}\right)^{\frac{1}{4}} H_\nu^1(\beta) = \text{Ai}\,(u) + \epsilon(u, \beta), \tag{2}$$

where

$$|\epsilon(u, \beta)| \le (\nu_2/\nu_1)(e^{2\nu_1 F(u,\beta)} - 1)E^{-1}(u)M_2(u), \tag{3}$$

$$F(u, \beta) = \frac{|z|}{\beta}\int_{\zeta \exp(\frac{2}{3}\pi i)}^{+\infty} |s^{-\frac{1}{2}}f(se^{-\frac{2}{3}\pi i})|\,|ds|, \tag{4}$$

$$f(\zeta) = \frac{5}{16\zeta^2} + \tfrac{1}{4}\zeta\frac{z^2(z^2 + 4)}{(z^2 - 1)^3},$$

$$E(u) = |\exp(\tfrac{2}{3}u^{\frac{3}{2}})|,$$

$$M_2^2(u) = E^2(u)\,|\text{Ai}^2(u)| + E^{-2}(u)\,|\text{Ai}^2(ue^{-\frac{2}{3}\pi i})|$$

for $-\frac{1}{3}\pi \le \arg u \le \pi$,

$$M(u) = M(\bar{u}) \quad \text{for} \quad |\arg(-u)| \le \tfrac{2}{3}\pi,$$

$$\nu_1 = \max_{|\arg z| \le \frac{1}{3}\pi} \{\pi\,|z|^{\frac{1}{2}} M_2^2(z)\},$$

and

$$\nu_2 = \max_{-\frac{1}{3}\pi \le \arg z \le \pi} \{\pi E(z)M(z)\,|z^{\frac{1}{2}}\,\text{Ai}\,(z)|\}.$$

4. APPROXIMATION OF THE $\nu_n(\beta)$

In our application of Theorem 1, we take $f(u, \beta)$ as the left-hand side of (2) and $g(u) = \text{Ai}\,(u)$. It is clear that the continuous dependence of f and ϵ on the parameter β does not affect the application of the theorem. If $\rho < \frac{1}{2}(3)^{\frac{1}{2}}\,|a_n|$, where a_n is the nth negative zero of the Airy function Ai (u), then the entire disk $|u - a_n| \le \rho$ is contained in the sector $|\arg(-u)| < \frac{1}{3}\pi$. It has been shown[12] that $f(u, \beta)$ is a holomorphic function of u for $|u - a_n| \le \rho < 3^{\frac{1}{2}}\,|a_n|/2$.

Here, $m = \min |\text{Ai}\,(u)|$, $E(\beta) = \max |\epsilon(u, \beta)|$, and $M = \max |\text{Ai}'\,(u)|$, where $|u - a_n| = \rho$. Since $E(\beta)$ is a decreasing function of β from (3) and (4), we can choose β large enough so that $m > E(\beta)$. Consequently, there exists a simple zero c of $f(u, \beta)$ such that $|c - a_n| \le \rho$ and $|c - a_n| \le E(\beta)\rho^2 M/m[m - E(\beta)]$. Since the coefficient of $H_\nu^1(\beta)$ on the left-hand side of (2) is never zero for $|\arg(-u)| < \frac{1}{3}\pi$, c must be the desired zero of $H_\nu^1(\beta)$ as a function of u. If we let $c = \nu^{\frac{2}{3}}e^{\frac{2}{3}\pi i}b$, then b is a zero of $H_\nu^1(\beta)$ as a function of ζ and

$$b = (a_n + \delta)e^{-\frac{2}{3}\pi i}z^{\frac{2}{3}}/\beta^{\frac{2}{3}}, \tag{5}$$

where $|\delta| \le \rho$ and

$$|\delta| \le E(\beta)\rho^2 M/m[m - E(\beta)]. \tag{6}$$

We now obtain an expression for the zero of $H_\nu^1(\beta)$ as a function of the order ν by using $\nu_n(\beta) = \beta/z(b)$.

If we make use of the known[11] Maclaurin's series for $z(\zeta)$ in $\nu_n = \beta/z(b)$, then

$$\nu_n(\beta) = \beta + 2^{-\frac{1}{3}}\beta b + \tfrac{7}{10}2^{-\frac{2}{3}}\beta b^2 + \tfrac{139}{700}\beta b^3 + \beta b^4 R_4(b), \tag{7}$$

where

$$R_4(b) = \frac{1}{2\pi i}\int_c \frac{dw}{z(w)w^4(w - b)}, \tag{8}$$

c being a circle with center at the origin and radius $R < (\frac{3}{2}\pi)^{\frac{2}{3}}$. The result of replacing one b in the second through fourth terms of (7) by (5) is

$$\begin{aligned}\nu_n(\beta) = \beta &+ (2)^{-\frac{1}{3}}\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}z^{\frac{2}{3}} \\ &+ \tfrac{7}{10}(2^{-\frac{2}{3}})\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}z^{\frac{2}{3}}b \\ &+ \tfrac{139}{700}\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}z^{\frac{2}{3}}b^2 + \beta b^4 R_4(b).\end{aligned} \tag{9}$$

Now we employ Maclaurin's series for $z^{\frac{2}{3}}(b)$ in (9) and combine similar terms to obtain

$$\begin{aligned}\nu_n(\beta) = \beta &+ \frac{\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}}{2^{\frac{1}{3}}} + \frac{2^{\frac{1}{3}}\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}b}{60} \\ &+ \frac{61\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}b^2}{6300} + \beta b^4 R_4(b) \\ &+ \beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}b^3\left(\frac{S_3}{2^{\frac{1}{3}}} + \frac{7S_2}{10 \times 2^{\frac{2}{3}}} + \frac{139S_1}{700}\right),\end{aligned}$$

where

$$S_m(b) = \frac{1}{2\pi i}\int_c \frac{z^{\frac{2}{3}}(w)\,dw}{w^m(w - b)}. \tag{10}$$

Replacing one b in the third and fourth term of the expression above by (5) and utilizing Maclaurin's series for $z^{\frac{2}{3}}(b)$ again, we have

$$\begin{aligned}\nu_n(\beta) = \beta &+ \frac{\beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}}{2^{\frac{1}{3}}} \\ &+ \frac{2^{\frac{1}{3}}(a_n + \delta)^2 e^{-\frac{4}{3}\pi i}}{60\beta^{\frac{1}{3}}} - \frac{(a_n + \delta)^2 e^{-\frac{4}{3}\pi i}b}{700\beta^{\frac{1}{3}}} \\ &+ \frac{(a_n + \delta)^2 e^{-\frac{4}{3}\pi i}b^2}{\beta^{\frac{1}{3}}}\left(\frac{2^{\frac{1}{3}}S_2}{60} + \frac{61S_1}{6300}\right) \\ &+ \beta^{\frac{1}{3}}(a_n + \delta)e^{-\frac{2}{3}\pi i}b^3\left(\frac{S_3}{2^{\frac{1}{3}}} + \frac{7S_2}{10 \times 2^{\frac{2}{3}}} + \frac{139S_1}{700}\right) \\ &+ \beta b^4 R_4(b).\end{aligned} \tag{11}$$

The bound on $|\epsilon(u, \beta)|$ in (3) is simplified if we use the result[10] that $\nu_2/\nu_1 \leq 1$ and let E^{-1} and M_2 be the maximums of $E^{-1}(u)$ and $M_2(u)$ for $|u - a_n| \leq \rho$, P_r and Q_r be the maximum and minimum of $|z(\zeta)|$ for $|\zeta| = r$, and I_r be the maximum of the integral in $F(u, \beta)$ for $|\zeta| \leq r$. Now, $|u - a_n| \leq \rho$ implies $|\zeta/z^{\frac{2}{3}}| \leq (|a_n| + \rho)/\beta^{\frac{2}{3}}$. If we assume that $|\zeta/z^{\frac{2}{3}}| \leq (|a_n| + \rho)/\beta_0^{\frac{2}{3}}$ implies $|\zeta| \leq r$, then $\beta \geq \beta_0$ implies

$$E(\beta) \leq (e^{2\nu_1 P_r I_r/\beta} - 1)E^{-1}M_2. \tag{12}$$

Using (6) and the inequality $e^x - 1 \leq x/(1 - x)$ applied to the right-hand side of (12), we conclude that

$$\delta| \leq 2\nu_1 P_r I_r E^{-1} M_2 \rho^2 M/\beta m(1 - 2\nu_1 P_r I_r/\beta_0) \times \{m - [\exp(2\nu_1 P_r I_r/\beta_0) - 1]E^{-1}M_2\},$$

which we express as

$$|\delta| \leq D(\beta_0, \rho)/\beta. \tag{13}$$

From (11) and (13) we obtain the theorem below.

Theorem 2: Suppose $0 \leq \arg \nu \leq \frac{1}{2}\pi$, $\rho < 3^{\frac{1}{2}}|a_n|/2$, and $\beta \geq \beta_0$ where $|\zeta/z^{\frac{2}{3}}| \leq (|a_n| + \rho)/\beta_0^{\frac{2}{3}}$ implies $|\zeta| \leq r$ and

$$(e^{2\nu_1 P_r I_r/\beta} - 1)E^{-1}M_2 < m.$$

Then there exists a simple zero $\nu_n(\beta)$ of $H_\nu^1(\beta)$ with an asymptotic approximation given by (1) such that

$$|\alpha_n(\beta)| \leq \frac{D}{2^{\frac{1}{3}}\beta^{\frac{2}{3}}} + \frac{2^{\frac{1}{3}}(2|a_n| + \rho)D}{60B^{\frac{4}{3}}} + \frac{(|a_n| + \rho)^3 P_r^{\frac{3}{2}}}{700\beta} + \frac{(|a_n| + \rho)^4 P_r^{\frac{4}{3}}}{\beta^{\frac{5}{3}}}\left(\frac{2^{\frac{1}{3}}|S_2|}{60} + \frac{61|S_1|}{6300}\right) + \frac{(|a_n| + \rho)^4 P_r^{\frac{8}{3}}}{\beta^{\frac{5}{3}}}|R_4| + \frac{(|a_n| + \rho)^4 P_r^2}{\beta^{\frac{5}{3}}} \times \left(\frac{|S_3|}{2^{\frac{1}{3}}} + \frac{7|S_2|}{10 \times 2^{\frac{2}{3}}} + \frac{139|S_1|}{700}\right). \tag{14}$$

5. ERROR BOUNDS FOR THE APPROXIMATION TO THE FIRST ZERO

In this section, we use computed values of the constants occurring on the right-hand side of (14) to find an error bound for $|\alpha_1(\beta)|$. The values of m, M, E^{-1}, M_2, P_r, Q_r, and I_r have been calculated and tabulated[12] for various values of ρ and r. It has been proved that $\nu_1 \geq 1.25$, and it has been calculated that $\nu_1 \leq 1.288$.[12] All numbers given in this paper have been rounded to obtain the weakest inequalities.

The first negative zero of Ai (u) is $a_1 = -2.33810$. If we choose $\rho = 0.1$, then $\rho < 3^{\frac{1}{2}}|a_1|/2$, $m = 0.070$, $M = 0.710$, and $E^{-1}M_2 = 0.292$. If $\beta_0 = 20$, then $|\zeta/z^{\frac{2}{3}}| \leq 2.438/(20)^{\frac{2}{3}}$ implies $|\zeta| \leq 0.4$. Using $P_{0.4} = 1.35$ and $I_{0.4} = 0.1302$, we find $E(\beta) \leq 0.006$, from (12), and $D = 0.214$, from (13). From (8) and (10), it follows that $|R_4(b)| \leq [Q_R R^2(R - r)]^{-1}$ and

$$|S_m(b)| \leq P_R^{\frac{3}{2}}[R^{m-1}(R - r)]^{-1},$$

where $r < R < (\frac{3}{2}\pi)^{\frac{2}{3}}$. Using the above inequalities with $R = 2.6$ and $r = 0.4$, it has been shown[12] that $|S_3| \leq 0.087$, $|S_2| \leq 0.074$, $|S_1| \leq 0.56$, and $|R_4| \leq 0.206$. Incorporating the above values into (14) yields $|\alpha_1(\beta)| \leq 1.71/\beta^{\frac{2}{3}}$ for $\beta \geq 20$. It follows immediately that

$$|\nu_1(\beta) - (\beta + 1.856\beta^{\frac{1}{3}}e^{\frac{1}{3}\pi i})| \leq 1.78/\beta^{\frac{1}{3}}$$

and $|\nu_1(\beta) - \beta| \leq 2.10\beta^{\frac{1}{3}}$ for $\beta \geq 20$.

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[1] H. M. Nussenzveig, Ann. Phys. (N.Y.) **34**, 23 (1965).
[2] G. N. Watson, Proc. Roy. Soc. (London) **A95**, 83 (1918).
[3] T. Regge, Nuovo Cimento **14**, 951 (1958).
[4] H. Bremmer, *Terrestrial Radio Waves* (Elsevier, New York, 1949).
[5] W. Franz, Z. Naturforsch. **9a**, 705 (1954).
[6] W. Magnus and L. Kotin, Numerische Math. **2**, 228 (1960).
[7] J. Keller, S. I. Rubinow, and M. Goldstein, J. Math. Phys. **4**, 829 (1963).
[8] J. A. Cochran, Numerische Math. **7**, 238 (1965).
[9] H. W. Hethcote, SIAM J. Math. Anal. **1**, 147 (1970).
[10] F. W. J. Olver, J. Soc. Indust. Appl. Math. **12**, 200 (1964).
[11] F. W. J. Olver, Phil. Trans. Roy. Soc. (London) **A247**, 328 (1964).
[12] H. W. Hethcote, Doctoral Dissertation, University of Michigan, 1968.

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General Theorem on Bifurcation and Its Application to the Hartree Equation of the Helium Atom

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The existence of a globally extended branch of pointwise positive solutions of a class of nonlinear eigenvalue problems is established. The branch bifurcates from the lowest eigenvalue of the associated linearized problem. The general theorem is then applied to the Hartree equation of the helium atom, giving a rigorous proof for the existence of a solution of this equation.

I. INTRODUCTION

The purpose of this article is to give a rigorous proof for the existence of a pointwise positive solution for the nonlinear Hartree equation of the helium atom, which is of the form

$$-\tfrac{1}{2}\Delta u(x) - \frac{2}{r(x)}\,u(x) + u(x)\int \frac{u^2(y)}{r(x-y)}\,dy = \lambda u(x),$$

with the auxiliary condition

$$\|u\|^2 = \int u^2(y)\,dy = 1.$$

A solution of this equation is called a self-consistent field. For the connection of this equation with the Schrödinger equation of the helium atom, see, for example, Hartree's book.[1] Numerical iterative calculations indicate convergence of the procedure, and the λ calculated is in good agreement with variationally calculated values for the Schrödinger equation, whose lowest eigenvalue is connected with the lowest eigenvalue of the above nonlinear equation; but no rigorous proof has been given for the existence of such a solution. The proof is constructed along the lines exposed in Refs. 2–5. In these places, the nonlinear eigenvalue problem is supposed to be of the form

$$Bu + C(u) = \lambda u,$$

where B is a linear self-adjoint operator and C is a nonlinear operator, homogeneous of degree greater than one and satisfying a special estimate

$$\|C(u) - C(v)\| \leq K(\|u\|^{m-1} + \|v\|^{m-1})\,\|u - v\|,$$

where m is the degree of C:

$$C(tu) = t^m C(u).$$

From this, it follows immediately that C is a bounded operator, which is certainly not true for the nonlinear term of the Hartree equation which is not defined everywhere. But on the domain D_Δ of the Laplacian, which is the natural domain for the solutions of this equation, the nonlinear term is bounded with respect to the graph norm of the Laplacian; or, precisely stated,

$$\sup_{u\in D_\Delta} \frac{\|C(u)\|}{\|u\|_\Delta} < \infty,$$

where

$$\|u\|_\Delta^2 = \|u\|^2 + \|\Delta u\|^2 \quad \text{for} \quad u \in D_\Delta.$$

So, before entering the discussion proper, we should adapt standard bifurcation analysis, as presented in the papers mentioned above, to this more general situation.

II. THE GENERAL THEOREM

Let G be a bounded or unbounded region of $\mathbb{R}^n$. Furthermore, we define the graph norm $\|u\|_S$ for any self-adjoint operator S by

$$\|u\|_S = \alpha\,\|Su\| + \beta\,\|u\|, \qquad \forall\, u \in D_S, \quad \alpha > 0, \quad \beta \geq 1.$$

Consider an equation of the form

$$Bu + C(u) = \lambda u$$

in the real Hilbert space $L^2(G)$, where B and C have the following properties:

(1) B is self-adjoint and bounded below, the lower bound μ_0 being an isolated eigenvalue. The resolvent $(B-\mu)^{-1}$ is strictly positive for $\mu < \mu_0$; that is, nonnegative functions are transformed into strictly positive functions by $(B-\mu)^{-1}$.

(2) The nonlinear operator C is generated by an m-linear form $C(u_1, u_2, \cdots, u_m)$ defined on D_B; that is, $C(u) = C(u, u, \cdots, u)$ and this m-linear form is such that $C(u, u, \cdots, u, h) = q_u h$, where q_u is a bounded measurable function.

(3) There is a self-adjoint operator S which has the same domain as B, such that

(a) $\|C(u_1, u_2, \cdots, u_m)\| \leq K_0\,\|u_1\|_S\,\|u_2\|_S \cdots \|u_m\|_S$, for $u_i \in D_B$,

and suppose that $\|C(u)\| \leq K_1 \|u\|^{m-1} \|u\|_S$, where α can be chosen as small as one wishes, independently of K_1. The first inequality implies that

$$\|C(u) - C(v)\| \leq K_2(\|u\|_S^{m-1} + \|v\|_S^{m-1}) \|u - v\|_S$$

and that C is continuously differentiable in the sense of Frechet as a mapping from D_B into $L^2(G)$:

$$C(u + h) - C(u) = d_u Ch + R(u, h)$$

and

$$\lim_{\|h\|_S \to 0} \frac{\|R(u, h)\|}{\|h\|_S} = 0, \quad \forall\, u,\, h \in D_B.$$

(b) C is relatively compact with respect to S; that is, from $\|u_i\|_S < \text{const}$ follows the existence of a subsequence $u_{i'}$ such that $C(u_{i'})$ converges strongly.

(c) $d_u C$ is symmetric and relatively compact with respect to S and $(d_u C \cdot h, h) > (q_u h, h) > 0, \forall\, u, h \in D_B$ and $h \neq 0,\ u > 0$.

(4) $B + q_u$, with $u \in D_B$, where q_u is regarded as a multiplicative operator, has no eigenvalues in the interior of the essential spectrum of B, whose infimum shall be denoted by μ_e, which is not supposed to be an isolated point of the essential spectrum. Under these assumptions, the following result holds true.

Theorem: There exists an interval (μ_0, μ_c), $\mu_c \leq \mu_e$ such that:

(a) On the interval (μ_0, μ_c), there is a unique branch of solutions u_λ, everywhere positive, where $\|u_\lambda\|_S$ and $\|u_\lambda\|$ are continuous functions of λ.

(b) $\|u_\lambda\|$ is monotonically increasing with λ, and $\|u_\lambda\|_S$ and $\|u_\lambda\|$ tend to infinity if $\mu_c < \mu_e$. If $\mu_c = \mu_e$, then $\|u_\lambda\|$ and $\|u_\lambda\|_S$ may either both stay bounded or both diverge.

(c) There are no other positive solutions for $\mu_0 < \lambda < \mu_c$.

Proof:

(a) Bifurcation analysis: Let μ be a simple isolated eigenvalue of B with eigenvector v normalized to one. Then the equation

$$Bu + C(u) = \lambda u$$

can be split up in two equations, namely,

$$w = (B - \mu)^{-1} P(\delta w - C(w + \epsilon v)) = F(w, \delta, \epsilon),$$
$$\delta\epsilon = (C(w + \epsilon v), v), \tag{1}$$

where $u = w + \epsilon v$, $\lambda = \mu + \delta$, and P is the projection onto $[v]^\perp$. F is a mapping from D_S into D_S, which can be estimated in the graph norm. One has to use hypothesis (3a) of the theorem and the fact that

$$\|\omega\| \leq \|\omega\|_S, \quad \|(B - \mu)^{-1} P\| = M_1,$$
$$\|S(B - \mu)^{-1} P\| = M_2.$$

The last equality stems from the fact that $S(B - \mu)^{-1}$ is a bounded operator by the closed graph theorem. Thus one is led to the following estimates for F:

$$\|F(\omega, \delta, \epsilon)\|_S \leq (\alpha M_2 + \beta M_1)(\delta \|\omega\|_S + K_2 \|\omega + \epsilon v\|_S^m)$$
$$\|F(\omega, \delta, \epsilon) - F(\omega', \delta, \epsilon)\|_S \leq (\alpha M_2 + \beta M_1)[\delta + K_2(\|\omega + \epsilon v\|_S^{m-1} + \|\omega' + \epsilon v\|_S^{m-1})] \|\omega - \omega'\|_S. \tag{2}$$

From these estimates, it follows that there are constants δ_0, ϵ_0, and ν_0 such that, for $|\delta| < \delta_0$, $|\epsilon| < \epsilon_0$, and $\|\omega\|_S < \nu_0$, F is a contraction mapping, so that there is a unique solution $\omega(\delta, \epsilon)$ with $\|\omega(\delta, \epsilon)\|_S \leq K\epsilon^m$. The second equation of (1) can be treated as in Ref. 4. Thus, the results which are derived there for a bounded nonlinear term $C(u)$ remain valid in this case.

(b) By hypothesis (1) of our theorem, the lower bound of $B + f$, where f is a bounded measurable function, is simple if it is an isolated eigenvalue and the corresponding eigenfunction can be chosen positive. To prove this, we remark that $B + f$ is bounded below, because B and f are. Then we choose μ and μ' such that $\mu' + f > 0$ and $\mu + \mu'$ is smaller than the lower bound of $B + f$ and B and such that $\|(B - \mu)^{-1}(\mu' - f)\| < 1$. Then we write

$$[B - \mu - (\mu' - f)]^{-1} = (B - \mu)^{-1}[1 + (\mu' - f)(B - \mu)^{-1} + \cdots].$$

Because $(B - \mu)^{-1}$ is strictly positive, the above equality proves that $(B + f - \mu - \mu')^{-1}$ is strictly positive and so, by [10], if the lower bound of $B + f$ is an isolated eigenvalue, then it is simple and the corresponding eigenfunction can be chosen positive.

(c) From hypothesis (2) of the theorem, we conclude that every solution of $Bu + C(u) = \lambda u$ is at the same time an eigenvector of the linear operator $B + q_u$ because $C(u) = q_u \cdot u$. In (a), we have proven that the results of standard bifurcation theory as in Refs. 2–4 are applicable. So, by repeating the respective arguments in Ref. 5, we get the existence of a branch of positive solutions u_λ in some interval $(\mu_0, \mu_0 + \gamma)$.

(d) Next, we show that the branch we have constructed in (c) can be extended to some maximal interval (μ_0, μ_c) with $\mu_c \leq \mu_e$. To see this, we consider the two equations

$$Bu_\lambda + C(u_\lambda) = \lambda u_\lambda,$$
$$B(u_\lambda + h) + C(u_\lambda + h) = (\lambda + \delta)(u_\lambda + h), \tag{3}$$

where u_λ is a positive solution of the first equation. From (b), we know that, if $B + q_u$ has a lowest isolated eigenvalue, its eigenfunction is positive, so that the higher eigenvalues cannot have positive eigenfunctions because such a function would not be orthogonal to the first one. Therefore, our u_λ is necessarily the first eigenvalue of $B + q_{u_\lambda}$. Further, $d_u C$ is relatively compact with respect to S. This is equivalent to saying that it is relatively compact with respect to B since $\|u\|_B$ and $\|u\|_S$ are equivalent because of the closed graph theorem. But a relatively compact, symmetric perturbation does not change the essential spectrum of B. So, below μ_c, $B + d_{u_\lambda} C$ has only eigenvalues of finite multiplicity, and the first one is strictly bigger than that of $B + q_{u_\lambda}$ because of $(d_{u_\lambda} Ch, h) > (q_{u_\lambda} h, h)$. From that, we conclude that λ is in the resolvent set of $(B + d_{u_\lambda} C - \lambda)$. So, we take the difference of the two equations in (3) and invert, arriving at

$$h = (B + d_{u_\lambda} C - \lambda)^{-1}[\delta(u_\lambda + h) - R(u_\lambda, h)]. \quad (4)$$

As is easily checked, the right-hand side is a contraction mapping in the graph norm for δ and $\|h\|_S$ sufficiently small. Therefore, it has a solution h_δ, with $\|h_\delta\|_S$ being a continuous function of δ and $\|h_\delta\|_S \to 0$ for $\delta \to 0$. This means that u_λ is continuous in the graph norm. From that, it follows that $B + q_{u_\lambda}$ converges relatively uniformly[6] to $B + q_{u_\mu}$ if $\lambda \to \mu$. From this, we conclude that, because λ was the first eigenvalue of $B + q_{u_\lambda}$ which is simple, it has to stay the first one, so that the functions are always positive. This shows that the branch we had constructed in (c) can be extended to a maximal interval (μ_0, μ_c), where $\mu_c \leq \mu_e$, because we know from hypothesis (4) that $B + q_{u_\lambda}$ has only eigenvalues $\lambda \leq \mu_e$.

(e) Let us now assume $\mu_c < \mu_e$. Thus, μ_c is below the essential spectrum of B and can therefore be, at most, an eigenvalue of finite multiplicity if it is an eigenvalue at all. Let Q be the projection on its eigenspace ($Q = 0$ if μ_c is not eigenvalue) and let $P = 1 - Q$. Our equation $Bu_\lambda + C(u_\lambda) = \lambda u_\lambda$ can be rewritten as

$$Pu_\lambda = (B - \mu_c)^{-1} P((\lambda - \mu_c)u_\lambda + C(u_\lambda)),$$
$$0 = Q((\lambda - \mu_c)u_\lambda + C(u_\lambda)).$$

Now let $\mu_c < \mu_e$. Since C is relatively compact with respect to S, we can choose a sequence λ_i such that $C(u_{\lambda_i})$ converges strongly. $\lambda_i - \mu_c \to 0$; thus, Pu_{λ_i} converges strongly. From this sequence, we can once again select a subsequence $\lambda_{i'}$ such that $Qu_{\lambda_{i'}}$ converges strongly, because it is restricted to a finite-dimensional subspace. So $u_{\lambda_{i'}}$ converges strongly. Rewriting our equation now as

$$u_\lambda = (B - \mu)^{-1}[(\lambda - \mu)u_\lambda - C(u_\lambda)], \quad (5)$$

where μ is from the resolvent set of B, we conclude, by applying S to this equation, that u_λ converges even in the graph norm. Therefore, it is a solution of our equation and, by the same continuity argument as before, it belongs to the first eigenvalue of the associated linear comparison operator. Therefore, it is positive and, by (d), we can continue to the right, contradicting the definition of μ_c. So $\|u_\lambda\|_S \to \infty$ for $\lambda \to \mu_c$ if $\mu_c < \mu_e$. If $\mu_c = \mu_e$, the extension argument fails, because $(B + d_{u_\lambda} C - \lambda)$ need not be invertible for $\lambda = \mu_e$ since the limit point of the essential spectrum is not shifted by the strictly positive operator $d_{u_\lambda} C$.

(f) Multiplying Eq. (5) by S and taking the norm, we get the estimate

$$\|Su_\lambda\| \leq M(K\|u_\lambda\| + K_1 \|u_\lambda\|^{m-1} \|u_\lambda\|_S).$$

Using hypothesis (3a), we can rewrite it, bringing all $\|Su\|$ to the left side, as

$$\|Su_\lambda\|(1 - \alpha M K_1 \|u_\lambda\|^{m-1}) \leq \|u_\lambda\|(KM + K_1 \beta \|u_\lambda\|^{m-1}). \quad (6)$$

Now, let us assume that $\|u_\lambda\|$ remains bounded while $\|Su_\lambda\|$ goes to infinity; then we immediately get a contradiction if we choose α small enough in equality (6) to make the left side positive. Thus, both expressions remain finite or both diverge.

(g) To prove that $\|u_\lambda\|$ increases monotonically, let us calculate its derivative:

$$\frac{d\|u_\lambda\|^2}{d\lambda} = \lim_{\delta \to 0} 2\left(u_\lambda, \frac{h_\delta}{\delta}\right).$$

Introducing (4) into this expression, we get

$$\frac{d}{d\lambda}\|u_\lambda\|^2 = 2((B + d_{u_\lambda} C - \lambda)u_\lambda, u_\lambda),$$

which is positive because the lowest eigenvalue of $B + d_{u_\lambda} C$ is larger than λ.

(h) The proof that, for $\mu_0 \leq \lambda \leq \mu_c$, there are no other positive solutions reads exactly as in Ref. 5, and is not repeated here.

Remark: If m is odd, there is a second branch starting at μ_0 and going to the right, consisting simply of $-u_\lambda$. If m is even, then a second branch starting at μ_0 goes to the left, but secondary bifurcation may occur on this branch.

III. THE HARTREE EQUATION

To apply the general theorem to the Hartree equation, the assumptions (1)–(4) have to be verified. But in order to do this, one has to transform this equation into a 1-dimensional form. For that purpose, we observe that the linear part is reduced by the subspace of spherically symmetric functions and that the nonlinear term transforms this subspace into itself. To verify the last statement, we introduce the series expansion

$$\frac{1}{r(x-y)} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta), \quad \sphericalangle(x, y) = \theta,$$

$$r_> = \max(r(x), r(y)), \quad r_< = \min(r(x), r(y)),$$

in the integral $\int u^2(y)\, dy/r(x-y)$. This results in

$$\begin{aligned}\int \frac{u^2(y)}{r(x-y)}\, dy &= \int_0^\infty r^2\, dr \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, u^2(r) \\ &\quad \times \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta) \\ &= \int_0^\infty r^2\, dr u^2(r) \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} \\ &\quad \times \int_0^\pi \sin\theta\, d\theta\, P_l(\cos\theta) \int_0^{2\pi} d\phi \\ &= 4\pi \int_0^\infty r^2 u^2(r) \frac{1}{r_>}\, dr \\ &= 4\pi \left(\frac{1}{r} \int_{s<r} u^2(s) s^2\, ds + \int_{s>r} u^2(s) s\, ds \right) \\ &= q_u(r). \end{aligned} \tag{7}$$

By restricting the Hartree equation to the subspace of spherically symmetric functions, this equation becomes

$$\left(-\frac{1}{2r} \frac{d^2}{dr^2} r - \frac{2}{r} + q_u(r) \right) u(r) = \lambda u(r).$$

Substituting, as is usually done, $x(r) = ru(r)$, we see that this equation becomes an equation in $L^2(0, \infty)$:

$$-\left(\frac{1}{2} \frac{d}{dr^2} - \frac{2}{r} + q_x(r) \right) x(r) = \lambda x(r);$$

$$q_x(r) = 4\pi \left(\frac{1}{r} \int_{s<r} x^2\, ds + \int_{s>r} \frac{x^2}{s}\, ds \right),$$

with the boundary condition $x(0) = 0$. In the domain D'_Δ of the second derivative d^2/dr^2, with the above boundary condition, the graph norm $\|x\|'_\Delta$ is introduced:

$$\|x\|'_\Delta = \alpha \left(\int_0^\infty (x'')^2\, ds \right)^{\frac{1}{2}} + \beta \left(\int_0^\infty x^2\, ds \right)^{\frac{1}{2}}.$$

We note that

$$\begin{aligned}\|u\|^2 &= \int dy u^2(y) = 4\pi \int r^2 u^2(r)\, dr \\ &= 4\pi \int x^2\, ds = 4\pi \|x\|^2, \\ \|u\|_\Delta &= 4\pi \|x\|'^2_\Delta. \end{aligned}$$

The Laplacian in three dimensions has a very special property. The functions in its domain are bounded in terms of the graph norm (see, for example, Ref. 7):

$$|u(x)| \le C(\gamma^{-\frac{1}{2}} \|\Delta u\| + \gamma^{\frac{3}{2}} \|u\|), \quad \gamma > 0,$$
$$\text{or} \quad |u(x)| \le C_1 \|u\|_\Delta, \quad \forall\, \alpha > 0.$$

Furthermore, r^{-1} is relatively bounded with respect to Δ:

$$\|r^{-1}u\| \le \alpha \|\Delta u\| + \beta \|u\|,$$

where α can be made arbitrarily small or

$$\|r^{-1}u\| \le C_2 \|u\|_\Delta, \quad \forall\, \alpha > 0.$$

These two inequalities carry over to $L^2(0, \infty)$:

$$|x(r)/r| \le C'_1 \|x\|'_\Delta; \quad \|x/r\| \le C'_2 \|x\|'_\Delta, \quad \forall\, \alpha > 0. \tag{8}$$

After these preliminaries, assumptions (1)–(4) of the general theorem are verified.

(1) $B = -\frac{1}{2}d^2/dr^2 - 2/r$, which is self-adjoint and bounded below by -2, which is an isolated eigenvalue. The essential spectrum is absolutely continuous and starts at zero, extending to infinity. $(-\frac{1}{2}d^2/dr^2 - 2/r - \mu)^{-1}$ is strictly positive for $\mu < -2$.

(2) The nonlinear term is generated by the 3-linear form

$$C(x_1, x_2, x_3) = x_3 \left(\frac{4\pi}{r} \int_{s<r} x_1 x_2\, ds + 4\pi \int_{s>r} \frac{x_1 x_2}{s}\, ds \right)$$

and

$$C(x, x, h) = q_x h,$$

where

$$q_x = 4\pi \left(\frac{1}{r} \int_{s<r} x^2\, ds + \int_{s>r} \frac{x^2}{s}\, ds \right)$$

and q_x is bounded

$$\begin{aligned} 0 \le q_x &= 4\pi \left(\frac{1}{r} \int_{s<r} x^2\, ds + \int_{s>r} \frac{x^2}{s}\, ds \right) \le 4\pi \int_0^\infty \frac{x^2}{s}\, ds \\ &\le 4\pi \|x\| \left\| \frac{x}{r} \right\| \le 4\pi C'_2 \|x\| \|x\|'_\Delta. \end{aligned} \tag{9}$$

Here, r^{-1} has been taken under the integral sign in the first integral and (2) has been used. By taking s^{-1} in front of the second integral another inequality results:

$$0 \le q_x(r) \le \frac{4\pi}{r} \int_0^\infty x^2\, ds = \frac{\|u\|^2}{r}. \tag{10}$$

(3) We take operator S to be $-d^2/dr^2$, which has the same domain as $-\frac{1}{2}d^2/dr^2 - 2/r$. The required boundedness property for the 3-linear form then holds true:

$$\left\| x_3 \left(\frac{4\pi}{r} \int_{s<r} x_1 x_2 \, ds + 4\pi \int_{s>r} \frac{x_1 x_2}{s} \, ds \right) \right\|$$
$$\leq 4\pi \left[\left\| \frac{x_3}{r} \right\| \|x_1\| \, \|x_2\| + \|x_3\| \left\| \frac{x_2}{r} \right\| \|x_1\| \right]$$
$$\leq 8\pi C_2' \|x_1\|_\Delta' \|x_2\|_\Delta' \|x_3\|_\Delta'$$

and

$$\|x q_x\| \leq 8\pi C_2' \|x\|^2 \|x\|_\Delta'. \tag{11}$$

This is proven for the first integral in the following way:

$$\left\| \frac{x_3}{r} \int_{s<r} x_1 x_2 \, ds \right\| \leq \left\| \frac{x_3}{r} \right\| \cdot \sup_r \left| \int_{s<r} x_1 x_2 \, ds \right|$$

and

$$\sup_r \left| \int_{s<r} x_1 x_2 \, ds \right| \leq \sup_r \left(\int_{s<r} x_1^2 \, ds \right)^{\frac{1}{2}} \left(\int_{s<r} x_2^2 \, ds \right)^{\frac{1}{2}}$$
$$\leq \|x_1\| \, \|x_2\|.$$

The second integral is handled in the same manner. $C(x)$ is relatively compact with respect to $-d^2/dr^2$. To prove this, we observe that q_x is differentiable with respect to r:

$$\frac{d}{dr} q_x(r) = -\frac{4\pi}{r^2} \int_{s<r} x^2 \, ds + \frac{4\pi}{r} x^2 - 4\pi \frac{x^2}{r}$$
$$= -\frac{4\pi}{r^2} \int_{s<r} x^2 \, ds,$$
$$|q_x'(r)| \leq 4\pi \int \frac{x^2}{s^2} \, ds = \left\| \frac{x}{r} \right\|^2 \leq C_2'^2 \|x\|'^2. \tag{12}$$

Therefore, q_x is a bounded continuous function by (3) and its tail at infinity is square integrable by (4). This implies that $q_x \in L^2(0, \infty)$ and that q_x is majorized by some fixed function from $L^2(0, \infty)$ which depends only upon $\|x\|_\Delta'$. Furthermore, its derivative is bounded by $\|x\|_\Delta'$. Let us then assume that the sequence x_i is bounded in the graph norm, $\|x_i\|_\Delta'^2 < \text{const}$; then q_{x_i} is bounded by some fixed L^2 function, its derivatives are uniformly bounded by a constant, and, therefore, the q_{x_i} are equicontinuous and uniformly bounded. By the Ascoli–Arzela theorem, there is a subsequence which converges pointwise and uniform on each compact set. By the dominated convergence theorem, this convergence is strong even in $L^2(0, \infty)$. The x_i, as well, are uniformly bounded and equicontinuous, so that the same reasoning applies; thus, there is a subsequence which converges pointwise. It is therefore possible to choose a subsequence such that $x_{i'} q_{x_{i'}}$ converges strongly. Thus, $C(x)$ is relatively compact with respect to $-d^2/dr^2$.

The Frechet derivative of $C(x)$ is easily computed:

$$d_x C \cdot h = q_x h + x \left(\frac{4\pi}{r} \int_{s<r} x h \, ds + 4\pi \int_{s>r} \frac{xh}{s} \, ds \right).$$

It is a symmetric operator, and the integral operator on the right-hand side is strictly positive. This is most easily recognized by remembering that $C(x)$ is the restriction of

$$C(u) = u \int \frac{u^2(y)}{r(x-y)} \, dy$$

to spherically symmetric functions, with the substitution $x = ru$. The Frechet derivative of this operator is given by

$$d_u C \cdot h = h(x) \int \frac{u^2(y)}{r(x-y)} \, dy + 2u(x) \int \frac{u(y)h(y)}{r(x-y)} \, dy,$$

which is manifestly symmetric, and the integral operator is strictly positive, because its kernel is $u(x)u(y)$ times the Green's function of the Laplacian. From this, it follows that

$$(d_x C \cdot h, h) > (q_x h, h) \geq 0$$
$$\text{for} \quad x, h \in D' \quad \text{and} \quad h \neq 0.$$

To check that $d_x C$ is relatively compact with respect to second differentiation, we note that $q_x h_i$ has a strongly convergent subsequence if $\|h_i\|_\Delta'$ is bounded. That implies that there is a uniformly bounded pointwise convergent subsequence $h_{i'}$. Multiplied by the function q_x, which belongs to $L^2(0, \infty)$, this gives strong convergence. The second term in the Frechet derivative converges because $\|h_i\|_\Delta'$ bounded implies the existence of a weakly convergent subsequence $h_{i'}$. This in turn implies convergence of

$$\int_{s<r} x h_{i'} \, ds \quad \text{and} \quad \int_{s>r} \frac{x h_{i'}}{s} \, ds$$

for all r. From this, we conclude, by the same reasoning as above, that

$$\frac{4\pi x}{r} \int_{s<r} x h_{i'} \, ds + 4\pi x \int_{s>r} \frac{x h_{i'}}{s} \, ds$$

converges strongly.

(4) If we look at

$$-\tfrac{1}{2}\Delta - \frac{2}{r} + q_x \quad \text{with} \quad x \in D_\Delta'$$

but arbitrary otherwise, we can apply the theorem in Ref. 8 assuring that there are no eigenvalues bigger

than zero. The required hypotheses on the potential function $V(r)$ are:

(a) V is a sum of a $L^\infty(R^3)$ and a $L^2(R^3)$ function;
(b) V is continuous;
(c) $\lim V(r) = 0$, as $r \to \infty$;
(d) $\limsup r\, dV(r)/dr = 0$, $r \to \infty$.

All four conditions are easily checked for our

$$V(r) = -2/r + q_\varkappa(r).$$

Now, if

$$-\tfrac{1}{2}\Delta - 2/r + q_\varkappa(r)$$

has no positive eigenvalues, then

$$-\frac{1}{2}\frac{d^2}{dr^2} - \frac{2}{r} + q_\varkappa(r)$$

has none.

Thus, conditions (1)–(4) of the general theorem are fulfilled and the theorem applies. There is a branch coming out of -2 and its norm is monotonically increasing. The branch consists of pointwise positive functions, and these are the only positive solutions for $-2 < \lambda < 0$.

To establish the existence of a solution of the Hartree equation with the auxiliary condition $\|u\| = 1$, one must make sure that the norm of the branch reaches one; but this is not yet proven. The general theorem gives an alternative: Either $\|u\|$ goes to infinity or, if the branch extends up to zero, the norm $\|u\|$ may stay bounded. To decide this question, one has to make a rather detailed study of the equation.

Let us write the equation in the form

$$x_\lambda'' = Q_\lambda x_\lambda, \quad Q_\lambda = 2[-2/r + q_\varkappa(r) - \lambda]. \quad (13)$$

It follows immediately that the solutions of this equation are infinitely differentiable for $r \neq 0$ because the equation implies the existence of the nth derivative if the derivatives up to order $n-2$ exist. Furthermore, we already know that the branch we are looking at consists of strictly positive functions which vanish at the origin. This implies that the zeros of x_λ'' are those of Q_λ, because the x_λ have no zero for $r \neq 0$. Let us study the behavior of Q_λ:

$$Q_\lambda' = +\frac{2}{r^2}\left(2 - 4\pi\int_{s<r} x_\lambda^2\, ds\right),$$

where we have used (12). Assume that $\|u_\lambda\| \leq K < 2$, so that Q_λ is monotonically increasing from $-\infty$ to -2λ, and

$$-2/r + q_\lambda(r) \leq -(2-K)/r. \quad (14)$$

If $\|u_\lambda\| = 2$, Q_λ is still monotonically increasing from $-\infty$ to -2λ, but there is no majorizing potential as in (14). If $\|u_\lambda\| > 2$, then Q_λ' changes sign somewhere. Thus, it is monotonically increasing from $-\infty$ to some finite maximum and then monotonically decreasing to -2λ.

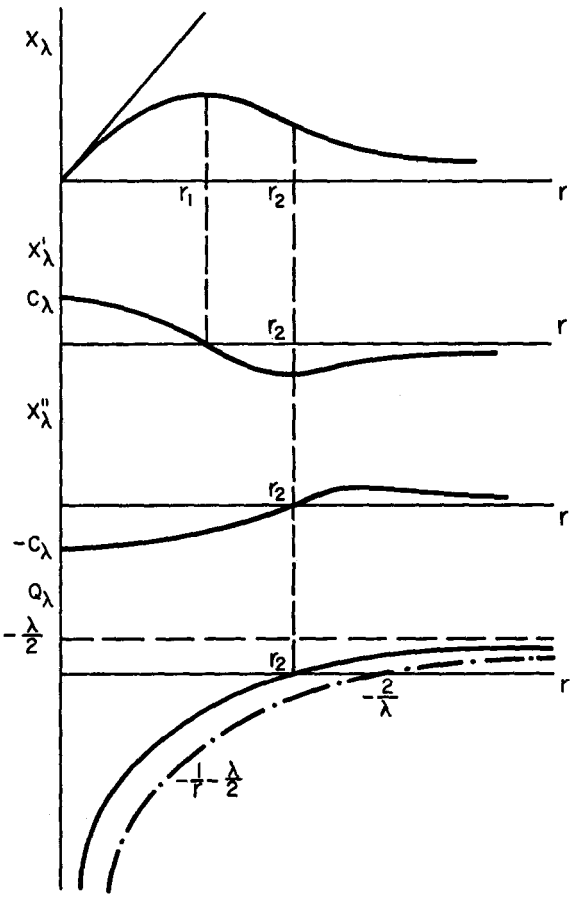

FIG. 1.

From this we conclude that, for any $\lambda < 0$, Q_λ has exactly one zero. This, in turn, implies that x_λ' has only one zero, because x_λ is zero at $r = 0$ and at $r = \infty$ and positive elsewhere: Therefore, x_λ' has an uneven number of zeros and, if it had more than one, x_λ'' would have more than one. Now we note that

$$C_\lambda \equiv x'(0) = \lim_{r\to 0}\frac{x_\lambda(r) - x_\lambda(0)}{r} = \lim_{r\to 0}\frac{x_\lambda(r)}{r}$$
$$= -\lim_{r\to 0} Q_\lambda x_\lambda = -x_\lambda''(0).$$

What has been said of the x_λ allows us to draw a qualitative picture of these functions as is done in Fig. 1. From the fact that $x_\lambda'(0) = C_\lambda$ and $x_\lambda''(0) = -C_\lambda$, a trivial estimate follows:

$$x_\lambda(r) \leq C_\lambda r. \quad (15)$$

Now, let r_1 be the zero of x_λ', r_2 that of x_λ'', and r_3 that of Q_λ' if it has one. Then it is true that

$$r_1 \leq r_2 \leq r_3. \quad (16)$$

Remembering that q_x is a positive function, we have

$$Q_\lambda(r) \geq 4(-r^{-1} - \tfrac{1}{2}\lambda), \tag{17}$$

which implies

$$r_2 \leq -2/\lambda. \tag{18}$$

Let $r \leq r_2$. Then integration of (7) gives

$$\int_0^r x_\lambda'' \, ds = x_\lambda'(r) - C_\lambda = \int_0^r Q_\lambda x_\lambda \, ds \geq \int_0^r \left(-\frac{4}{s}\right) x_\lambda$$

$$\geq C_\lambda \int_0^r (-4) \, ds = -4C_\lambda r. \tag{19}$$

For $r = r_1$, this results in

$$r_1 \geq \tfrac{1}{4}. \tag{20}$$

We now derive an estimate similar to that in Chap. VIII of Ref. 9. Multiplying (7) by x_λ' and integrating over $r \geq -2/\lambda$, where Q_λ is positive, we get

$$-x_\lambda'^2(r) = \int_r^\infty Q_\lambda (x_\lambda^2)' \, ds \leq -4(-r^{-1} - \tfrac{1}{2}\lambda) x_\lambda^2(r),$$

$$\text{for} \quad r \geq -2/\lambda.$$

This gives

$$-x_\lambda'(r)/x_\lambda(r) \geq 2(-r^{-1} - \tfrac{1}{2}\lambda)^{\frac{1}{2}} \geq (-r^{-1} - \tfrac{1}{2}\lambda),$$

$$\text{for} \quad r \geq -2/\lambda,$$

and, after one further integration from r to R, we end up with

$$-\ln x_\lambda(R) + \ln x_\lambda(r) \geq \int_r^R (-s^{-1} - \tfrac{1}{2}\lambda) \, ds$$

$$= \ln \frac{R}{r} - \tfrac{1}{2}\lambda(R - r)$$

or

$$x_\lambda(R) \leq x_\lambda(r)(R/r) e^{\frac{1}{2}(R-r)\lambda}, \quad \text{for} \quad R > r \geq -2/\lambda.$$

Remembering (15), we can eliminate the $x_\lambda(r)$ and, by taking $r = -2/\lambda$ and replacing R by r, we get

$$x_\lambda(r) \leq C_\lambda e r e^{\frac{1}{2}r\lambda}, \quad r \geq -2/\lambda,$$

$$\leq C_\lambda r, \qquad r \leq -2/\lambda. \tag{21}$$

This gives the important result

$$\|x_\lambda\|^2 \leq C_\lambda^2 \cdot F(\lambda). \tag{22}$$

On the other hand, by integrating (19) once again from zero to $r < r_1$, we get

$$x_\lambda(r) \geq C_\lambda(r - 2r^2), \quad r \leq r_1. \tag{23}$$

We know that, in our case, $\mu_c = 0$. Let us assume that $\mu_c < 0$. We know from the general theorem that, in this case, $\|x_\lambda\| \to \infty$ for $\lambda \to \mu_c$. Equation (22) shows us that, here, $C_\lambda \to \infty$ for $\lambda \to \mu_c$ because $F(\mu_c) < \infty$.

On the other hand, we have by (23)

$$q_{x_\lambda}(r) \geq \frac{4\pi}{r} \int_{s<r} x_\lambda^2 \, ds \geq \frac{4\pi C_\lambda^2}{r} \int_0^r (s - 2s^2) \, ds,$$

$$\text{for} \quad r \leq \tfrac{1}{4},$$

where the right-hand side tends to infinity for $\lambda \to \mu_c$ because of C_λ. But then the zero of

$$Q_\lambda(r) = 2[-2/r + q_{x_\lambda}(r) - \lambda]$$

would move below $\frac{1}{4}$, which is impossible because of (20) and (16). Thus, $\mu_c = 0$.

Now assume that, for $\lambda \to 0$, we have $\|u_\lambda\| \leq 1$. Then we know, from (14), that there is a majorizing potential for the linear comparison operator. Moreover, the x_λ are strictly positive functions, so that (12) becomes a strict inequality such that

$$-\frac{1}{2}\frac{d^2}{dr^2} - \frac{2}{r} + q_{x_\lambda}(r) < -\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}.$$

From that, we conclude that the lowest eigenvalue of our equation is bounded above by $-\frac{1}{2}$ in contradiction to our assumption that $\lambda \to 0$ or, stated differently, that there is a u_λ on the branch with $\|u_\lambda\| = 1$ and $\lambda < -\frac{1}{2}$. On the other hand, we can now show that these u_λ (and $-u_\lambda$, of course) are the only solutions for $\lambda < -\frac{1}{2}$. Let x_λ be a solution of our equation which changes sign; then it is necessarily a higher eigenfunction of the linear comparison operator

$$-\frac{1}{2}\frac{d^2}{dr^2} - \frac{2}{r} + q_{x_\lambda}.$$

But the higher eigenvalues of this operator are bounded below by the second eigenvalue of

$$-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r},$$

which is $-\frac{1}{2}$. So we have shown that solutions x_λ which change sign have $\lambda \geq -\frac{1}{2}$.

Remark: Our analysis leaves open the question of whether $\lim \|u_\lambda\|$, as $\lambda \to 0$, is finite or infinite. Also, it does not extend in its present form to analogous equations in $\mathbb{R}^n$ for $n > 3$, because the estimates for $|u(x)|$ in Sec. III are specific for $\mathbb{R}^3$.

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The author is indebted to N. Bazley and B. Zwahlen for their kind interest.

[1] D. R. Hartree, *The Calculation of Atomic Structures* (Wiley, New York, 1957).
[2] M. A. Krasnosel'skii, *Positive Solutions of Operator Equations* (Noordhoff, Gröningen, The Netherlands, 1964).
[3] G. H. Pimbley, *Eigenfunction Branches of Nonlinear Operators and their Bifurcations, Lecture Notes in Mathematics, No. 104* (Springer, Berlin, 1969).
[4] N. Bazley and B. Zwahlen, J. Appl. Math. Phys. **20**, 281 (1969).
[5] N. Bazley and B. Zwahlen, "A Branch of Positive Solutions of Nonlinear Eigenvalue Problems," Manuscripta Math. (to be published).
[6] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Ungar, New York, 1955).
[7] T. Kato, *Perturbation Theory for Linear Operators* (Springer, Berlin, 1966).
[8] B. Simon, Commun. Pure Appl. Math. **22**, 537 (1969).
[9] E. C. Titchmarsh, *Eigenfunction Expansions* (Oxford U.P., London, 1962), Part I.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 11, NUMBER 8 AUGUST 1970

Generalized Racah Tensors and the Structure of Mixed Configurations*

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(Received 26 September 1969)

Generalized Racah tensors are defined after the manner of Elliott and Feneuille. The linear combinations $^{\pm}\mathbf{w}^{(\kappa k)}(l, l')$ used by them are redefined to permit the correct embedding of the group R_4 in the higher groups that may be used to classify the states of mixed configurations. A number of points regarding the transformation properties of states and operators are clarified and related to the problem of the symmetrization of the Coulomb repulsion in mixed configuations.

1. INTRODUCTION

The theory of continuous groups has been applied extensively to the calculation of the properties of single configurations of electrons or nucleons.[1] In many practical cases the single configuration approximation is physically inappropriate and it is necessary to consider a multiconfiguration model that allows for configuration mixing. Notable examples are the case of the $(2s + 2p)^N$ configurations in a Coulomb field or of $(s + d)^N$ nucleon configurations in a harmonic oscillator potential. In these cases, it is desirable to consider sets of configurations collectively.

The application of continuous groups to the calculation of the properties of particular mixed configurations has been considered by a number of authors.[2–4] In the present paper, we wish to give a systematic account of a number of problems that arise in the extension of the application of continuous groups in going from the single-configuration to multiconfiguration approximation. In particular, we shall examine the general transformation properties of the tensor operators and states appropriate to the description of multiconfigurations together with the obtaining of expressions for the Casimir operators in terms of the group generators. An examination of problems associated with the embedding of the R_4 group in the higher Lie groups leads to a more careful treatment of the phase definitions of the tensor operators that form the group generators. Finally, application to the symmetry description of the Coulomb interaction is considered.

2. GENERALIZED TENSOR OPERATORS

Following Elliott[2] and Feneuille,[3] let us define the tensor operators $\mathbf{v}^{(k)}(A, B)$ and $\mathbf{w}^{(\kappa k)}(A, B)$ in terms of their reduced matrix elements between single-particle wavefunctions:

$$\langle C\| v^{(k)}(A, B) \|D\rangle = \delta(A, C)\delta(B, D)[k]^{\frac{1}{2}}, \quad (1a)$$

$$\langle sC\| w^{(\kappa k)}(A, B) \|sD\rangle = \delta(A, d)\delta(B, D)[\kappa, k]^{\frac{1}{2}}, \quad (1b)$$

with the usual notation

$$[x, y, \cdots, z] \equiv (2x + 1)(2y + 1) \cdots (2z + 1).$$

We use capital Latin letters to indicate arbitrary values of the single-particle angular momentum.

A component $w^{(\kappa k)}_{\pi q}(A, B)$ operating on a single electron wavefunction gives

$$\begin{aligned} w^{(\kappa k)}_{\pi q}(A, B)\,|slm_sm_l\rangle &= \sum_{l', m'_l, m'_s} \delta(A, l')\delta(B, l)(-1)^{l'+s-m'_l-m'_s} \\ &\times [\kappa, k]^{\frac{1}{2}} \begin{pmatrix} s & \kappa & s \\ -m'_s & \pi & m_s \end{pmatrix} \begin{pmatrix} l' & k & l \\ -m'_l & q & m_l \end{pmatrix} \\ &\times |sl'm'_sm'_l\rangle, \end{aligned} \quad (2)$$

from which we may deduce the general commutator

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[3] G. H. Pimbley, *Eigenfunction Branches of Nonlinear Operators and their Bifurcations, Lecture Notes in Mathematics, No. 104* (Springer, Berlin, 1969).
[4] N. Bazley and B. Zwahlen, J. Appl. Math. Phys. **20**, 281 (1969).
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[6] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Ungar, New York, 1955).
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A component $w^{(\kappa k)}_{\pi q}(A, B)$ operating on a single electron wavefunction gives

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from which we may deduce the general commutator

expression

$$[w^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B),\, w^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)]$$
$$= \sum_{\kappa_3,k_3,\pi_3,q_3} (-1)^{2s+\kappa_3+k_3-\pi_3-q_3}[\kappa_1,\kappa_2,\kappa_3,k_1,k_2,k_3]^{\frac{1}{2}}$$
$$\times \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa_3 \\ \pi_1 & \pi_2 & -\pi_3 \end{pmatrix} \begin{pmatrix} k_1 & k_2 & k_3 \\ q_1 & q_2 & -q_3 \end{pmatrix} \begin{Bmatrix} \kappa_1 & \kappa_2 & \kappa_3 \\ s & s & s \end{Bmatrix}$$
$$\times \Bigg[\delta(B,C)(-1)^{A+D+\kappa_1+\kappa_2+k_1+k} \begin{Bmatrix} k_1 & k_2 & k_3 \\ D & A & B \end{Bmatrix} w^{(\kappa_3 k_3)}_{\pi_3 q_3}(A,D)$$
$$- \delta(A,D)(-1)^{B+C+\kappa_3+k_3} \begin{Bmatrix} k_1 & k_2 & k_3 \\ C & B & A \end{Bmatrix} w^{(\kappa_3 k_3)}_{\pi_3 q_3}(C,B) \Bigg]. \tag{3}$$

If we define the linear combinations

$$^{\pm}\mathbf{w}^{(\kappa k)}(A,B) = \mathbf{w}^{(\kappa k)}(A,B) \pm (-1)^{\kappa+k+A-B}\mathbf{w}^{(\kappa k)}(B,A), \tag{4}$$

then we obtain the following commutators:

$$[^{+}w^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B),\, ^{\pm}w^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)]$$
$$= \sum_{\kappa k \pi q} (-1)^{\kappa-\pi+k-q+A+D+2s}[\kappa_1,\kappa_2,\kappa,k_1,k_2,k]^{\frac{1}{2}}$$
$$\times \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa \\ \pi_1 & \pi_2 & -\pi \end{pmatrix} \begin{Bmatrix} \kappa_1 & \kappa_2 & \kappa \\ s & s & s \end{Bmatrix}$$
$$\times \Bigg[\delta(B,C)(-1)^{k_1+k_2+\kappa_1+\kappa_2} \begin{Bmatrix} k_1 & k_2 & k \\ D & A & B \end{Bmatrix} {}^{\mp}w^{(\kappa k)}_{\pi q}(A,D)$$
$$\pm \delta(A,D) \begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} {}^{\mp}w^{(\kappa k)}_{\pi q}(B,C)$$
$$\pm \delta(B,D)(-1)^{\kappa_1+k_1} \begin{Bmatrix} k_1 & k_2 & k \\ C & A & B \end{Bmatrix} {}^{\mp}w^{(\kappa k)}_{\pi q}(A,C)$$
$$+ \delta(A,C) \begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} {}^{\mp}w^{(\kappa k)}_{\pi q}(B,D) \Bigg] \tag{5a}$$

and

$$[^{-}w^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B),\, ^{\pm}w^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)]$$
$$= \sum_{\kappa k \pi q} (-1)^{\kappa-\pi+k-q+A+D+2s}[\kappa_1,\kappa_2,\kappa,k_1,k_2,k]^{\frac{1}{2}}$$
$$\times \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa \\ \pi_1 & \pi_2 & -\pi \end{pmatrix} \begin{Bmatrix} \kappa_1 & \kappa_2 & \kappa \\ s & s & s \end{Bmatrix}$$
$$\times \Bigg[\delta(B,C)(-1)^{k_1+k_2+\kappa_1+\kappa_2} \begin{Bmatrix} k_1 & k_2 & k \\ D & A & B \end{Bmatrix} {}^{\pm}w^{(\kappa k)}_{\pi q}(A,D)$$
$$\mp \delta(A,D) \begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} {}^{\pm}w^{(\kappa k)}_{\pi q}(B,C)$$
$$\pm \delta(B,D)(-1)^{\kappa_1+k_1} \begin{Bmatrix} k_1 & k_2 & k \\ C & A & B \end{Bmatrix} {}^{\pm}w^{(\kappa k)}_{\pi q}(A,C)$$
$$- \delta(A,C)(-1)^{\kappa_2+k_2} \begin{Bmatrix} k_1 & k_2 & k \\ D & B & A \end{Bmatrix} {}^{\pm}w^{(\kappa k)}_{\pi q}(B,D) \Bigg]. \tag{5b}$$

We note that the set $^{-}\mathbf{w}^{(\kappa k)}(A,B)$ is closed under commutation, but that the set $^{+}\mathbf{w}^{(\kappa k)}(A,B)$ is, in general, not closed, in the sense that its commutators can produce terms of the form $^{-}\mathbf{w}^{(\kappa k)}(A,B)$, etc. We could, of course, choose different sets; e.g., for two configurations the set $^{+}\mathbf{w}^{(\kappa k)}(A,B)$ $(A \neq B)$ and $\mathbf{w}^{(\kappa k)}(A,A)$, $\mathbf{w}^{(\kappa k)}(B,B)$ $(\kappa + k$ odd) will be closed, but we hope to demonstrate shortly that the set of all $^{-}\mathbf{w}^{(\kappa k)}(A,B)$ is the correct choice for all mixed configurations.

The choices

$$^{-}\mathbf{w}^{(\kappa k)}(A,B) = \mathbf{w}^{(\kappa k)}(A,B) - (-1)^{\kappa+k}\mathbf{w}^{(\kappa k)}(B,A), \tag{6a}$$
$$^{-}\mathbf{w}^{(\kappa k)}(A,B) = \mathbf{w}^{(\kappa k)}(A,B) - (-1)^{A+B+\kappa+k}\mathbf{w}^{(\kappa k)}(B,A), \tag{6b}$$
$$^{+}\mathbf{w}^{(\kappa k)}(A,B) = \mathbf{w}^{(\kappa k)}(A,B) + \mathbf{w}^{(\kappa k)}(B,A) \tag{6c}$$

have been taken by Feneuille,[3] Morrison,[4] and Elliott,[2] respectively. Alper and Sinanoğlu[5] have also used (6c) in their recent work on R_4. The above choices all have their disadvantages. It is shown in the next section that Eq. (6a) does not contain the generators of the group R_4, but is equivalent to that of Eq. (4) where orbitals of the same parity are involved. The choice of Eq. (6b) is equivalent to that of Eq. (4) for integral A and B, but does not reduce to Judd's operators[1] for half-integral values of A and B. The linear combination given in Eq. (6c) must be rejected, as it fails to close under commutation.

The linear combinations defined by Eq. (4) satisfy the closure requirements in all cases, yield the appropriate generators for R_4 as a subgroup and will correctly reduce to the special cases studied by Judd,[1] Feneuille,[3] and Morrison.[4]

Later, we shall have occasion to use both the operators $\mathbf{w}^{(\kappa k)}_i(A,B)$ and

$$\mathbf{W}^{(\kappa k)}(A,B) \equiv \sum_i \mathbf{w}^{(\kappa k)}_i(A,B),$$

where $\mathbf{w}^{(\kappa k)}_i(A,B)$ is the operator that acts only between states of the ith electron and $\mathbf{W}^{(\kappa k)}(A,B)$ acts between states of all electrons. Both sets of operators satisfy the commutation relations Eqs. (3) and (5). It is easily shown that $\mathbf{w}^{(0k)}(A,B) \equiv 2^{-\frac{1}{2}}\mathbf{v}^{(k)}(A,B)$ and all the commutation relations given in terms of $\mathbf{w}^{(0k)}(A,B)$ may be reduced to those for $\mathbf{v}^{(k)}(A,B)$ by omitting the quantum numbers dependent on spin.

3. INFINITESIMAL OPERATORS FOR R_4

We now wish to use the properties of the $\mathbf{v}^{(k)}(A,B)$ tensor operators to construct a set of infinitesimal operators for the 4-dimensional rotation group R_4

which leave invariant the quadratic form $x_1^2 + x_2^2 + x_3^2 + x_4^2$. The Lie algebra for R_4 may be defined in terms of six infinitesimal operators[6]

$$J_{\lambda\mu} = i\left(x_\mu \frac{\partial}{\partial x_\lambda} - x_\lambda \frac{\partial}{\partial x_\mu}\right), \quad \lambda, \mu = 1, 2, 3, 4. \quad (7)$$

Putting

$$J_0 = J_{23}, \quad J_{\pm 1} = (\pm\sqrt{2})(J_{31} \pm iJ_{12}),$$
$$N_0 = J_{41}, \quad N_{\pm 1} = (\pm\sqrt{2})(J_{42} \pm iJ_{43})$$

leads to the set of commutation relations

$$[J_i, J_j] = -\epsilon_{ijk}J_k = [N_i, N_j],$$
$$[J_i, N_j] = -\epsilon_{ijk}N_k. \quad (8)$$

Now, we obtain two sets of operators which satisfy these commutation relations and at the same time fix the phases of our ${}^{-}\mathbf{V}^{(k)}(A, B)$ operators.

It is well known that not only $\mathbf{L} = (1/\hbar)r \times p$, but also the Runge–Lenz vector[7]

$$\mathbf{A} = \left(\frac{z^2e^4m}{-2h^2E}\right)^{\frac{1}{2}}\left(\frac{1}{2Ze^2mh}(\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) + \frac{\mathbf{r}}{r}\right) \quad (9)$$

commute with the hydrogenic Hamiltonian. The matrix elements of $\mathbf{A}$ between single-electron states may be calculated following Biedenharn[8] or from first principles to give

$$\langle nlm|\, A_Z \,|nl'm'\rangle = \langle nl'm'|\, A_Z \,|nlm\rangle = \left(\frac{(n-l-1)(n+l+1)(l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right)^{\frac{1}{2}}. \quad (10)$$

Using this result, we may readily show that

$$\mathbf{A} = \sum_{l=0}^{n-2}[(n-l-1)(n+l+1)(l+1)/3]^{\frac{1}{2}} \times [\mathbf{V}^{(1)}(l, l+1) - \mathbf{V}^{(1)}(l+1, l)]. \quad (11)$$

This, taken with the known result[2]

$$\mathbf{L} = \sum_{l=0}^{n-1}[l(l+1)(2l+1)/3]^{\frac{1}{2}}\mathbf{V}^{(1)}(l, l), \quad (12)$$

gives us a set of six operators that satisfy the commutation relations of Eq. (8). The phase choice for $\mathbf{A}$ means that $\mathbf{A}$ is a simple linear combination of the ${}^{-}\mathbf{V}^{(1)}(l, l')$ operators defined in Eq. (4). Other choices of phases make it impossible to form an operator $\mathbf{A}$ out of the operators of the large rotation group formed by the set of all ${}^{-}\mathbf{V}^{(k)}(l, l')$ operators. We must now take up the study of these larger groups.

4. CONSTRUCTION OF ROOT FIGURES USING $\mathbf{V}^{(k)}(A, B)$ AND $\mathbf{W}^{(\kappa k)}(A, B)$ OPERATORS

In this section we largely follow the arguments of Chaps. 5 and 6 of Judd's text[1] and construct root figures using general sets of the operators $\mathbf{V}^{(k)}(A, B)$ and $\mathbf{W}^{(\kappa k)}(A, B)$. These operators for $A, B, \cdots, F = l_1, l_2, \cdots, l_n$ form the infinitesimal operators of the groups U_X and U_{2X}, respectively, where

$$X = \sum_{l=1}^{n}(2l_i + 1)$$

and l is integral or half-integral.

First, let us consider the case of the $\mathbf{V}^{(k)}(A, B)$ type operators. Using the methods of Jucys *et al.*,[9] we may show that the linear combinations

$$\Gamma_{ab}(A, B) = \sum_{k,q}(-1)^{A-a}[k]^{\frac{1}{2}}\begin{pmatrix} A & k & B \\ -a & q & b \end{pmatrix}V_q^{(k)}(A, B) \quad (13)$$

satisfy the commutation relations

$$[\Gamma_{ab}(A, B), \Gamma_{cd}(C, D)] = \delta(B, C)\delta(b, c)\Gamma_{ad}(A, D) - \delta(A, D)\delta(a, d)\Gamma_{cb}(C, B). \quad (14)$$

The self-commuting Weyl operators[10] $H_{I,i} = \Gamma_{ii}(I, I)$ have eigenvalues $0, \pm 1$ to give us the roots

$$\pm\mathbf{e}_{Aa} \pm \mathbf{e}_{Bb}$$

with $\Gamma_{ab}(A, B)$, these roots being appropriate to U_X.

The subgroups of U_X formed by the set of tensors ${}^{-}\mathbf{V}^{(k)}(A, B)$ are a somewhat more complicated problem. We define the linear combination

$$\Theta_{ab}(A, B) = \sum_{k,q}[k]^{\frac{1}{2}}(-1)^{A-a}\begin{pmatrix} A & k & B \\ -a & q & b \end{pmatrix}{}^{-}V^{(k)}(A, B), \quad (15)$$

giving

$$\Theta_{ab}(A, B) = (-1)^{A+B+a+b+1}\Theta_{-b-a}(B, A),$$

which are, therefore, not all linearly independent for $A \equiv B$. Forming the commutator gives

$$[\Theta_{ab}(A, B), \Theta_{cd}(C, D)] = \delta(B, C)\delta(b, c)\Theta_{ad}(A, D) - \delta(A, D)\delta(a, d)\Theta_{cb}(C, B) + (-1)^{A+B+a+b+1}\{\delta(A, C)\delta(-a, c)\Theta_{-bd}(B, D) - \delta(B, D)\delta(-b, d)\Theta_{c-a}(C, A)\}. \quad (16)$$

It can easily be shown that the operators $H_{I,i} = \Theta_{ii}(I, I)$ with $i > 0$ acting on the remaining operators $\Theta_{ab}(A, B)$, with $a \neq 0 \neq b$, yield all the roots

$$\pm\mathbf{e}_{Aa} \pm \mathbf{e}_{Bb}.$$

For the case where the angular momentum set $A, B, \cdots$ is half-integral, the set of roots includes the

roots $\pm 2\mathbf{e}_{Aa}$ coming from

$$\Theta_{a-a}(A, A) = (-1)^{2A+1}\Theta_{-aa}(A, A)$$

for $a \neq 0$. The complete set of roots then gives the customary root figures for the symplectic group Sp_X where X is an even integer.

In the case of the rotation group R_X, the roots $\pm 2\mathbf{e}_{Aa}$ do not occur, since $(-1)^{2A+1} = -1$. However, there remain operators of the form $\Theta_{a0}(A, B)$ with $a \neq 0$ and $\Theta_{00}(A, B) = -\Theta_{00}(BA)$ (hence, $A \neq B$). We must complement the above Weyl operators $H_{I,i}$ with a set $H_{IJ} = (-1)^{\frac{1}{2}(A+B+1)}\Theta_{00}(A, B)$,

$$(-1)^{\frac{1}{2}(C+D+1)}\Theta_{00}(C, D),$$

etc., which satisfy $H_{IJ} = H_{JI}$. [It will be noted that we must have this phase choice which often leads to imaginary operators but real roots. The simplest case for which this occurs is for $(s + d)^n$ when the characters of R_6 are complex.] The operators

$$\Theta_{i0}(C, A) \pm (-1)^{\frac{1}{2}(A+B+1)}\Theta_{i0}(C, B)$$

with $C \neq 0$ give the roots $\pm\mathbf{e}_{AB}$ $\pm\mathbf{e}_{Cc}$. For every set of four angular momenta A, B, C, D, etc., considered, we must also have the combinations

$$\Theta_{00}(C, A) \pm (-1)^{\frac{1}{2}(A+B+1)}\Theta_{00}(C, B) + (-1)^{\frac{1}{2}(C+D+1)}[\Theta_{00}(D, A) \pm (-1)^{\frac{1}{2}(A+B+1)}\Theta_{00}(D, B)]$$

and

$$\Theta_{00}(C, A) \pm (-1)^{\frac{1}{2}(A+B+1)}\Theta_{00}(C, B) - (-1)^{\frac{1}{2}(C+D+1)}[\Theta_{00}(D, A) \pm (-1)^{\frac{1}{2}(A+B+1)}\Theta_{00}(D, B)]$$

which gives the roots $\pm\mathbf{e}_{AB}$ $\pm\mathbf{e}_{CD}$. This completes the root figure for the even-dimensional rotation groups. In the case of an odd number of angular momenta, we have finally the operators $\Theta_{a0}(A, L)$ and $\Theta_{00}(L, A) \pm (-1)^{\frac{1}{2}(A+B+1)}\Theta_{00}(L, B)$, giving the roots $\pm\mathbf{e}_{Aa}$ and $\pm\mathbf{e}_{AB}$ required for the root figure of the odd-dimensional rotation group.

Now, let us consider the $\mathbf{W}^{(\kappa k)}(A, B)$ operators. In a similar fashion to the above, we define the operators

$$\Theta_{\alpha\beta ab}(AB) = \sum_{\kappa,k,\pi,q} (-1)^{s-m_s+A-a}[\kappa, k]^{\frac{1}{2}} \times \begin{pmatrix} s & \kappa & s \\ -\alpha & \pi & \beta \end{pmatrix}\begin{pmatrix} A & k & B \\ -a & q & b \end{pmatrix} \times {}^{-}W^{(\kappa k)}_{\pi q}(A, B). \quad (17)$$

These lead to the establishment of the root figure for Sp_{2X}. Several choices exist for the phases of the Weyl H operators. We shall choose

$$H_{Aa} = \Theta_{\frac{1}{2}\frac{1}{2}aa}(A, A), \quad -A \leq a \leq A.$$

This choice is made so that

$$\sum_{A,a} H_{Aa} = 2^{\frac{1}{2}} \sum_{A} [A]^{\frac{1}{2}} W^{(10)}_{00}(A, A) = 2S_z,$$

thus ensuring that the function of highest weight belonging to a representation of Sp_{2X} will have the highest possible spin.

5. CASIMIR'S OPERATORS AND EIGENVALUES

The structure constants $c^{\tau}_{\sigma\rho}$ of a group are defined by the commutation properties of the infinitesimal operators X_σ, viz.,

$$[X_\sigma, X_\rho] = \sum_{\tau} c^{\tau}_{\sigma\rho} X_\tau .$$

The metric tensor $g_{\sigma\lambda}$ is obtained in terms of the structure constants as[1]

$$g_{\sigma\lambda} = c^{\tau}_{\sigma\rho} c^{\rho}_{\tau\lambda} .$$

For semisimple groups the metric tensor has its inverse $g^{\rho\lambda} = (g_{\sigma\lambda})^{-1}$ and the Casimir operator[11] G is defined as

$$G = g^{\rho\lambda} X_\rho X_\lambda .$$

From its construction, it is evident that G commutes with all the operators of the group. Racah[12] has shown that the eigenvalues of the Casimir operator may be expressed in the form $\mathbf{K}^2 - \mathbf{R}^2$ where $\mathbf{R} = \frac{1}{2}\sum \boldsymbol{\alpha}^+$ and $K_i = R_i + w_i$, with $\boldsymbol{\alpha}^+$ being a positive root and w_i the ith component of the highest weight of the representation.

The eigenvalues λ_w of the Casimir operator $G(R_n)$, $n = 2\nu$ or $2\nu + 1$, or of $G(Sp_n)$, $n = 2\nu$, may be found by acting the Casimir operator on the eigenket $|W\rangle \equiv |w_1 \cdots w_\nu\rangle$ which forms a basis for the representation $[w_1 \cdots w_\nu]$ of R_n or $\langle w_1 \cdots w_\nu\rangle$ of Sp_n to yield for R_n,

$$\lambda_w = \frac{1}{2(n-2)} \sum_{i=1}^{\nu} w_i(w_i + n - 2i), \quad (18)$$

and for Sp_n,

$$\lambda_w = \frac{1}{2(n-2)} \sum_{i=1}^{\nu} w_i(w_i + n - 2i + 2). \quad (19)$$

The Casimir operator may be conveniently expressed in terms of the operators defined in Eq. (15) (for R_X or Sp_X) as

$$2(X-2)G = \tfrac{1}{2}\sum_{A,B}\sum_{a,b} \Theta_{ab}(A, B)\Theta_{ba}(B, A) \quad (20)$$

$$= 2\sum_{A}\sum_{k\,\text{odd}} (\mathbf{V}^{(k)}(A, A))^2 + (-1)^{k+1}\sum_{A<B}\sum_{k} ({}^{-}\mathbf{V}^{(k)}(A, B))^2, \quad (21)$$

and for Sp_{2X} we use the operators of Eq. (17) to obtain

$$\begin{aligned}4(X-1)G(Sp_{2X}) &= \tfrac{1}{2}\sum_{A,B}\sum_{a,b}\sum_{\alpha,\beta}\Theta_{\alpha\beta ab}(A,B)\Theta_{\beta\alpha ba}(B,A)\\ &= 2\sum_{A}\sum_{\kappa,k}(\mathbf{W}^{(\kappa k)}(A,A))^2\\ &\quad+(-1)^{\kappa+k+1}\sum_{A<B}\sum_{\kappa,k}(^{-}\mathbf{W}^{(\kappa k)}(A,B))^2, \quad (22)\end{aligned}$$

where $\kappa + k$ is *odd* in the first summation.

The above results are useful for constructing eigenfunctions symmetrized with respect to the relevant representations of the transformation group used to classify the multiconfiguration states.

6. TRANSFORMATION PROPERTIES OF STATES AND OPERATORS

In this section, we derive a correspondence between the transformation properties of the $^{\pm}W^{(\kappa k)}_{\pi q}(A,B)$ operators and the symmetric and antisymmetric combinations of two particle states.

Following Fano and Racah,[13] we denote the vector coupled states of particle 1 in orbital A and particle 2 in orbital B, coupled to spin and orbital ranks κ and k with z projections π and q, respectively, by $(12\,|\,AB\kappa k\pi q\rangle$. We then define the symmetric (+) and antisymmetric (−) combinations as

$$|AB\kappa k\pi q\rangle^{\pm} = (12\,|\,AB\kappa k\pi q\rangle \pm (21\,|\,AB\kappa k\pi q\rangle. \quad (23)$$

Acting $^{-}W^{(\kappa_1 k_1)}_{\pi_1 q_1}$ on a ket $|CD\kappa_2 k_2\pi_2 q_2\rangle^{\pm}$ gives a result equivalent to the commutator

$$[^{-}W^{(\kappa_1 k_1)}_{\pi_1 q_1}(A,B),\ ^{\mp}W^{(\kappa_2 k_2)}_{\pi_2 q_2}(C,D)]$$

and thus proves that the operators $^{\pm}W^{(\kappa k)}_{\pi q}(A,B)$ have the same symmetry transformation properties under the operations of Sp_{2X} and its subgroups as the 2-particle states $|AB\kappa k\pi q\rangle^{\mp}$, i.e., the operators $^{+}W^{(\kappa k)}_{\pi q}(A,B)$ transform like fermions and the $^{-}W^{(\kappa k)}_{\pi q}(A,B)$ like bosons.

As the operators $^{+}\mathbf{W}^{(\kappa k)}(A,B)$ transform the sets $^{+}\mathbf{W}^{(\kappa k)}(A,B)$ and $^{-}\mathbf{W}^{(\kappa k)}(A,B)$ into each other, it is apparent that they must, together, span a single representation $\{\lambda\}$ of the unitary group U_{2X}. The operators connect states of the same number of particles, and so we have

$$\{\lambda\}\{1^n\} \supset \{1^n\} \quad \text{for all } n.$$

Thus,

$$\{1^n\}\{1^n\}^* \equiv \{1^n\}\{1^{2X-n}\} \supset \{\lambda\}.$$

We find that the complete set of tensors $\mathbf{W}^{(\kappa k)}(A,B)$ transform as the $\{21^{2X-2}0\}$ representation of U_{2X} with the exception of the scalar operator

$$\sum_{A}[A]^{\frac{1}{2}}W^{(00)}_{00}(A,A)$$

which transforms as $\{0\}$.

We have the branching rules for $U_{2X} \to Sp_{2X}$:

$$\{21^{2X-2}0\} \to \langle 2\rangle + \langle 11\rangle,$$
$$\{0\} \to \langle 0\rangle. \quad (24)$$

Similar comments will apply to the set of tensors $\mathbf{V}^{(k)}(A,B)$ under the operators of U_X. The branching rule

$$\{21^{X-2}0\} \to [2] + [11] \quad (25)$$

is then required.

The transformation properties of the 2-particle states and single-particle operators have been found to be very similar. When states or operators are coupled, care must be taken to ensure correct normalization. We therefore adopt the combinations

$$2^{-\frac{1}{2}}\,|AB\kappa k\pi q\rangle^{\pm} \quad \text{and} \quad (2^{-\frac{1}{2}})\,^{\pm}W^{(\kappa k)}_{\pi q}(A,B), \quad A \neq B, \quad (26)$$

and

$$\tfrac{1}{2}\,|AA\kappa k\pi q\rangle^{\pm} \equiv |AA\kappa k\pi q\rangle$$

and

$$\tfrac{1}{2}\,^{\pm}W^{(\kappa k)}_{\pi q}(A,A) \equiv W^{(\kappa k)}_{\pi q}(AA). \quad (27)$$

An example of the use of coupling the normalized operators for the Coulomb interaction in the R_4 scheme will be given in a later paper.

7. GENERAL CLASSIFICATION SCHEMES

The algebra of the generalized Racah tensors gives a powerful tool for studying the properties of mixed configurations. The nucleon configurations $(s+d)^N$ have been studied by Elliott[2] using the scheme

$$U_{24} \to SU_4 \times (SU_6 \to SU_3 \to R_3),$$

while Feneuille[3] has studied the equivalent problem for electron configurations, but using the alternative scheme

$$U_{12} \to Sp_{12} \to SU_2 \times (R_6 \to R_5 \to R_3).$$

This latter scheme is of dubious physical significance in atoms since it fails to mix the eigenfunctions of the ^1D states of the d^2 and ds configurations which are known to couple strongly.

The chain of groups

$$U_{2n^2} \to Sp_{2n^2} \to SU_2 \times (R_{n^2} \to R_4 \to R_3) \quad (28)$$

is useful in studying electrons moving in a Coulomb field, where in the case of the nonrelativistic hydrogen atom the orbitals associated with the principal quantum number n are all degenerate. In this scheme, the single particle eigenfunctions transform as

$$|\{1\}\langle 1\rangle S[10\cdots 0][n-1,0]LM_SM_L\rangle,$$

TABLE I. Decompositions of irreducible representations for $Sp_{18} \to SU_2 \times R_9$.

$f^{\langle\lambda\rangle}$	Sp_{18}	$SU_2 \times R_9$
1	0	^{1}[0000]
18	1	^{2}[1000]
152	2	^{3}[1100]^1[2000]
798	3	^{4}[1110]^2[2100]
2907	4	^{5}[1111]^3[2110]^1[2200]
7752	5	^{6}[1111]^4[2111]^2[2210]
15504	6	^{7}[1110]^5[2111]^3[2211]^1[2220]
23256	7	^{8}[1100]^6[2110]^4[2211]^2[2221]
25194	8	^{9}[1000]^7[2100]^5[2210]^3[2221]^1[2222]
16796	9	^{10}[0000]^8[2000]^6[2200]^4[2220]^2[2222]

where $L = 0, 1, \cdots, n$ and the group labels are written in the order indicated by Eq. (28), using the bracket notation of Littlewood.[14]

In the particular case of $n = 3$, which arises in the classification of the states of the $(3s + 3p + 3d)^n$ configurations, we need to use the group scheme

$$U_{18} \to Sp_{18} \to SU_2 \times (R_9 \to R_4 \to R_3). \quad (29)$$

The branching rules for $Sp_{18} \to SU_2 \times R_9$ and $R_9 \to O_4$ are given in Tables I and II, respectively. The latter branching rules were easily evaluated in terms of the plethysm[14]

$$[20] \otimes [\lambda] \equiv (\{2\} - \{0\}) \otimes [\lambda].$$

A full description of this method has been given elsewhere.[15] To complete the classification, we note that under $O_4 \to R_4$

$$[pq]' \to [pq] + [p - q], \quad q > 0,$$
$$[p0]' \to [p0],$$

while under $R_4 \to R_3$,

$$[pq] \to p, p - 1, \cdots, |q|.$$

We note that the problem of duplicated R_4 representations in the $R_9 \to R_4$ branching rules becomes appreciable for all but the simplest R_9 representations. The situation will obviously worsen as configurations involving higher values of the principal quantum number n are considered.

8. THE COULOMB INTERACTION

After the states of a mixed configuration have been classified by their transformation properties under a chain of groups, it is desirable to partition the Hamiltonian into parts which have well-defined transformation properties under the same group chain. Now, we consider in general terms the Coulomb repulsion.

The Coulomb interaction between electrons may be written in the form

$$H_c = \sum_{i>j}^{N} \frac{e^2}{r_{ij}} = e^2 \sum_k \sum_{i>j}^{N} \frac{r_<^k}{r_>^{k+1}} (\mathbf{C}_i^{(k)} \cdot \mathbf{C}_j^{(k)}), \quad (30)$$

where

$$\mathbf{C}_i^{(k)} = \sum_{A,B} (-1)^A \begin{pmatrix} A & k & B \\ 0 & 0 & 0 \end{pmatrix} [A, B]^{\frac{1}{2}} [k]^{-\frac{1}{2}} \mathbf{v}_i^{(k)}(A, B)$$
$$= \tfrac{1}{2} \sum_{A,B} (-1)^A \begin{pmatrix} A & k & B \\ 0 & 0 & 0 \end{pmatrix} [A, B]^{\frac{1}{2}} [k]^{-\frac{1}{2}}$$
$$\times (\mathbf{v}_i^{(k)}(A, B) + (-1)^{A-B} \mathbf{v}_i^{(k)}(B, A)). \quad (31)$$

Because $A + k + B$ is even, we have a sum of operators of the form ${}^p\mathbf{v}_i^{(k)}(A, B)$, where p is the parity of k, which is the same as that of $A - B$.

Using

$$(\mathbf{V}^{(k)}(A, B) \cdot \mathbf{V}^{(k)}(C, D))$$
$$= \sum_{i \neq j} (\mathbf{v}_i^{(k)}(A, B) \cdot \mathbf{v}_j^{(k)}(C, D))$$
$$+ \delta(A, D)\delta(B, C)(-1)^{A-B}[k][A]^{-\frac{1}{2}} V_0^{(0)}(A, A), \quad (32)$$

we obtain

$$H_c = \tfrac{1}{4} \sum_k \sum_{A,B,C,D} R^{(k)}(AB; CD)(-1)^{A+B}$$
$$\times [A, B, C, D]^{\frac{1}{2}} [k]^{-1} \begin{pmatrix} A & k & C \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} B & k & D \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times [({}^p\mathbf{V}^{(k)}(A, C) \cdot {}^p\mathbf{V}^{(k)}(B, D))$$
$$- 2\delta(A, D)\delta(B, C) V_0^{(0)}(A, A)], \quad (33)$$

TABLE II. Decompositions of irreducible representations for $R_9 \to R_4$

$f^{[\lambda]}$	R_9	O_4
1	[0000]	[00]
9	[1000]	[20]
36	[1100]	[31][11]
84	[1110]	[40][33][31][20][11]
126	[1111]	[42][40][31][22][20]^2[00]
44	[2000]	[40][22][20]
231	[2100]	[51][42][40][31]^2[22][20]^2[11]
594	[2110]	[60][53][51]^2[42]^2[40]^3[33][31]^4[22][20]^4[11]^2
924	[2111]	[62][60][53][51]^3[44][42]^3[40]^5[33][31]^5[22]^3 [20]^5[11]^2[00]
495	[2200]	[62][60][51][44][42]^2[40]^3[31]^2[22]^2[20]^3[00]^2
1650	[2210]	[71][64][62]^2[60]^3[53]^2[51]^4[44][42]^5[40]^3 [33]^2[31]^6[22]^3[20]^7[11]^2[00]^2
2772	[2211]	[73][71]^2[64][62]^3[60]^4[55][53]^4[51]^3[44][42]^7 [40]^{10}[33]^4[31]^{11}[22]^3[20]^8[11]^5
1980	[2220]	[80][73][71][66][64][62]^2[60]^4[53]^2[51]^4[44]^2 [42]^5[40]^3[33]^2[31]^5[22]^3[20]^6[11][00]^3
4158	[2221]	[82][80][75][73]^2[71]^3[64]^2[62]^5[60]^7[55] [53]^6[51]^{10}[44]^2[42]^9[40]^{12}[33]^4[31]^{12}[22]^4 [20]^9[11]^4[00]
2772	[2222]	[84][82][80][73][71]^2[64]^2[62]^4[60]^4[55][53]^3 [51]^6[44]^2[42]^6[40]^3[33][31]^5[22]^4[20]^6[11] [00]

where the $R^{(k)}(AB; CD)$ are the usual Condon and Shortley radial integrals.[16]

For a set of configurations involving orbitals of the same parity, all of the operators appearing in Eq. (33) are of the form ${}^{+}\mathbf{V}^{(k)}(A, B)$, which transform like the antisymmetric 2-particle states constructed from the same set of orbitals. This result is entirely analogous to that known for a single configuration! However, for configurations involving orbitals of differing parities, we have also the set of tensors ${}^{-}\mathbf{V}^{(k)}(A, B)$, $A \neq B$, to consider. These tensors, unlike those of ${}^{+}\mathbf{V}^{(k)}(A, B)$, are generators of the group R_X and as such preserve the representation label of R_X as a "good" quantum number.

9. CONCLUSIONS

Our chief object has been to remove some of the confusion that exists in the literature concerning the application of continuous groups in atomic spectroscopy and to recast some known results in a more general form. The phase choice for the linear combinations of the $\mathbf{W}^{(\kappa k)}(A, B)$ tensors has been defined to allow the construction of the root figures of the groups R_X and Sp_X for all cases. The Casimir operators of the relevant groups have been derived in terms of the tensorial forms of the group generators and the transformation properties of states and operators derived.

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[1] B. R. Judd, *Operator Techniques in Atomic Spectroscopy* (McGraw-Hill, New York, 1962).
[2] J. P. Elliott, Proc. Roy. Soc. (London) **A245**, 128 (1958).
[3] S. Feneuille, J. Phys. **28**, 61, 315 (1967).
[4] J. C. Morrison, J. Math. Phys. **10**, 1431 (1969).
[5] J. S. Alper and O. Sinanoğlu, Phys. Rev **177**, 77 (1969).
[6] W. Pauli, Ergeb. Exakt. Naturw. **37**, 85 (1965).
[7] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), 3rd ed.
[8] L. C. Biedenharn, J. Math. Phys. **2**, 433 (1961).
[9] A. Jucys, J. Levinsonas, and V. Vanagas, *Mathematical Apparatus of the Theory of Angular Momentum* (Vilna, 1960). A translation by Sen and Sen has been published in the Israel Program for Scientific Translations (Jerusalem, 1962).
[10] H. Weyl, Math. Z. **23**, 271 (1925).
[11] H. Casimir, Proc. Koninkl. Akad. Amsterdam **34**, 844 (1931).
[12] G. Racah, Ergeb. Exakt. Naturw. **37**, 28 (1965).
[13] U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic, New York, 1959).
[14] D. E. Littlewood, *The Theory of Group Characters* (Oxford U.P., London, 1950), 2nd ed.
[15] B. G. Wybourne, *Symmetry Principles and Atomic Spectroscopy* (Wiley, New York, 1970).
[16] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Oxford U.P., New York, 1950), 2nd ed.

Is the Group R_4 an Approximate Symmetry for Many-Electron Theory?*

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The 4-dimensional rotation group R_4 is used to analyze the structure of the $(2s + 2p)^N$ shell and to determine the relevance, if any, of the R_4 group as an approximate symmetry group for many-electron theory. It is found that while the R_4 symmetrized states of the $(2s + 2p)^N$ complex approximately diagonalize the Coulomb energy matrix for interactions within the complex, the inclusion of the inner $1s^2$ shell effects leads to a large symmetry violating term, which invalidates the R_4 group as an approximate symmetry for many-electron theory.

I. INTRODUCTION

It is well known that the energy levels of a hydrogen atom, in the nonrelativistic approximation, may be grouped in the series

$$1s;\ 2s,\ 2p;\ 3s,\ 3p,\ 3d;\ 4s,\ 4p,\ 4d,\ 4f;\cdots \qquad (1)$$

with orbitals having the same principal quantum number n, having a total orbital degeneracy of n^2. Fock[1] and Bargmann[2] have shown that for the bound states of a single electron moving in a pure Coulomb potential, the group appropriate to the symmetry description of the Hamiltonian is the rotation group in four dimensions R_4. Indeed, the orbital eigenfunctions associated with the principal quantum number n span the n^2-dimensional representation $[n-1, 0]$ of R_4. Perelomov and Popov[3] have shown that the symmetry of both the discrete and continuous spectra of the hydrogen atom may be described in terms of the noncompact homogeneous Lorentz group $O(3, 1)$. Here, we shall restrict our attention to the bound states only and thus only R_4 will be considered.

It is of some interest to examine the role of the R_4 group, if any, in the many-electron theory of atoms. In Layzer's[4–6] development of the theory of complex spectra the "*complex of configurations*" involving a definite set of principal quantum numbers, n and parity played a central role. His definition of a complex derives ultimately from the degeneracies associated with the hydrogen atom. Moshinsky,[7] following upon the work of Biedenharn,[8] has suggested that the group R_4 could be used as a starting point for treating the electron correlation problem. Wulfman[9] has suggested that the doubly excited helium metastable states, studied by Lipsky and Russek,[10] may be usefully labeled according to the representations of the group R_4.

More recently Alper and Sinanoğlu[11,12] have made a detailed study of the role of the group R_4 in the many-electron theory of atomic structure giving particular attention to the Coulomb interaction in the $(2s + 2p)^N$ and $(3s + 3p + 3d)^N$ configurations. They have concluded that the group R_4 does indeed have relevance as an approximate symmetry in many electron systems and that it clearly exposes the Z and N dependence of the nondynamical electron correlation.

In the present paper, we wish to examine the significance of the R_4 group as an approximate symmetry group for the Coulomb interaction of a many-electron system. We shall first give a systematic treatment of the group-theoretical properties of the Coulomb interaction in the $(2s + 2p)^N$ complex correcting a number of significant errors of substance in the original work of Alper and Sinanoğlu and then consider the question, "Is the group R_4 an approximate symmetry for many electron theory?"

II. INFINITESIMAL OPERATORS OF R_4

The transformations of the group R_4 leave invariant the quadratic form $x_1^2 + x_2^2 + x_4^2 + x_3^2$. The Lie algebra for the group R_4 may be defined in terms of the six infinitesimal operators[13]

$$J_{\lambda\mu} = i\left(x_\mu \frac{\partial}{\partial x_\lambda} - x_\lambda \frac{\partial}{\partial x_\mu}\right). \qquad (2)$$

We may write these six operators as components of two spherical tensors $\mathbf{J}^{(1)}$ and $\mathbf{N}^{(1)}$ by putting

$$J_0^{(1)} = J_{23}, \quad J_{\pm 1}^{(1)} = \pm 2^{-\frac{1}{2}}(J_{31} \pm iJ_{12})$$

and

$$N_0^{(1)} = J_{41}, \quad N_{\pm 1}^{(1)} = \pm 2^{-\frac{1}{2}}(J_{42} \pm iJ_{43})$$

to yield the commutation algebra

$$[J_q^{(1)}, J_{q'}^{(1)}] = -\epsilon_{qq'q''}J_{q''}^{(1)} = [N_q^{(1)}, N_{q'}^{(1)}]$$

and

$$[J_q^{(1)}, N_{q'}^{(1)}] = -\epsilon_{qq'q''}N_{q''}^{(1)}. \qquad (3)$$

Let us now introduce single particle tensor operators $\mathbf{w}^{(\kappa k)}(ll')$ and $\mathbf{W}^{(\kappa k)}(ll')$ defined in Ref. 14. Then, if we let

$$\mathbf{J}^{(1)} = \sum_{l=1}^{n-1} a_l \mathbf{v}^{(1)}(ll) \tag{4a}$$

and

$$\mathbf{N}^{(1)} = \sum_{l=0}^{n-2} b_l [\mathbf{v}^{(1)}(l, l+1) - \mathbf{v}^{(1)}(l+1, l)], \tag{4b}$$

where l ranges over all the orbital quantum numbers associated with the designated principal quantum number n, and demand that the commutation rules of Eq. (3) be satisfied. We readily find that the components of the tensor operators

$$\mathbf{J}^{(1)} = \sum_{l=1}^{n-1} [\tfrac{1}{3}(l+1)(2l+1)]^{\frac{1}{2}} \mathbf{v}^{(1)}(ll), \tag{5}$$

$$\mathbf{N}^{(1)} = \sum_{l=0}^{n-2} [\tfrac{1}{3}(n-l-1)(n+l+1)(l+1)]^{\frac{1}{2}} \times [\mathbf{v}^{(1)}(l, l+1) - \mathbf{v}^{(1)}(l+1, l)] \tag{6}$$

will form the infinitesimal operators of R_4. [Note that Alper and Sinanoğlu give the linear combination of tensor operators in Eq. (6) with the opposite sign and thus do not obtain the correct generators for the R_4 group.[14]]

The Weyl[15] self-commuting operators H_1 and H_2 are $J_0^{(1)}$ and $N_0^{(1)}$. The operators

$$E_{\pm 1}^{+} = J_{\pm 1}^{(1)} + N_{\pm 1}^{(1)}, \quad E_{\pm 1}^{-} = J_{\pm 1}^{(1)} - N_{\pm 1}^{(1)} \tag{7}$$

are simultaneous eigenfunctions of H_1 and H_2 and may be used to construct the root figure. The eigenvalues p and q of the operators H_1 and H_2 are used to label the irreducible representations of R_4 after the manner of Racah.[16] p and q are both integers or half-integers with $p \geq |q|$. While p is necessarily positive, q may be positive or negative. In this scheme of labeling, we find upon making the restriction $R_4 \rightarrow R_3$ that

$$[pq] \rightarrow [p] + [p-1] + \cdots + [|q|]. \tag{8}$$

III. GROUP CLASSIFICATION OF STATES

It follows from the above equation that the irreducible representation $[n-1, 0]$ of R_4 decomposes under restriction to R_3 according to the rule

$$[n-1, 0] \rightarrow s + p + d + \cdots + (n-1), \tag{9}$$

where we give the R_3 terms in the usual spectroscopic notation. Thus, the orbital states associated with the principal quantum number n transform together as the $[n-1, 0]$ representation of R_4.

Taking into account the spin of the electron, we would expect the eigenfunctions associated with the distribution of N electrons among the n electron shells associated with the principal quantum number n to transform according to the antisymmetric representation $\{1^N\}$ of U_{2n^2}. Butler and Wybourne[14] have shown that the states associated with the principal quantum number n may be classified using the group chain

$$U_{2n^2} \rightarrow Sp_{2n^2} \rightarrow SU_2 \times [R_{n^2} \rightarrow R_4 \rightarrow R_3], \tag{10}$$

and have given tables for the classification of states associated with $n = 2$ and 3.

The classification is complete for the $(2s + 2p)^N$ complexes but duplications occur as many as eleven times in the $(3s + 3p + 3d)^N$ complexes. Here we shall be primarily concerned with the structure of the $(2s + 2p)^N$ complexes.

IV. CONSTRUCTION OF R_4 SYMMETRIZED STATES

The states of the $(2s + 2p)^N$ complexes may be uniquely labeled by the scheme of quantum numbers

$$|(2s + 2p)^N [pq] SLM_S M_L\rangle,$$

or suppressing the quantum numbers $M_S M_L$, the terms are specified by

$$|(2s + 2p)^N [pq] SL\rangle. \tag{11}$$

We first note that the matrix elements of a scalar 2-particle operator $G = \sum_{i>j}^{N} g_{ij}$ between states of any N electron complex X^N, where $X \equiv l_1 + l_2 + \cdots + l_k$, may be expressed as a linear combination of 2-electron matrix elements in X^2 weighted by the appropriate 2-particle coefficients of fractional parentage to give

$$\begin{aligned}
&\langle X_\alpha^N [pq] SL | \, G \, | X_{\alpha'}^N [pq]' SL\rangle \\
&\quad = \tfrac{1}{2} N(N-1) \sum_{[\overline{pq}]\overline{SL}[pq]'', [pq]''S''L''} \\
&\quad \times \langle X_\alpha^N [pq] SL \{ | \, X^{N-2} [\overline{pq}] \overline{SL}; X^2 [pq]'' S'' L''\rangle \\
&\quad \times \langle X^2 [pq]'' S'' L'' | \, g_{12} \, | X^2 [pq]''' S'' L''\rangle \\
&\quad \times \langle X^{N-2} [\overline{pq}] \overline{SL}; X^2 [pq]''' S'' L' | \} \, X_{\alpha'}^N [pq]' SL\rangle.
\end{aligned} \tag{12}$$

Inspection of the above equation indicates that R_4 symmetry can only be conserved in X^N if the scalar interaction g_{12} is diagonalized in the 2-electron basis $|X^2 [pq] SL\rangle$. Thus the question, "is the group R_4 an approximate symmetry in many-electron theory?," can be answered by investigating the structure of the X^2 configuration alone.

The states symmetrized according to the scheme of Eq. (11) may be expanded as a linear combination of the usual single configuration states. The relevant linear combination may be readily determined either by use of Biedenharn's formula for the R_4

TABLE I. R_4 symmetrized eigenfunctions of $(2s + 2p)^1$ and $(2s + 2p)^2$.

$\|[10]\,^2P\rangle$	$= \|2s\,^2S\rangle$
$\|[10]\,^2S\rangle$	$= -\|2p\,^2P\rangle$
$\|[11]\,^3P\rangle$	$= 2^{-\frac{1}{2}}(\|2p^2\,^3P\rangle + \|2s2p\,^3P\rangle)$
$\|[1-1]\,^3P\rangle$	$= 2^{-\frac{1}{2}}(\|2p^2\,^3P\rangle - \|2s2p\,^3P\rangle)$
$\|[20]\,^1D\rangle$	$= \|2p^2\,^1D\rangle$
$\|[20]\,^1P\rangle$	$= -\|2s2p\,^1P\rangle$
$\|[20]\,^1S\rangle$	$= \frac{1}{2}(3^{\frac{1}{2}})\,\|2s^2\,^1S\rangle - \frac{1}{2}\,\|2p^2\,^1S\rangle$
$\|[00]\,^1S\rangle$	$= \frac{1}{2}\,\|2s^2\,^1S\rangle + \frac{1}{2}(3^{\frac{1}{2}})\,\|2p^2\,^1S\rangle$

Wigner coefficients[8] or by use of his result for the reduced matrix elements of the operator $N^{(1)}$ defined by Eq. (6). Either method readily yields the results of Table I for the $(2s + 2p)$ and $(2s + 2p)^2$ complexes. The phases defined in Biedenharn's paper are identical to those of Condon and Shortley. It is important to notice that with this convention, the phases of the 1-electron states in the R_4 scheme are not simply those of conventional orbitals. Our results differ from those of Wulfman[9] and of Alper and Sinanoğlu[11,12] owing, in the first case, to a numerical error and, in the second, to an incorrect choice of group generators and in the transcription of Biedenharn's results. The difference in phase for the linear combinations of the $|[20]\,^1S\rangle$ and $|[00]\,^1S\rangle$ states is of critical importance in assessing the relevance of R_4 symmetry in many-electron theory, since these are the only states belonging to different R_4 representations that can interact in $(2s + 2p)^2$ and thus give rise to a configuration mixing.

We note that the states $|[11]\,^3P\rangle$ and $|[1-1]\,^3P\rangle$ involve a linear combination of *odd* and *even* parity states. However, we may always form states of well defined parity by forming the linear combinations

$$|[pq]'SL\rangle^{\pm} = 2^{-\frac{1}{2}}(|[pq]SL\rangle \pm |[p-q]SL\rangle), \quad q > 0. \tag{13}$$

There is no difficulty in obtaining the appropriate linear combinations for more complex 2-electron configurations. At this point, it should be noted that the linear combinations given by Alper and Sinanoğlu[11] for $(3s + 3p + 3d)^2$ while forming an orthonormal set do not have consistently defined phases.

V. R_4 SYMMETRIZATION OF THE COULOMB INTERACTION

In a previous paper,[14] we derived the transformation properties of the double-tensor operators $\mathbf{w}^{(\kappa k)}(A, B)$ under the groups of interest here. In Table II we give the transformation properties of the operators using

TABLE II. Symmetrization of 1-particle tensor operators for $(s + p)^N$.

U_8	Sp_8	$SU_2 \times R_4$	$SU_2 \times R_3$	Symmetrized operator
$\{21^6\}$	$\langle 1^2\rangle$	$^3[11]$	^3P	$2^{-\frac{1}{2}}[\mathbf{w}^{(11)}(pp) + \overset{+}{\mathbf{w}}{}^{(11)}(sp)]$
		$^3[1-1]$	^3P	$2^{-\frac{1}{2}}[\mathbf{w}^{(11)}(pp) - \overset{+}{\mathbf{w}}{}^{(11)}(sp)]$
		$^1[20]$	^1D	$\mathbf{w}^{(02)}(pp)$
			^1P	$-\overset{+}{\mathbf{w}}{}^{(01)}(sp)$
			^1S	$\frac{1}{2}(3^{\frac{1}{2}})\mathbf{w}^{(00)}(ss) - \frac{1}{2}\mathbf{w}^{(00)}(pp)$
	$\langle 2\rangle$	$^1[11]$	^1P	$2^{-\frac{1}{2}}[\mathbf{w}^{(01)}(pp) + \bar{\mathbf{w}}^{(01)}(sp)]$
		$^1[1-1]$	^1P	$2^{-\frac{1}{2}}[\mathbf{w}^{(01)}(pp) - \bar{\mathbf{w}}^{(01)}(sp)]$
		$^3[20]$	^3D	$\mathbf{w}^{(12)}(pp)$
			^3P	$-\bar{\mathbf{w}}^{(11)}(sp)$
			^3S	$\frac{1}{2}(3^{\frac{1}{2}})\mathbf{w}^{(10)}(ss) - \frac{1}{2}\mathbf{w}^{(10)}(pp)$
		$^3[00]$	^3S	$\frac{1}{2}\mathbf{w}^{(10)}(ss) + \frac{1}{2}(3^{\frac{1}{2}})\mathbf{w}^{(10)}(pp)$
$\{0\}$	$\langle 0\rangle$	$^1[00]$	^1S	$\frac{1}{2}\mathbf{w}^{(00)}(ss) + \frac{1}{2}(3^{\frac{1}{2}})\mathbf{w}^{(00)}(pp)$

the abbreviation

$$\overset{\pm}{\mathbf{w}}{}^{(\kappa k)}(l, l') = 2^{-\frac{1}{2}}[\mathbf{w}^{(\kappa k)}(l, l') \pm (-1)^{\kappa+k+l-l'}\mathbf{w}^{(\kappa k)}(l', l)].$$

Now the Coulomb interaction may be written

$$\begin{aligned} H_c = &\sum_{i>j} F_0(2s, 2s)[\mathbf{v}_i^{(0)}(ss) \cdot \mathbf{v}_j^{(0)}(ss)] \\ &+ 3F_0(2p, 2p)[\mathbf{v}_i^{(0)}(pp) \cdot \mathbf{v}_j^{(0)}(pp)] \\ &+ 3^{\frac{1}{2}}F_0(2s, 2p)\{[\mathbf{v}_i^{(0)}(ss) \cdot \mathbf{v}_j^{(0)}(pp)] \\ &\qquad + [\mathbf{v}_i^{(0)}(pp) \cdot \mathbf{v}_j^{(0)}(ss)]\} \\ &+ 6F_2(2p, 2p)[\mathbf{v}_i^{(2)}(pp) \cdot \mathbf{v}_j^{(2)}(pp)] \\ &+ 2G_1(2s, 2p)[\bar{\mathbf{v}}_i^{(1)}(sp) \cdot \bar{\mathbf{v}}_j^{(1)}(sp)]. \end{aligned} \tag{14}$$

The Coulomb interaction as written has well-known spin and orbital symmetry—namely scalar—but we wish to split the interaction up into parts of precise R_4 symmetries. This may be done readily, as we know the symmetry of the single operators and the R_4-Wigner coefficients.[8] When coupling, the sum is over all subgroup representations and thus, we must introduce $\overset{+}{\mathbf{v}}{}^{(1)}(sp)$ and $\mathbf{v}^{(1)}(pp)$.

The operators ϵ_k and e_k symmetrized with respect to R_3 and R_4 are given in Tables III and IV. The

TABLE III. R_3 symmetrized operators.

$$\epsilon_0 = \sum_{i>j} (\mathbf{v}_i^{(0)}(ss) \cdot \mathbf{v}_j^{(0)}(ss))$$

$$\epsilon_1 = \sum_{i\neq j} (\mathbf{v}_i^{(0)}(ss) \cdot \mathbf{v}_j^{(0)}(pp))$$

$$\epsilon_2 = \sum_{i>j} (\mathbf{v}_i^{(0)}(pp) \cdot \mathbf{v}_j^{(0)}(pp))$$

$$\epsilon_3 = \sum_{i>j} (\overset{+}{\mathbf{v}}{}^{(1)}(sp) \cdot \overset{+}{\mathbf{v}}{}^{(1)}(sp))$$

$$\epsilon_4 = \sum_{i>j} (\mathbf{v}_i^{(2)}(pp) \cdot \mathbf{v}_j^{(2)}(pp))$$

$$\epsilon_5 = \sum_{i>j} (\bar{\mathbf{v}}_i^{(1)}(sp) \cdot \bar{\mathbf{v}}_j^{(1)}(sp))$$

$$\epsilon_6 = \sum_{i>j} (\mathbf{v}_i^{(1)}(pp) \cdot \mathbf{v}_j^{(1)}(pp))$$

TABLE IV. R_4 symmetrized operators.

Sp_8	R_4	$2S+1_L$	normalization	
$\langle 0\rangle$	[00]	^1S	$\frac{1}{2}$	$e_0=\epsilon_0+3^{\frac{1}{2}}\epsilon_1+3\epsilon_2$
$\langle 22\rangle+\langle 0\rangle$	[00]	^1S	$\frac{1}{6}$	$e_1=3\epsilon_0-3^{\frac{1}{2}}\epsilon_1+\epsilon_2-4\epsilon_3+4\epsilon_4$
$\langle 22\rangle+\langle 0\rangle$	[00]	^1S	$3^{-\frac{1}{2}}$	$e_2=2\epsilon_6+2\epsilon_5$
$\langle 11\rangle$	[20]	^1S	$2(3^{-\frac{1}{2}})$	$e_3=3\epsilon_0+3^{\frac{1}{2}}\epsilon_1-3\epsilon_2$
$\langle 22\rangle+\langle 11\rangle$	[20]	^1S	$2(3^{-\frac{1}{2}})$	$e_4=3\epsilon_0-3^{\frac{1}{2}}\epsilon_1+\epsilon_2-2\epsilon_3-2\epsilon_4$
$\langle 22\rangle+\langle 11\rangle$	[20]	^1S	$2(3^{-\frac{1}{2}})$	$e_5=2\epsilon_6-2\epsilon_5$
$\langle 22\rangle$	[40]	^1S	$6(5^{-\frac{1}{2}})$	$e_6=15\epsilon_0-5(3^{\frac{1}{2}})\epsilon_1+5\epsilon_2+10\epsilon_3+2\epsilon_4$

possible symplectic group symmetries for these operators are also given. They may be derived using the appropriate plethysms.

Writing

$$H_c=\sum_{k=0}^{6}e_kE_k \tag{15}$$

and comparing this with Eq. (14) we may solve for the coefficients E_k in terms of the Slater integrals (Table V). Contrary to Alper and Sinanoğlu,[11] we note that the exploitation of the R_4 symmetry does not lead to any reduction in the number of parameters required to characterize the Coulomb field. This invalidates the results of their Tables III and V.

TABLE V. Radial coefficients for R_4 symmetry.

$E_0=\frac{1}{10}[F_0(2s,2s)+6F_0(2s,2p)+9F_0(2p,2p)]$
$E_1=\frac{1}{48}[F_0(2s,2s)-2F_0(2s,2p)+F_0(2p,2p)+40F_2(2p,2p)]$
$E_2=\frac{1}{2}G_1(2s,2p)$
$E_3=\frac{1}{8}[F_0(2s,2s)+2F_0(2s,2p)-3F_0(2p,2p)]$
$E_4=\frac{1}{16}[F_0(2s,2s)-2F_0(2s,2p)+F_0(2p,2p)-20F_2(2p,2p)]$
$E_5=-\frac{1}{2}G_1(2p,2p)$
$E_6=\frac{1}{48}[F_0(2s,2s)-2F_0(2s,2p)+F_0(2p,2p)+4F_2(2p,2p)]$
$E_7=\frac{1}{4}[I(2s)+3I(2p)+2F_0(1s,2s)+6F_0(1s,2p)-G_0(1s,2s)-3G_1(1s,2p)]$
$E_8=\frac{1}{4}[I(2s)-I(2p)+2F_0(1s,2s)-2F_0(1s,2p)-G_1(1s,2s)+G_1(1s,2p)]$

This process of symmetrizing with respect to higher groups can be carried out whenever we know the coupling coefficients. The operators must have a common normalization for this procedure and for this reason the factor required for the normalization of the operators is included in Table IV.

VI. MATRIX ELEMENTS FOR $(2s+2p)^2$

The matrix elements for the e_k may be readily calculated using standard methods[16] to give the results of Table VI. We note that we may factorize the matrix element of e_i as[16]

$$\langle\gamma_2W_2L_2M_2|\,e_i^{WLM}\,|\gamma_1W_1L_1M_1\rangle = \langle LM, L_1M_1\,|\,L_2M_2\rangle\langle WL, W_1L_1\,|\,W_2L_2\rangle \times\langle\gamma_2W_2\|\,e_i^W\,\|\gamma_1W_1\rangle, \tag{16}$$

thus reducing the number of calculations required. We have now separated the Hamiltonian into R_4 symmetry preserving $(e_0E_0+E_1e_1+E_2e_2)$ and symmetry breaking $(E_3e_3+E_4e_4+e_5E_5+e_6E_6)$ terms. The R_4 model will only be valid if the last part is small. In order to obtain some feeling for the size of the radial integrals, we present in Table VII the values of the E_i obtained using either hydrogen-like orbitals or the Hartree–Fock radial integrals found for neutral beryllium by Condon and Odabasi.[17]

The ^1S energy levels are of particular interest since the R_4 model gives a prediction of the mixing of the $|2s^2\,^1S\rangle$ and $|2p^2\,^1S\rangle$ states. Using the hydrogenic radial integrals, the relevant energy matrices in the two schemes are

	$\|[20]\,^1S\rangle$	$\|[00]\,^1S\rangle$
$\|[20]\,^1S\rangle$	108	$-16\sqrt{3}$
$\|[00]\,^1S\rangle$	$-16\sqrt{3}$	80

	$\|2p^2\,^1S\rangle$	$\|2s^2\,^1S\rangle$
$\|2p^2\,^1S\rangle$	111	$-15\sqrt{3}$
$\|2s^2\,^1S\rangle$	$-15\sqrt{3}$	77

where the matrix elements have units of $Ze^2/512a_0$. In

TABLE VI. Matrix elements of $(s+p)^2$.

	e_0	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8
$\langle[11]\,^3P\|\,e_i\,\|[11]\,^3P\rangle$	1	−3	−1	.	.	.	.	2	.
$\langle[1-1]\,^3P\|\,e_i\,\|[1-1]\,^3P\rangle$	1	−3	−1	.	.	.	.	2	.
$\langle[11]\,^3P\|\,e_i\,\|[1-1]\,^3P\rangle$	.	.	.	−1	2	−1	.	.	−2
$\langle[20]\,^1D\|\,e_i\,\|[20]\,^1D\rangle$	1	1	1	−1	.	1	2	2	−2
$\langle[20]\,^1P\|\,e_i\,\|[20]\,^1P\rangle$	1	1	1	1	.	−1	−10	2	2
$\langle[20]\,^1S\|\,e_i\,\|[20]\,^1S\rangle$	1	1	1	2	.	−2	−20	2	4
$\langle[20]\,^1S\|\,e_i\,\|[00]\,^1S\rangle$	.	.	.	$3^{\frac{1}{2}}$	$2(3^{\frac{1}{2}})$	$3^{\frac{1}{2}}$	.	.	$2(3^{\frac{1}{2}})$
$\langle[00]\,^1S\|\,e_i\,\|[00]\,^1S\rangle$	1	9	−3	.	.	.	.	2	.

TABLE VII. Radial integrals.

	Hydrogenic $Ze^2/512a_0$ a.u.	Hartree-Fock[a] a.u.
E_0	$\frac{1421}{16}$	0.3152
E_1	$\frac{73}{48}$	0.0047
E_2	$\frac{15}{2}$	0.0511
E_3	$-\frac{33}{8}$	0.0094
E_4	$-\frac{35}{8}$	−0.0061
E_5	$-\frac{15}{2}$	−0.0511
E_6	$\frac{41}{240}$	−0.00067
E_7	—	−0.5444
E_8	—	−0.0344

[a] Derived from Condon and Odabasi.[17]

this case, the R_4 scheme is less diagonal than the configuration scheme.

Using the H–F orbitals we obtain

$\|[20]\,^2S\rangle$	$\|[00]\,^1S\rangle$	$\|2p^2\,^1S\rangle$	$\|2s^2\,^1S\rangle$
0.5054	−0.0933	0.3607	−0.1773
−0.0933	0.2046	−0.1773	0.3493

in atomic units. Diagonalization of the matrices gives the groundstate eigenfunction for beryllium as

$$|^1S\rangle_0 = 0.953\,|[00]\,^1S\rangle + 0.275\,|[20]\,^1S\rangle \equiv 0.715\,|2s^2\,^1S\rangle + 0.700\,|2p^2\,^1S\rangle, \quad (17)$$

suggesting that for these Hartree–Fock orbitals the R_4 scheme is very much better than the configurational scheme.

Multiconfiguration calculations[18–20] for the beryllium atom yield for the groundstate[21]

$$|^1S\rangle_0 = 0.953|\,2s^2\,^1S\rangle + 0.299\,|2p^2\,^1S\rangle \equiv 0.736\,|[00]\,^1S\rangle + 0.676\,|[20]\,^1S\rangle, \quad (18)$$

indicating in this case that the configurational scheme is superior. Comparison of Eqs. (17) and (18) suggests that there is a contradiction between the R_4 and the multiconfiguration schemes. To resolve this discrepancy, we shall re-examine some of the approximations involved in the R_4 scheme.

VII. INCLUSION OF CLOSED-SHELL EFFECTS

Equation (14) gives a complete description of the Coulomb interaction within the $(2s + 2p)^N$ complex but fails to include contributions to the Hamiltonian from the $1s^2$ shell. To take into account these effects for the configuration $1s^2 2s^X 2p^{N-X}$, we must add to Eq. (14) the terms[22]

$$H_c' = 2I(1s) + F_0(1s, 1s) + XI(2s) + 2XF_0(1s, 2s) - XG_0(1s, 2s) + (N - X)I(2p) + 2(N - X)F_0(1s, 2p) - (N - X)G_1(1s, 2p). \quad (19)$$

We now express Eq. (19) as a linear combination of operators having well-defined R_4 symmetry by first noting that the numbers X and $N - X$ may be replaced by their operator equivalents

$$X = V_0^{(0)}(2s2s) \quad \text{and} \quad N - X = 3^{\frac{1}{2}}V_0^{(0)}(2p2p).$$

Inspection of Table II shows that we may construct two operators

$$e_7 = V_0^{(0)}(2s2s) + 3^{\frac{1}{2}}V_0^{(0)}(2p2p) \quad (20a)$$

and

$$e_8 = 3V_0^{(0)}(2s2s) - 3^{\frac{1}{2}}V_0^{(0)}(2p2p), \quad (20b)$$

having [00] and [20] R_4 symmetry, respectively, to give

$$H_c' = 2I(1s) + F_0(1s, 1s) + e_7E_7 + e_8E_8, \quad (21)$$

where

$$E_7 = \tfrac{1}{4}[I(2s) + 2F_0(1s, 2s) - G_0(1s, 2s) + 3I(2p) + 6F_0(1s, 2p) - 3G_1(1s, 2p)],$$

$$E_8 = \tfrac{1}{4}[I(2s) - I(2p) + 2F_0(1s, 2s) - 2F_0(1s, 2p) - G_0(1s, 2s) + G_1(1s, 2p)].$$

The first two terms in Eq. (21) are constant for the terms of a given $(2s + 2p)^N$ complex and thus cannot affect the result of Eq. (17). Similarly, since e_7 is just the number operator with eigenvalues N for all terms of the complex, its effect also leaves Eq. (17) invariant and thus can only alter the absolute energy of the complex.

The term e_8E_8 has [20] symmetry under R_4 and will thus have an off-diagonal matrix between the $|[00]\,^1S\rangle$ and $|[20]\,^1S\rangle$ states of $(2s + 2p)^2$, as follows from an inspection of Table VI. The integrals of Condon and Odabasi[17] lead to the values

$$E_7 = -0.5444 \quad \text{and} \quad E_8 = -0.0344 \text{ a.u.}$$

Explicit calculation using these values gives the groundstate eigenfunction of the beryllium atom as

$$|^1S\rangle_0' = 0.819\,|[00]\,^1S\rangle + 0.574\,|[20]\,^1S\rangle \equiv 0.907\,|2s^2\,^1S\rangle + 0.413\,|2p^2\,^1S\rangle. \quad (22)$$

This result is more in accord with that of the multiconfiguration calculation given in Eq. (18) and shows

that when the $1s^2$-shell effects are included the R_4 scheme ceases to be physical, and the configurational scheme becomes superior.

The term e_8E_8 clearly plays a major role in breaking the otherwise good R_4 symmetry. This result might well have been anticipated by noting that in the $(2s + 2p)^1$ complex the separation of the ^2S and ^2P terms will be, from Eq. (21), just $-4E_8$. Pure R_4 symmetry would require this splitting to be zero, while experimentally we find for the isoelectronic series[23]

	Li I	Be II	B III	C IV	
$-E_8 =$	3725	7958	12095	16150	cm^{-1}
	0.0170	0.0364	0.0551	0.0736	a.u.

which is by no means negligible.

VIII. CONCLUSION

Our principal conclusion is, contrary to previous assertions,[9,11,12] that the R_4 group does not yield an adequate approximate symmetry scheme for many-electron theory. In reaching this result, we have eliminated a number of errors in previous work and shown that the R_4 symmetry scheme approximately diagonalizes the energy matrix only when the effects of the inner shells are omitted. These latter effects lead to a large symmetry mixing term that renders the R_4 approximation of little physical significance for many-electron theory.

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[1] V. A. Fock, Z. Physik **98**, 145 (1935).
[2] V. Bargmann, Z. Physik **99**, 576 (1936).
[3] A. M. Perelomov and V. S. Popov, Zh. Eksp. Teor. Fiz. **50**, 179 (1966) [Sov. Phys.—JETP **23**, 118].
[4] D. Layzer, Ann. Phys. **8**, 271 (1959).
[5] D. Layzer, Ann. Phys. **17**, 177 (1962).
[6] D. Layzer, Z. Horak, M. N. Lewis, and D. P. Thompson, Ann. Phys. **29**, 101 (1964).
[7] M. Moshinsky, Phys. Rev. **126**, 1880 (1962).
[8] L. C. Biedenharn, J. Math. Phys. **2**, 433 (1961).
[9] C. E. Wulfman, Phys. Letters **26A**, 397 (1968).
[10] L. Lipsky and A. Russek, Phys. Rev. **142**, 59 (1966).
[11] J. S. Alper and O. Sinanoğlu, Phys. Rev. **142**, 77 (1969).
[12] J. S. Alper, Phys. Rev. **177**, 86 (1969).
[13] W. Pauli, Ergeb. Exakt. Naturw. **37**, 85 (1965).
[14] P. H. Butler and B. G. Wybourne, J. Math. Phys. **11**, 2513 (1970).
[15] H. Weyl, Math. Z. **23**, 271 (1925).
[16] B. R. Judd, *Operator Techniques in Atomic Spectroscopy* (McGraw-Hill, New York, 1963).
[17] E. U. Condon and H. Odabasi, *Selfconsistent Field Calculations for Energy Levels of 6, 7, and 8 Electron Isoelectronic Sequences*, Joint Institute of Laboratory Astrophysics Report, Boulder, Colorado, JILA No. 95, 1968.
[18] A. P. Jucys and V. I. Kavetskis, Akad. Nauk. Litovskoi SSR, Tr., Ser. B **1**(4), 9 (1956).
[19] E. Clementi and A. Veillard, J. Chem. Phys. **44**, 3050 (1966).
[20] N. Sabelli and J. Hinze, J. Chem. Phys. **50**, 684 (1969).
[21] It should be noted that the phase conventions in Refs. 12 and 20 are unspecified but evidently opposite to the Condon and Shortley phases[22] used in Ref. 18.
[22] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge U.P., New York, 1935).
[23] C. E. Moore, *Atomic Energy Levels* (National Bureau of Standards, Circular 467, Washington, 1949).

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Quantum Theory on a Network. II. A Solvable Model Which May Have Several Bound States per Node Point*

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This is a further development of a network model for electrons in solids. It is postulated that the electrons are restricted to move along 1-dimensional lines between atoms. The network for a given solid corresponds to that which one would use in a wire and ball model to exhibit the crystal structure. A potential of the form $V = -V_0 \operatorname{sech}^2 \gamma x$ is associated with each "atomic" node point. The atom can have 1, 2, 3, or more electronic bound states, depending on V_0 and γ. The wavefunctions have the usual Bloch form and involve hypergeometric functions. The density of states is plotted. Localized defect energy levels are also given for various types of atomic defects. An especially interesting feature of the model is that all the above-mentioned calculations are made exactly, without resorting to perturbation theory.

I. INTRODUCTION

One of the authors[1] has discussed a network model of electrons in molecules and crystals which has the nice feature that wavefunctions and energy levels can be calculated exactly. (This paper is referred to as I.) It is a generalization of the free-electron network model developed by Pauling,[2] Kuhn,[3] Platt,[4] Ruedenberg and Scherr,[5] Griffith,[6] Coulson,[7] and others. In the free-electron model, the electrons are restricted to move along 1-dimensional paths between network node points, the network being constructed to be topologically equivalent to the molecule or crystal of interest. The wavefunctions must be chosen to be continuous at the node points and to be such that Kirchoff's law is satisfied at the node points. In our generalization, a 1-dimensional potential is introduced along each internode bond. It is chosen in such a manner that bound states might exist at the node points and such that the wavefunctions can still be expressed in terms of classical special functions.

The 1-dimensional Schrödinger equation with the potential

$$V(x) = -V_0 \operatorname{sech}^2 \gamma x \tag{1}$$

can be solved in terms of hypergeometric functions. The special case $V_0 = \gamma^2\hbar^2/m$ was emphasized in I because the associated wavefunctions can be expressed in terms of elementary (circular and hyperbolic) functions. If the node points are not too close to each other, one band of bound states exists in this special case. While further remarks are made concerning this case here, we also allow V_0 to have other values so that situations with more than one band of bound states can be investigated. General aspects of the two parameter potential are discussed in Sec. II.

Section III is devoted to the application of (1) to square lattices and cubic lattices. We investigate the relation of the parameters to the spreading of bands and to the variation of distance between bands. The relationship of the density of states to the parameters of the potential is discussed also.

In Sec. IV, we consider a simple monatomic lattice with a defect which is characterized by a deviation in the parameters of the potential well from the values they have in the host atoms of the lattice. The values of the impurity energy levels are calculated as well as the localized wavefunctions in the neighborhood of the impurity. These localized electrons, of course, correspond to those found in semiconductors.

II. SOME GENERAL ASPECTS OF NETWORKS WITH BOND POTENTIALS $V = -V_0 \operatorname{sech}^2 \gamma x$

We have plotted the potential (1) in Fig. 1 for various values of V_0 and γ to give some idea of the relationship between the parameters and the shape of potential. The area between the potential and the axis $V(0) = 0$ is $2V_0/\gamma$, while the half-width of the potential is $\gamma^{-1} \tanh^{-1}(\frac{1}{2})$. As $\gamma \to \infty$ for fixed V_0, we have a deep narrow well, while as $\gamma \to 0$ we have free particles.

The 1-dimensional Schrödinger equation for the potential (1) is

$$\left(\frac{d^2}{dx^2} + 2\hbar^{-2}mE + 2mV_0\hbar^{-2} \operatorname{sech}^2 \gamma x\right)\psi(x) = 0. \tag{2}$$

If we let

$$k^2 = 2mE/\hbar^2 \quad \text{and} \quad s = \tfrac{1}{2}[-1 + (1 + 8mV_0/\hbar^2\gamma^2)^{\frac{1}{2}}], \tag{3}$$

the Schrödinger equation becomes

$$\left(\frac{d^2}{dx^2} + k^2 + s(s+1)\gamma^2 \operatorname{sech}^2 \gamma x\right)\psi(x) = 0, \tag{4}$$

which with $s = 1$ is the case investigated in some detail in I. It is well known[8,9] that the solution of this

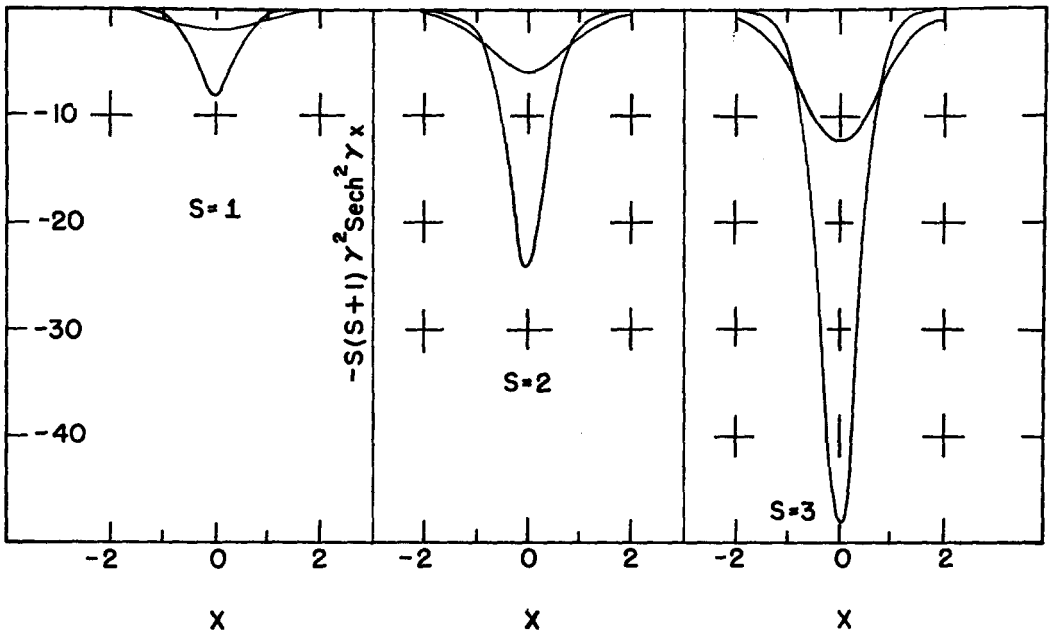


FIG. 1. Sketch of model "atomic" potential which we use in this paper. $s = 1$ corresponds to one bound state per atom, $s = 2$ two bound states, etc.

equation can be expressed in terms of hypergeometric functions. We write

$$\epsilon = (\hbar\gamma)^{-1}(-2mE)^{\frac{1}{2}} = ik/\gamma. \tag{5}$$

Then the solution of (2) is

$$\psi(x) = A[P(\epsilon, s, x) + DT(\epsilon, s, x)]. \tag{6a}$$

Here, A and D are arbitrary constants, while

$$P(\epsilon, s, x) = (\cosh^s \gamma x)^{-1} F_1, \tag{6b}$$

$$T(\epsilon, s, x) = (\sinh \gamma x)(\cosh^s \gamma x)^{-1} F_2, \tag{6c}$$

where, with $F(a, b, c; z)$ being the hypergeometric function,

$$F(a, b, c; z) = 1 + \frac{ab}{c}\frac{z}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \cdots, \tag{7}$$

$$F_1 \equiv F(-\tfrac{1}{2}s + \tfrac{1}{2}\epsilon, -\tfrac{1}{2}s - \tfrac{1}{2}\epsilon, \tfrac{1}{2}, -\sinh^2 \gamma x), \tag{6d}$$

$$F_2 \equiv F(-\tfrac{1}{2}s + \tfrac{1}{2}\epsilon + \tfrac{1}{2}, -\tfrac{1}{2}s - \tfrac{1}{2}\epsilon + \tfrac{1}{2}, \tfrac{3}{2}, -\sinh^2 \gamma x). \tag{6e}$$

The derivative of the wavefunction (6a) can be expressed in terms of four hypergeometric functions[10] F_1, F_2, F_3, and F_4 with

$$\frac{dF_1}{dx} = \tfrac{1}{2}\gamma(\epsilon^2 - s^2)F_3 \sinh 2\gamma x,$$

$$\frac{dF_2}{dx} = \tfrac{1}{6}\gamma[\epsilon^2 - (s-1)^2]F_4 \sinh 2\gamma x, \tag{8a}$$

$$F_3 \equiv F(-\tfrac{1}{2}s + \tfrac{1}{2}\epsilon + 1, -\tfrac{1}{2}s - \tfrac{1}{2}\epsilon + 1, \tfrac{3}{2}, -\sinh^2 \gamma x), \tag{8b}$$

$$F_4 \equiv F(-\tfrac{1}{2}s + \tfrac{1}{2}\epsilon + \tfrac{3}{2}, -\tfrac{1}{2}s - \tfrac{1}{2}\epsilon + \tfrac{3}{2}, \tfrac{5}{2}, -\sinh^2 \gamma x). \tag{8c}$$

Then some algebra yields

$$\psi'(x) = \gamma A[R(\epsilon, s, x) + DQ(\epsilon, s, x)], \tag{9a}$$

with

$$R(\epsilon, s, x) = [(\epsilon^2 - s^2)F_3 \sinh \gamma x \cosh \gamma x - sF_1 \tanh \gamma x]/\cosh^s \gamma x, \tag{9b}$$

$$Q(\epsilon, s, x) = \{(\cosh \gamma x - s \tanh \gamma x \sinh \gamma x)F_2 + \tfrac{1}{3}[\epsilon^2 - (s-1)^2]F_4 \cosh \gamma x \sinh^2 \gamma x\}/\cosh^s \gamma x. \tag{9c}$$

Both the wavefunction and its derivative can be evaluated at the origin by using $F(a, b, c, 0) = 1$. This gives

$$\psi(0) = A, \tag{10a}$$

$$\psi'(0) = \gamma AD, \tag{10b}$$

so that

$$\psi'(0)/\psi(0) = \gamma D. \tag{10c}$$

The hypergeometric functions are even functions of x, so that P and Q are even, while T and R are odd.

Now we introduce the network aspects of the problem, using the methods discussed in I to impose the boundary conditions on the wavefunction and its derivative. Consider the point halfway between nodes

separated by l. The value of the wavefunction is

$$\psi(\tfrac{1}{2}l) = \psi(0)(P_\alpha + DT_\alpha), \quad \text{with} \quad \alpha = \tfrac{1}{2}\gamma l, \tag{10d}$$

where we have omitted the parameters ϵ and s and have set $P_\alpha \equiv P(\alpha)$, etc. From the requirement of continuity of the wavefunction at the midpoint between nodes, we have (letting $\psi[i]$ be the wavefunction at the node i)

$$\psi[i](P_\alpha + D_{ij}T_\alpha) = \psi[j](P_\alpha + D_{ji}T_\alpha), \tag{11}$$

where D_{ij} is the constant associated with the wavefunction at node point $[i]$ along the bond connecting $[i]$ and $[j]$. Next, consider the value of the derivative of the wavefunction at the midpoint. The value of the derivative is

$$\psi'(\tfrac{1}{2}l) = \psi(0)(R_\alpha + DQ_\alpha). \tag{12}$$

Our convention is that the distance x is measured away from the node point so that continuity of the derivative at the midpoint implies that the derivatives with respect to each portion are of the same magnitude but opposite in sign:

$$(R_\alpha + D_{ij}Q_\alpha)\psi[i] = -(R_\alpha + D_{ji}Q_\alpha)\psi[j]. \tag{13}$$

By eliminating D_{ji} from (11) and (13), we obtain

$$D_{ij} = \{(P_\alpha Q_\alpha - T_\alpha R_\alpha)\psi[j] - (P_\alpha Q_\alpha + T_\alpha R_\alpha)\psi[i]\}/2T_\alpha Q_\alpha \psi[i]. \tag{14}$$

We are now in a position to discuss the boundary conditions at the ith node point. First, the wavefunction must be continuous as one goes from one segment connected to the ith node point to another. If $\{i_k\}$ is the set of nodes connected to the ith, the conservation of particles (or Kirchoff's law) leads to[5]

$$\sum_k \left(\frac{d \log f_{ii_k}}{dx_{ii_k}}\right)_0 = 0, \quad \text{all } i, \tag{15}$$

where f_{ij} is the wavefunction along the segment which connects nodes i and j and x_{ij} is the distance on the segments from node i in the direction of node j. The subscript 0 indicates that the derivative is to be evaluated at the node point i. If we refer to (10c), we see that (15) is equivalent to

$$\sum_k D_{ii_k} = 0, \tag{16}$$

so that

$$n_i f(\epsilon, s, \alpha)\psi[i] = \sum_k \psi[i_k], \tag{17}$$

where $f(\epsilon, s, \alpha)$, which we call a "form factor," is given by

$$f(\epsilon, s, \alpha) = (P_\alpha Q_\alpha + T_\alpha R_\alpha)/(P_\alpha Q_\alpha - T_\alpha R_\alpha). \tag{18}$$

Here n_i is the number of connections to the ith node and the sum is over the neighboring nodes connected to the ith node.

If we substitute the definitions of P, T, R, and Q into (15), the form factor is given in terms of the hypergeometric functions $F_j \equiv F_j(\alpha)$ [as defined by (6) and (8)], $\gamma x = \frac{1}{2}\gamma l \equiv \alpha$:

$$f(\epsilon, s, \alpha) = \frac{3F_1F_2(1 - 2s\tanh^2\alpha) + F_1F_4[\epsilon^2 - (s-1)^2]\sinh^2\alpha + 3F_2F_3(\epsilon^2 - s^2)\sinh^2\alpha}{3F_1F_2 + F_1F_4[\epsilon^2 - (s-1)^2]\sinh_1^2\alpha - 3F_2F_3(\epsilon^2 - s^2)\sinh^2\alpha}. \tag{19}$$

For integral values of s we can use the contiguity relations and formulas[10]

$$F(a, -a, \tfrac{1}{2}, \sin^2 z) = \cos 2az, \tag{20a}$$

$$F(a, 1-a, \tfrac{1}{2}, \sin^2 z) = \cos[(2a-1)z]/\cos z, \tag{20b}$$

$$F(a, 1-a, \tfrac{3}{2}, \sin^2 z) = \sin[(2a-1)z]/[(2a-1)\sin z], \tag{20c}$$

$$F(a, 2-a, \tfrac{3}{2}, \sin^2 z) = \sin[(2a-2)z]/[(a-1)\sin 2z] \tag{20d}$$

to express the wavefunction and the form factor in terms of elementary functions. For the free particle case $s = 0$, we have

$$\psi(x) = A(\cosh \epsilon\gamma x + D \sinh \epsilon\gamma x), \tag{21a}$$

$$f(\epsilon, 0, \alpha) = \cosh 2\epsilon\alpha. \tag{21b}$$

For $s = 1$, we have

$$\psi(x) = A[(\cosh \epsilon\gamma x - \epsilon^{-1}\tanh \gamma x \sinh \epsilon\gamma x) + D(\sinh \epsilon\gamma x - \epsilon^{-1}\tanh \gamma x \cosh \epsilon\gamma x)], \tag{22a}$$

$$f(\epsilon, 1, \alpha) = (\epsilon^2 - 1)^{-1}[(\epsilon^2 - 1 + 2\tanh^2\alpha) \times \cosh 2\epsilon\alpha - \epsilon^{-1}(2\epsilon^2 - \operatorname{sech}^2\alpha) \times \tanh\alpha \sinh 2\alpha\epsilon]. \tag{22b}$$

For $s = 2$, we have

$$\psi(x) = A([1 + 3(\epsilon^2 - 1)^{-1}\tanh^2\gamma x]\cosh \epsilon\gamma x - 3\epsilon(\epsilon^2 - 1)^{-1}\sinh \epsilon\gamma x + D\{[1 + 3(\epsilon^2 - 1)^{-1}\tanh^2\gamma x]\sinh \epsilon\gamma x - 3\epsilon(\epsilon^2 - 1)^{-1}\cosh \epsilon\gamma x\}), \tag{23a}$$

$$f(\epsilon, 2, \alpha) = [(\epsilon^2 - 1)(\epsilon^2 - 4)]^{-1} \times \{[\epsilon^4 + \epsilon^2(13 - 18\operatorname{sech}^2\alpha) + (4 - 36\operatorname{sech}^2\alpha + 36\operatorname{sech}^4\alpha)]\cosh 2\epsilon - 3\epsilon^{-1}\tanh\alpha[2\epsilon^4 + \epsilon^2(4 - 11\operatorname{sech}^2\alpha) - (4\operatorname{sech}^2\alpha - 6\operatorname{sech}^4\alpha)]\sinh 2\epsilon\alpha\}. \tag{23b}$$

So far, we have considered only bound states which correspond to negative values of the energy E. The

wavefunction and the form factor for the free-electron states, corresponding to positive energy, can be easily found by replacing ϵ by ik/γ in the above formulas. We notice that the form factor depends on the energy $E \sim -\epsilon^2$ rather than on ϵ itself. If we let $\kappa = k/\gamma$, then $\cos \kappa\gamma x$ replaces $\cosh \epsilon\gamma x$ and $\kappa^{-1} \sin \kappa\gamma x$ replaces $\epsilon^{-1} \sinh \epsilon\gamma x$, while $-\kappa^2$ replaces ϵ^2. As an example, the wavefunction and form factor for $s = 2$ are

$$\psi(x) = A\{(\kappa^2 + 1 - 3\tanh^2 \gamma x)\cos k\gamma x - 3\kappa \sin \kappa\gamma x + D[(\kappa^2 + 1 - 3\tanh^2 \gamma x)\sin \kappa\gamma x - 3\kappa \cos \kappa\gamma x]\}, \quad (24a)$$

$$f(\kappa, 2, \alpha) = \{[\kappa^4 - \kappa^2(13 - 18\,\mathrm{sech}^2 \alpha) + (4 - 36\,\mathrm{sech}^2 \alpha + 36\,\mathrm{sech}^4 \alpha)]\cos 2\kappa\alpha - 3\kappa^{-1}\tanh \alpha[2\kappa^4 - \kappa^2(4 - 11\,\mathrm{sech}^2 \alpha) - (4\,\mathrm{sech}^2 \alpha - 6\,\mathrm{sech}^4 \alpha)]\sin 2\kappa\alpha\}/(\kappa^2 + 1)(\kappa^2 + 4). \quad (24b)$$

The form factor is plotted in Figs. 2 and 3 as a function of the energy for several values of the parameters s and α.

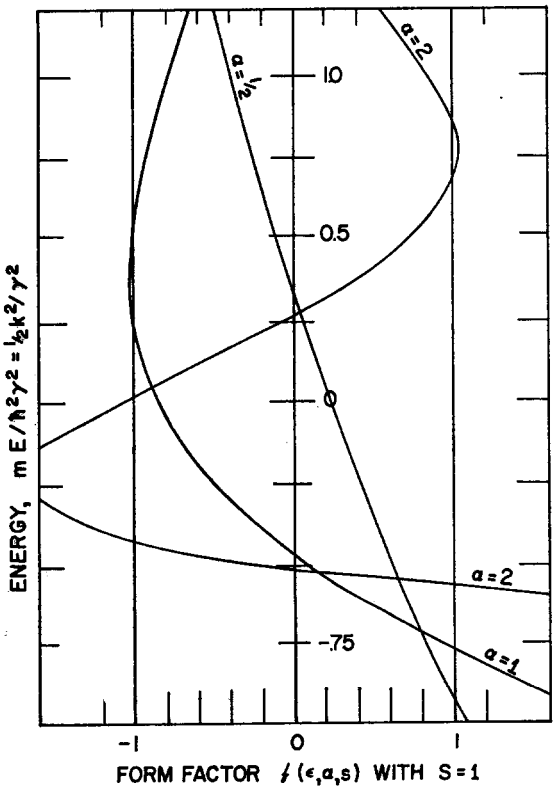


FIG. 2. Variation of forms factor with energy in network with one bound state per node point (i.e., per "atom"). The allowable values of the energy correspond to $-1 < f < 1$. Hence, energy bands for a given α exist for those energies for which f satisfies this inequality. Here $\alpha = \gamma l/2$, while l is the lattice spacing and $2\gamma^2$ the depth of the potential. Small α represents free electrons and large α represents the tight-binding limit.

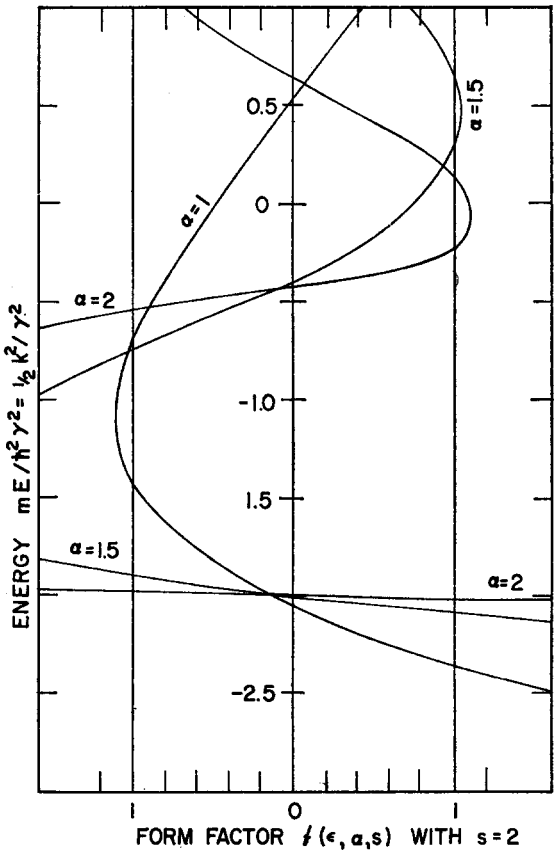


FIG. 3. Form factor when there are two bound states per atom. Again, the allowed energy levels are restricted to $-1 < f < 1$.

III. BAND STRUCTURE AND DENSITY OF STATES

Consider first a simple cubic lattice with a typical lattice point (j_1, j_2, j_3). Then (17) has the form

$$6f\psi[j_1, j_2, j_3] = \psi[j_1 - 1, j_2, j_3] + \psi[j_1 + 1, j_2, j_3] + \psi[j_1, j_2 - 1, j_3] + \psi[j_1, j_2 + 1, j_3] + \psi[j_1, j_2, j_3 - 1] + \psi[j_1, j_2, j_3 + 1]. \quad (25)$$

Using periodic boundary conditions in a network with N^3 node points, we find that (where A is a normalization constant)

$$\psi[j_1, j_2, j_3] = A \exp[2\pi i(s_1 j_1 + s_2 j_2 + s_3 j_3)/N], \quad s_1, s_2, s_3 = 1, 2, \cdots, N, \quad (26)$$

so that solutions of (25) have this form if f has one of the values

$$f = \tfrac{1}{3}\sum_{\alpha=1}^{3} \cos\left(\frac{2\pi s_\alpha}{N}\right). \quad (27)$$

As $N \to \infty$, the quantity $2\pi s/N$ can be replaced by the continuous variable ϕ with the range $0 < \phi < 2\pi$.

Or, as an alternative, if we introduce the lattice spacing l, we have $2\pi s/N \equiv 2\pi sl/lN = 2\pi sl/L \equiv ql$, where L is the length of an edge of our sample and $q = 2\pi s/L$. Then

$$f = \tfrac{1}{3}\sum_{\alpha=1}^{3}\cos\phi_\alpha \equiv \tfrac{1}{3}\sum_{1}^{3}\cos lq_\alpha. \qquad (28)$$

This is the basic equation from which the band structure and constant energy surfaces of a simple cubic lattice can be deduced.

Once the energy of interest [or ϵ, since ϵ is related to the energy by (5)] is chosen, the structure function f is obtained from (19). Since, for a given vector $\phi = (\phi_1, \phi_2, \phi_3)$ or $q = (q_1, q_2, q_3)$, the right-hand side of (28) is determined, the energy associated with that ϕ or q is that which gives the appropriate value of f. This can be read off graphs such as those given in Fig. 3. Since the right-hand side of (24) is restricted to values between -1 and $+1$, the allowed energies are those for which the form factor lies in this interval. By inspection of Fig. 3, we can see which values of the energy are allowed. Figures 4 and 5 show the location of the band edges as a function of α for $s = 1, 2$.

We see that, as we increase the depth of the well by increasing s for fixed α, we increase the number of bound states for each well. As we bring potential wells together (by decreasing l, i.e., α), we obtain a broadening of the bands.

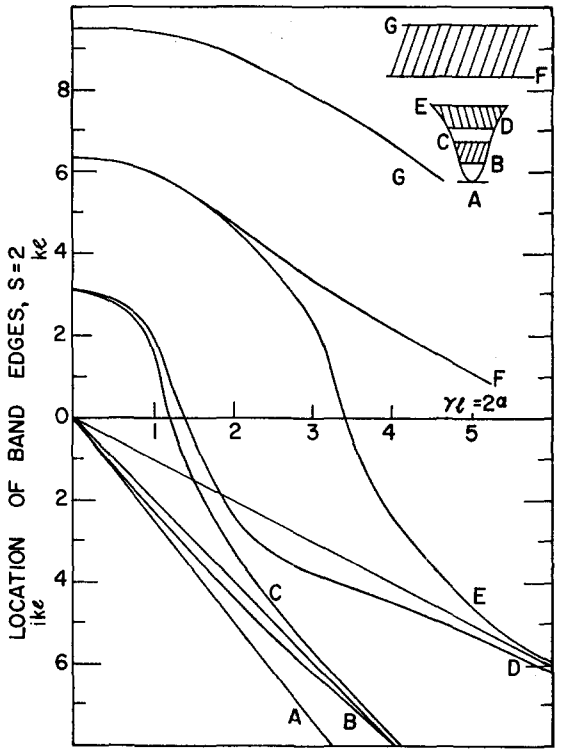


FIG. 5. Variation of location of band edges with γl when there are two bound states per "atom."

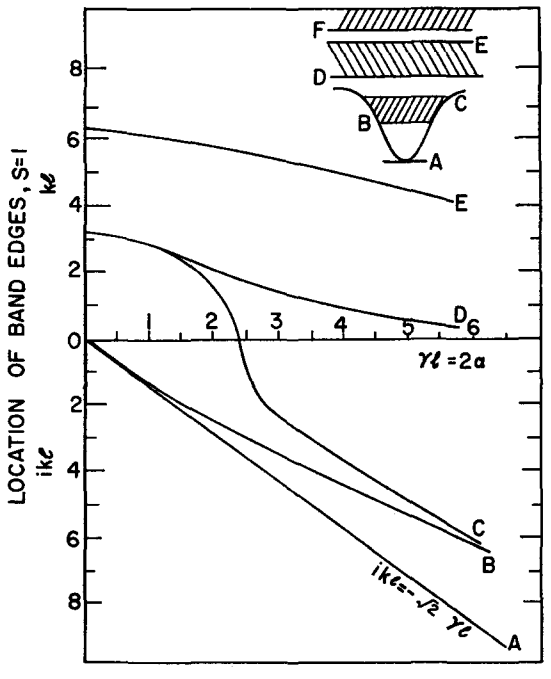


FIG. 4. Variation of location of band edges, with γl, where $2\gamma^2$ is the well depth of the potential well and l the distance between nearest-neighbor lattice points. This data corresponds to the case of one bound state per "atom." Notice that, as $\gamma \to \infty$ or $l \to \infty$, one obtains a tight-binding situation with a very narrow band associated with bound states. As $\gamma \to 0$ or $l \to 0$, one has a free-electron situation in which the gap between bands of bound states and free-electron states vanishes. A rapid change from one regime to another occurs when $\gamma l \simeq 2.5$.

The surfaces of constant energy (which in turn yield the Fermi surface of a material) can be determined immediately from (28) and (19). If an energy is specified and substituted into (19), the appropriate value of f is determined. With this constant f, a constant energy surface is defined in (28) which corresponds to the energy originally chosen. A typical constant-energy surface is plotted in Fig. 6.

It is well known from other solid-state problems, whose basic equations have the structure of (17) but in which the physical significance of f and ψ are somewhat different (for example, tight-binding approximation for electrons and random walks on lattices), that the analogs of (28) for body-centered- and face-centered-cubic lattices (BCC and FCC, respectively) with nearest-neighbor interactions only are[11–13]

$$f = \cos lq_1 \cos lq_2 \cos lq_3, \quad \text{BCC}, \qquad (29a)$$

$$f = \tfrac{1}{3}(\cos lq_1 \cos lq_2 + \cos lq_2 \cos lq_3 + \cos lq_3 \cos lq_1), \quad \text{FCC}. \qquad (29b)$$

Their constant-energy surfaces can be obtained in the manner discussed for the simple cubic lattice.

It was shown in I that the density of states of a simple cubic lattice can be derived from information

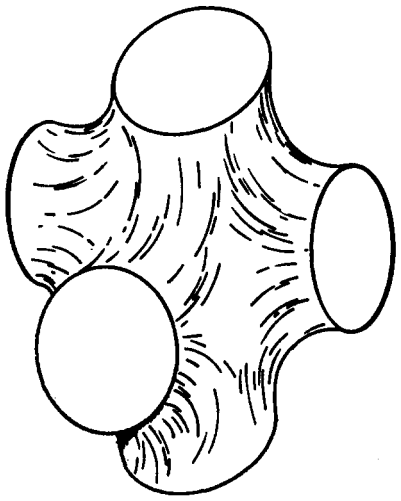


FIG. 6. A surface of constant energy for a simple cubic lattice.

on the form factor f and from the distribution function $P_3(x)$ of the variable

$$x_3 = \cos\phi_1 + \cos\phi_2 + \cos\phi_3 \tag{30}$$

as each ϕ ranges with equal likelihood through all values between 0 and 2η. Thus, in the band of bound states, the density of states $G_n(E)$ is given by

$$G_3(E) = -\left(\frac{1}{\epsilon}\right) P_3[3f(\epsilon, \alpha, s)] \frac{df}{d\epsilon} \tag{31}$$

and, in the conduction band, by

$$G_3(E) = \left(\frac{1}{\kappa}\right) P_3[3f(\kappa, \alpha, s)] \frac{df}{d\kappa}, \tag{32}$$

where

$$P_3(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{izx} [J_0(z)]^3 \, dz.$$

The properties of these distribution functions are summarized in I and, indeed, have been discussed by a number of authors including those listed in Refs. 14–16, as well as 12. The function $P_3(x)$ is plotted in Fig. 7(a).

The density of states for $s = 1$ is plotted in I for several values of α. Notice that, when s is an integer, f can be expressed in terms of elementary functions as can $df/d\epsilon$. Otherwise, it is very clumsy to deal with. In that case, calculations would be made on a computer and the best way to calculate derivatives would be through the aid of formulas such as

$$\frac{df}{d\epsilon} = h^{-1}\left(\frac{1}{2}(\Delta f_{-1} + \Delta f_0) - \frac{1}{2}\frac{1}{3!}(\Delta^3 f_{-2} + \Delta^3 f_{-1}) + \frac{2}{5!}(\Delta^5 f_{-3} + \Delta^5 f_{-2}) + \cdots\right) \tag{33}$$

for the derivative where f has the value f_0 when the values $\cdots, f_{-2}, f_{-1}, f_0$, and f_1 are known at points separated by intervals h. Also, $\Delta f_j = f_{j+1} - f_j$, $\Delta^2 f_j = \Delta f_{j+1} - \Delta f_j$, etc.

Since f is a smooth function, the derivative expansion converges rapidly. A variety of derivative formulas are given in Ref. 10, Chap. 25. The simple cubic lattice density of states for several values of s and α is plotted in Fig. 8.

Let $P_{BC}(x)$ and $P_{FC}(x)$ be the distribution functions of the body-centered and face-centered structure functions

$$X_{BC} = \cos\phi_1 \cos\phi_2 \cos\phi_3, \tag{34a}$$

$$X_{FC} = \cos\phi_1 \cos\phi_2 + \cos\phi_2 \cos\phi_3 + \cos\phi_3 \cos\phi_1. \tag{34b}$$

Then the respective densities of state are

$$G_{BC}(E) = -\frac{1}{\epsilon} P_{BC}[f(\epsilon, \alpha, s)] \frac{df}{d\epsilon}, \tag{35a}$$

$$G_{FC}(E) = -\frac{1}{\epsilon} P_{FC}[3f(\epsilon, \alpha, s)] \frac{df}{d\epsilon}. \tag{35b}$$

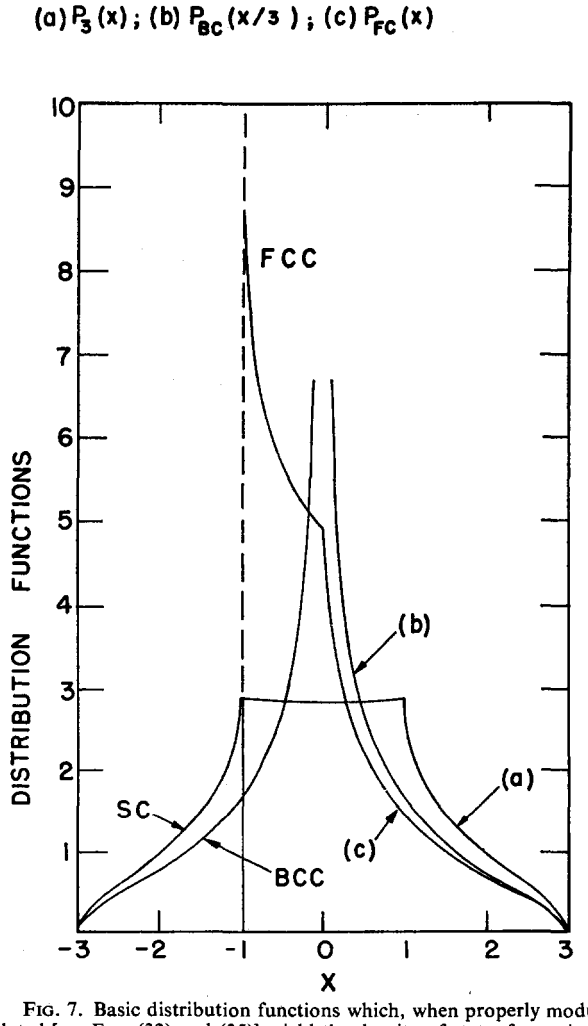


FIG. 7. Basic distribution functions which, when properly modulated [see Eqs. (32) and (35)], yield the density of states for various cubic lattices.

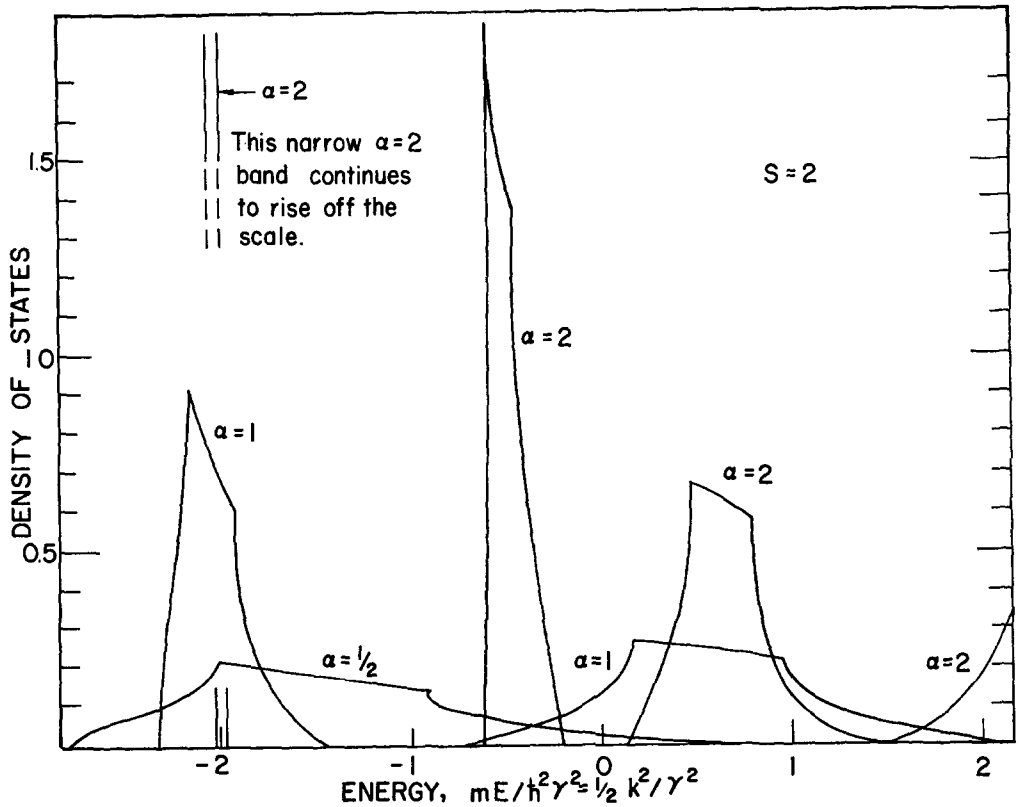


FIG. 8. Simple cubic lattice density of states with two bound states per atom ($s = 2$). Here $2\alpha = \gamma l$, where $2\gamma^2$ is the well depth and l is the lattice spacing.

The functions P_{BC} and P_{FC} have recently been discussed in detail by Jelitto[16] (his formulas, however, must be divided by $8\pi^3$ in order to satisfy our normalization).

The distribution functions $P_{BC}(x)$ and $P_{FC}(x)$ can be written, respectively, (letting $c_j \equiv \cos\phi_j$) as the Fourier transforms of

$$\langle \exp(i\alpha c_1 c_2 c_3)\rangle_{av}$$

and

$$\langle \exp i\alpha(c_1c_2 + c_2c_3 + c_3c_1)\rangle_{av}.$$

Jelitto has shown, for example, that

$$P_{BC}(x) = \left(\frac{2}{\pi}\right)^3 \int_x^1 (l^2 - x^2)^{-\frac{1}{2}} K'(l)\, dl, \qquad (36)$$

where

$$K'(l) = K((1 - l^2)^{\frac{1}{2}})$$

and where $K(z)$ is the elliptic integral of the first kind. The numerical integration of (36) has been carried out by Jelitto. The graph of $P_{BC}(x)$ is given in Fig. 7(b). A similar analysis[16] can be made of $P_{FC}(x)$. This is plotted in Fig. 7(c).

By combining Jelitto's formulas and our expression (19) for f, we find the density of states for BC and FC cubic lattices as plotted in Figs. 9 and 10.

IV. DEFECTS

A defect can be produced at a lattice point by introducing a different number of bound states, say $s \to t$, or by changing the parameter $\gamma \to \gamma'$ and, hence, $\alpha \to \beta$. We consider a lattice with one defect at the origin in an otherwise perfect network. Our defect corresponds to the case of a change in spring constant and mass in the theory of lattice vibrations. The methods developed for analyzing the effect of the defect on the frequency spectrum can be used to discuss the effect of the defect on the energy levels.

We consider the continuity of the wavefunction and its derivative at the node point and at the midpoint between nodes as in Sec. II. With a defect node at the origin of a lattice, there are three situations to consider:

(i) a perfect node connected to other perfect nodes (this case has been considered in Sec. II),

(ii) a defect node connected to perfect nodes, and

(iii) a perfect node connected to one defect node and other perfect nodes.

We derive the form factors relating the wavefunctions at the nodes for cases (ii) and (iii) and show how the set of difference equations for the network can be solved by a Green's-function method. The method

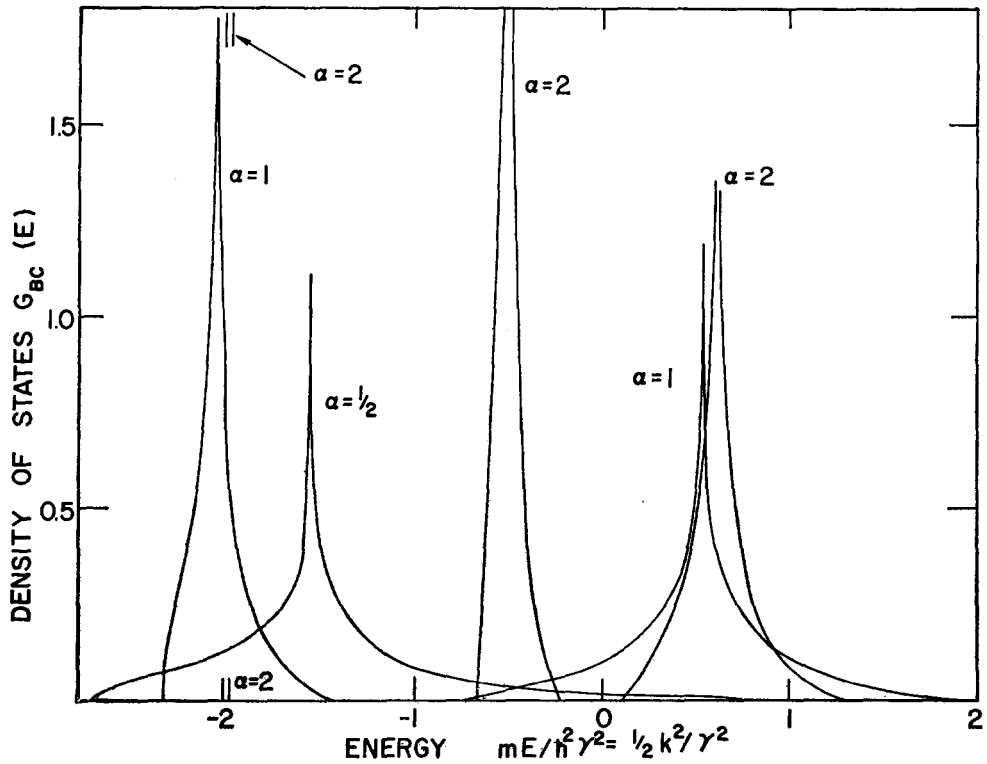


FIG. 9. Body-centered cubic lattice density of states, one bound state per atom ($s = 1$).

used is that developed by Lifshitz[17] and Montroll and Potts[18] for lattice vibrations in the presence of defects and by Slater and Koster[12] for the tight-binding model of electrons in crystals.

Let $s = t$ and $\gamma = \gamma'$ at the defect point. The solution of the Schrödinger equation and its derivative on each of the bonds attached to the defect are of the forms

$$\psi_D(x) = A[P(\epsilon, t, \gamma', x) + DT(\epsilon, t, \gamma', x)], \quad (37a)$$

$$\psi'_D(x) = A\gamma'[R(\epsilon, t, \gamma', x) + DQ(\epsilon, t, \gamma', x)], \quad (37b)$$

respectively, where P, T, R, and Q are defined by (6) and (9) with $s \to t$ and $\gamma \to \gamma'$. Now we consider the matching of this wavefunction with the wavefunction of the perfect lattice at the midpoint between nodes. With $\beta = \frac{1}{2}\gamma' l$, following the notation of Sec. II [see line below Eq. (10d)], we note that

$$\psi_D[0][P_\beta + D_{0j}T_\beta] = \psi_p[j][P_\alpha + D_{j0}T_\alpha], \quad (38a)$$

where j represents a node connected to the origin. Using the convention that distances are measured away from each node for each segment, we find that continuity of the derivatives gives

$$\beta\psi_D[0][R_\beta + D_{0j}Q_\beta] = -\alpha\psi_p[j][R_\alpha + D_{j0}Q_\alpha]. \quad (38b)$$

The elimination of D_{j0} from (38a) and (38b) gives

$$D_{0j} = \frac{\psi_p[j][\alpha P_\alpha Q_\alpha - \alpha R_\alpha T_\alpha] - \psi_D[0][\alpha Q_\alpha P_\beta + \beta T_\alpha R_\beta]}{[\alpha Q_\alpha T_\beta + \beta T_\alpha Q_\beta]\psi_D[0]} \quad (39)$$

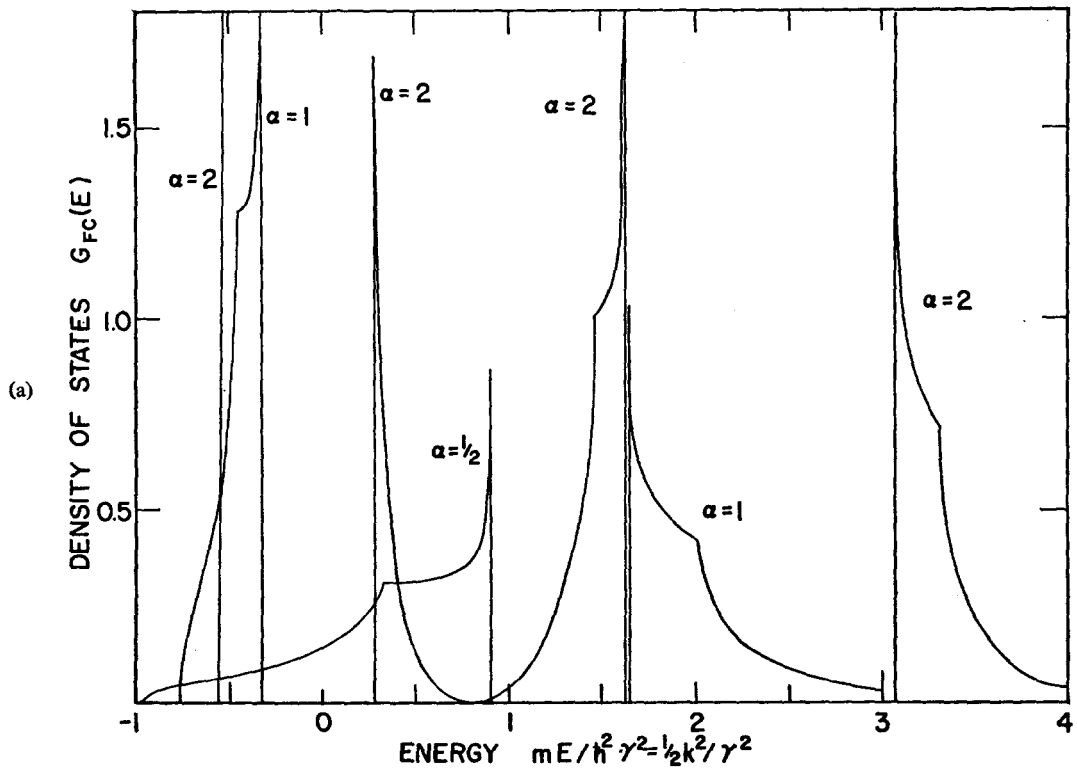
Since $\psi'(0)/\psi(0) = \gamma' D$, the boundary conditions at the defect node are $\sum_j D_{0j}$, which gives

$$n_0\left(\frac{\alpha P_\beta Q_\alpha + \beta T_\alpha R_\beta}{\alpha P_\alpha Q_\alpha - \alpha T_\alpha R_\alpha}\right)\psi[0] = \sum_j \psi[j]. \quad (40)$$

Here, $P_\beta \equiv P(\epsilon, t, \beta)$ and $P_\alpha \equiv P(\epsilon, s, \alpha)$, etc. The summation extends over all points connected to the origin. For $\alpha = \beta$, the form factor f reduces to the perfect-lattice case, as it must.

Next, we have to consider the form factor for the case in which a perfect-lattice point is connected to a defect as well as the other perfect-lattice points.

Let us represent a perfect-lattice point which is connected to our defect by i. Then, from (38a) and



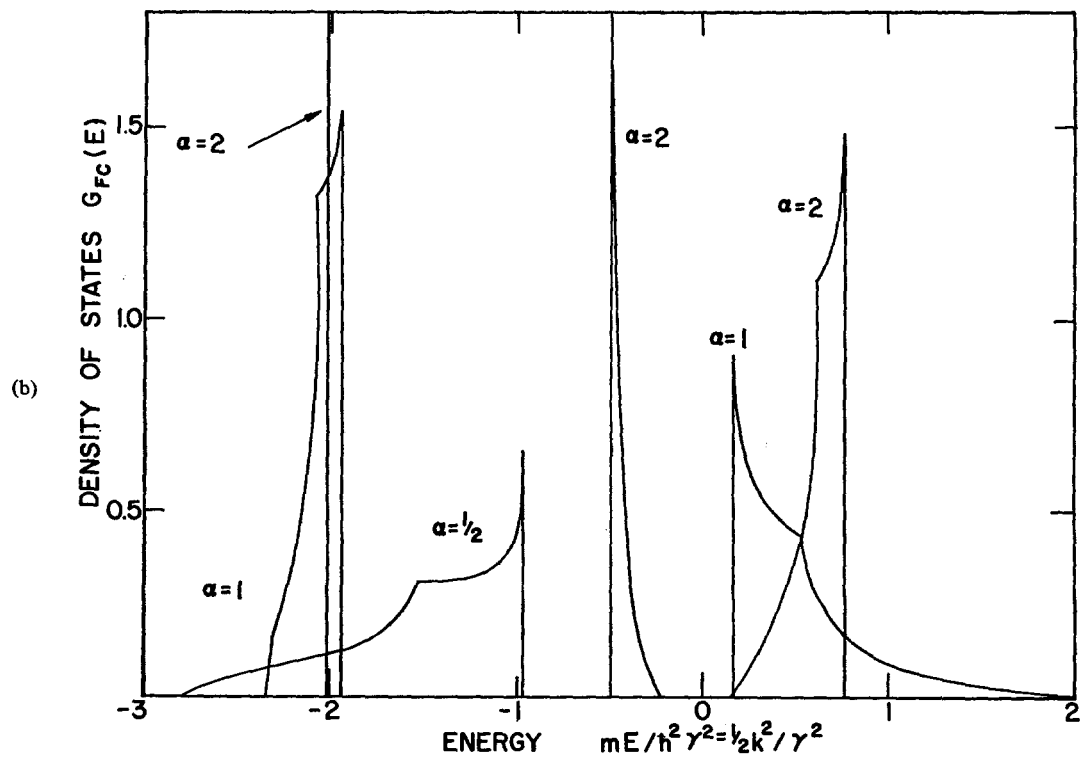


FIG. 10. (a) Face-centered cubic lattice density of states, one bound state per atom, $s = 1$. (b) Face-centered cubic lattice density of states, two bound states per atom, $s = 2$.

(38b), we find

$$D_{i0} = \frac{\psi[0](\beta Q_\beta P_\beta - \beta R_\beta T_\beta) - \psi[i](\beta Q_\beta P_\alpha + \alpha T_\beta R_\alpha)}{\psi[i](\beta Q_\beta T_\alpha + \alpha T_\beta Q_\alpha)} \tag{41a}$$

and, from (14), if j is any normal node point which is connected to i, we have

$$D_{ij} = \{(P_\alpha Q_\alpha - T_\alpha R_\alpha)\psi[j] - (P_\alpha Q_\alpha + T_\alpha R_\alpha)\psi[i]\}/2T_\alpha Q_\alpha \psi[i]. \tag{41b}$$

Then, by applying the conservation condition (16), we have

$$n_i f\psi[i] - \sum_k \psi[i_k] = (f - A)\psi[i] - (1 - c)\psi[0]. \tag{42}$$

The summation over k extends over all nodes connected to i (including the origin), and

$$A = \frac{2T_\alpha Q_\alpha(\beta Q_\beta P_\alpha + \alpha T_\beta R_\alpha)}{(P_\alpha Q_\alpha - T_\alpha R_\alpha)(\beta Q_\beta T_\alpha + \alpha T_\beta Q_\alpha)}, \tag{43a}$$

$$c = \frac{2\beta T_\alpha Q_\alpha(Q_\beta P_\beta - R_\beta T_\beta)}{(P_\alpha Q_\alpha - T_\alpha R_\alpha)(\beta Q_\beta T_\alpha + \alpha T_\beta Q_\alpha)}. \tag{43b}$$

We also define

$$f^* = (\alpha P_\beta Q_\alpha + \beta T_\alpha R_\beta)/(\alpha P_\alpha Q_\alpha - \alpha T_\alpha R_\alpha). \tag{43c}$$

If i is neither a defective node nor connected to a defective node, then the standard node-connection equations (17) are still valid.

As an example of the manner in which these equations are to be applied, let us consider a 1-dimensional chain. Then Eqs. (17), (40), and (42) can be written as

$$2f\psi[j] - \psi[j-1] - \psi[j+1] = (f - A)(\delta_{j,1} + \delta_{j,-1})\psi[j] + [2(f - f^*)\delta_{j,0} - (1 - c)(\delta_{j+1,0} + \delta_{j-1,0})]\psi[0]. \tag{44}$$

Under some conditions, a new bound state develops in which an electron or a deficiency of an electron develops around the defect position. This situation would correspond to the existence of a solution of (44) which would vanish as $|j| \to \infty$.

To find the new defect bound state, we start with the Green's function $g(j)$ which satisfies

$$2fg(j) - g(j-1) - g(j+1) = \delta_{j,0}, \qquad g(j) \to 0, \quad \text{as} \quad |j| \to \infty. \tag{45}$$

This Green's function is

$$g(j,f) = \frac{1}{4\pi}\int_{-\pi}^{\pi} \frac{\exp(ij\phi)\, d\phi}{f - \cos\phi}. \tag{46}$$

If $|f| > 1$, it is well known that

$$g(j,f) = \tfrac{1}{2}(\operatorname{sgn} f)^{j+1}(f^2 - 1)^{-\frac{1}{2}}[|f| - (f^2 - 1)^{\frac{1}{2}}]^{|j|} \tag{47a}$$

$$= (2\sinh z)^{-1}(\operatorname{sgn} f)^{j+1}\exp(-|j|z), \tag{47b}$$

where z is defined by

$$|f| = \cosh z. \tag{47c}$$

Incidentally,

$$g(j,f) = g(-j,f) \quad \text{and} \quad g(j,-f) = (-1)^{j+1}g(j,f). \tag{48}$$

If $F(j)$ is the right-hand side of (44), i.e.,

$$2f\psi[j] - \psi[j-1] - \psi[j+1] = F(j), \tag{49a}$$

then one can easily verify from (49a) that

$$\psi[j] = \sum_{j'=-\infty}^{\infty} g(j - j', f)F(j'), \tag{49b}$$

so that, after introducing $F(j)$ from the rhs of (44), we obtain

$$\psi[j] = (f - A)\{g(j+1)\psi[-1] + g(j-1)\psi[1]\} + [2(cf - f^*)g(j) + (1 - c)\delta_{j,0}]\psi[0]. \tag{50}$$

From these equations we see that, if we know the contribution of the wavefunction nodes 1, −1, and 0 due to the existence of the defect at the origin, the defect contribution to the wavefunction at any node point can be found. We also see, from (47), that the effect of the defect in a 1D chain dies out exponentially as one recedes from the defect. If the defect atom introduces a new electron, it is localized to within a distance $z^{-1} = (\cosh^{-1}|f|)^{-1}$. This distance depends on the energy level associated with the defect wavefunction. This level is found by solving an appropriate eigenvalue problem. The energy is then to be substituted into the formula which expresses the form factor as a function of energy to find f.

The value of the form factor f which gives us the localizability is obtained by successively letting $j = -1, 1, 0$ in Eq. (50). Three homogeneous equations result in $\psi[1]$, $\psi[0]$, and $\psi[-1]$. In order for these equations to have a solution, the determinant of the coefficients must vanish. Two independent characteristic equations follow from this condition:

$$(f - A)\{f - (\operatorname{sgn} f)(f^2 - 1)^{\frac{1}{2}}\} = 1 \tag{51}$$

and

$$(\operatorname{sgn} f)[f^* - f\lambda] = -(f^2 - 1)^{\frac{1}{2}}\lambda, \tag{52a}$$

where

$$\lambda = c - f^*(A - f) = (c - Af^*) + ff^*. \tag{52b}$$

Let us consider (51) first. It is compatible with

$$f^2 - 1 = A^2. \tag{53}$$

One must be a bit careful with signs. We always use the convention that $(x^2)^{\frac{1}{2}} = |x|$; then there are two cases:

(i) If $A > 0$, then $(f^2 - 1) = A^2$, so that

$$(f - A)(f - A \operatorname{sgn} f) = 1, \tag{54}$$

which is compatible with (53) if $f < 0$. In this case,

$$A > 0 \quad \text{implies} \quad f = -(1 + A^2)^{\frac{1}{2}}. \tag{55}$$

(ii) If $A < 0$, then $(f^2 - 1)^{\frac{1}{2}} = -A$, so that, in a similar manner,

$$A < 0 \quad \text{implies} \quad f = (1 + A^2)^{\frac{1}{2}}. \tag{56}$$

Now consider the second characteristic equation (52). It is easy to show that this is compatible with

$$f^2 = 1 + (c - Af^*)^2/(f^*)^2, \tag{57}$$

and that

$(c - Af^*)/f^* > 0$ implies

$$f = [1 + (f^*)^{-2}(c - Af^*)^2]^{\frac{1}{2}}, \tag{58}$$

$(c - Af^*)/f^* < 0$ implies

$$f = -[1 + (f^*)^{-2}(c - Af^*)^2]^{\frac{1}{2}}. \tag{59}$$

The parameters A, c, and f^* depend on the energy E or, equivalently, on ϵ. The same is true of the structure function f. Hence, if the right-hand and left-hand sides of Eqs. (53), (58), and (59) are plotted on the same figure as functions of E or ϵ, the intersection of the two curves gives the value of ϵ and E for the bound state due to the existence of the impurity in the lattice. The bound state energies are plotted as a function of various parameters in Fig. 11. The 3D bound state energies for simple cubic lattices are plotted in Fig. 12. The details of their calculations are given below Eq. (66b).

Let us now investigate the symmetry properties of the various nodal wavefunctions. First consider the case with f related to A by (56). Then it can be shown that (50) becomes

$$\psi[j] = (f - A)[g(j - 1) - g(j + 1)]\psi[1]. \tag{60}$$

We first assume that $f > 1$. Then, from (60) and (47), we have

$$\begin{aligned}\psi[j] &= 2(f - A)(f^2 - 1)^{\frac{1}{2}} g(j)\psi[1] \\ &= 2(A - f)Ag(j)\psi[1], \quad \text{if} \quad j > 1,\end{aligned} \tag{61}$$

since $A < 0$ when $f > 1$. Similarly, we find that

$$\psi[-j] = -2A(A - f)g(j)\psi[1], \quad \text{if} \quad j > 1, \tag{62}$$

so that $\psi[j]$ is an odd function of j with

$$\psi[j] = -\psi[-j]. \tag{63}$$

When $A > 0$ and $F < -1$, one finds [using (47)] that

$$\begin{aligned}\psi[j] &= -2(f - A)(f^2 - 1)^{\frac{1}{2}} g(j)\psi[1] \\ &= 2A(A - f)g(j, f)\psi[1]\end{aligned} \tag{64}$$

and that $\psi[j]$ is an odd function of j, i.e.,

$$\psi[j] = -\psi[-j]. \tag{65}$$

Now we consider the case associated with the second characteristic equation (53). In this case,

$$\psi[j] = f^* g(j, f)\psi[0]/g(1, f) \tag{66a}$$

which is an even function of j.

The number of lattice spacings from the origin over which the defect wavefunction remains localized is [from (47b)]

$$1/z = 1/\cosh^{-1} |f|. \tag{66b}$$

The above results can be generalized to 2D and 3D lattices. While the ideas are the same, the equations become a bit longer. The 2D and 3D analogs of Eq. (50) are

$$\begin{aligned}\psi[j_1, j_2] = (f - A)\{&g(j_1 + 1, j_2)\psi[-1, 0] \\ &+ g(j_1 - 1, j_2)\psi[1, 0] \\ &+ g(j_1, j_2 + 1)\psi[0, -1] \\ &+ g(j_1, j_2 - 1)\psi[0, 1]\} \\ &+ [4(fc - f^*)g(j_1, j_2) \\ &+ (1 - c)\delta_{j_1,0}\delta_{j_2,0}]\psi[0, 0],\end{aligned} \tag{67}$$

$$\begin{aligned}\psi[j_1, j_2, j_3] = (f - A)\{&g(j_1 + 1, j_2, j_3)\psi[-1, 0, 0] \\ &+ g(j_1 - 1, j_2, j_3)\psi[1, 0, 0] \\ &+ g(j_1, j_2 + 1, j_3)\psi[0, -1, 0] \\ &+ g(j_1, j_2 - 1, j_3)\psi[0, 1, 0] \\ &+ g(j_1, j_2, j_3 + 1)\psi[0, 0, -1] \\ &+ g(j_1, j_2, j_3 - 1)\psi[0, 0, 1]\} \\ &+ [6(fc - f^*)g(j_1, j_2, j_3) \\ &+ (1 - c)\delta_{j_1,0}\delta_{j_2,0}\delta_{j_3,0}]\psi[0, 0, 0].\end{aligned} \tag{68}$$

The Green's functions are

$$g(j_1, j_2; f) = \frac{1}{2(2\pi)^2} \iint_{-\pi}^{\pi} \frac{\exp i(j_1\phi_1 + j_2\phi_2)\, d\phi_1\, d\phi_2}{2f - \cos\phi_1 - \cos\phi_2}, \tag{69a}$$

$$g(j_1, j_2; f) = \frac{1}{2(2\pi)^3} \iiint_{-\pi}^{\pi} \frac{\exp i(j_1\phi_1 + j_2\phi_2 + j_3\phi_3)\, d\phi_1\, d\phi_2\, d\phi_3}{3f - \cos\phi_1 - \cos\phi_2 - \cos\phi_3}, \tag{69b}$$

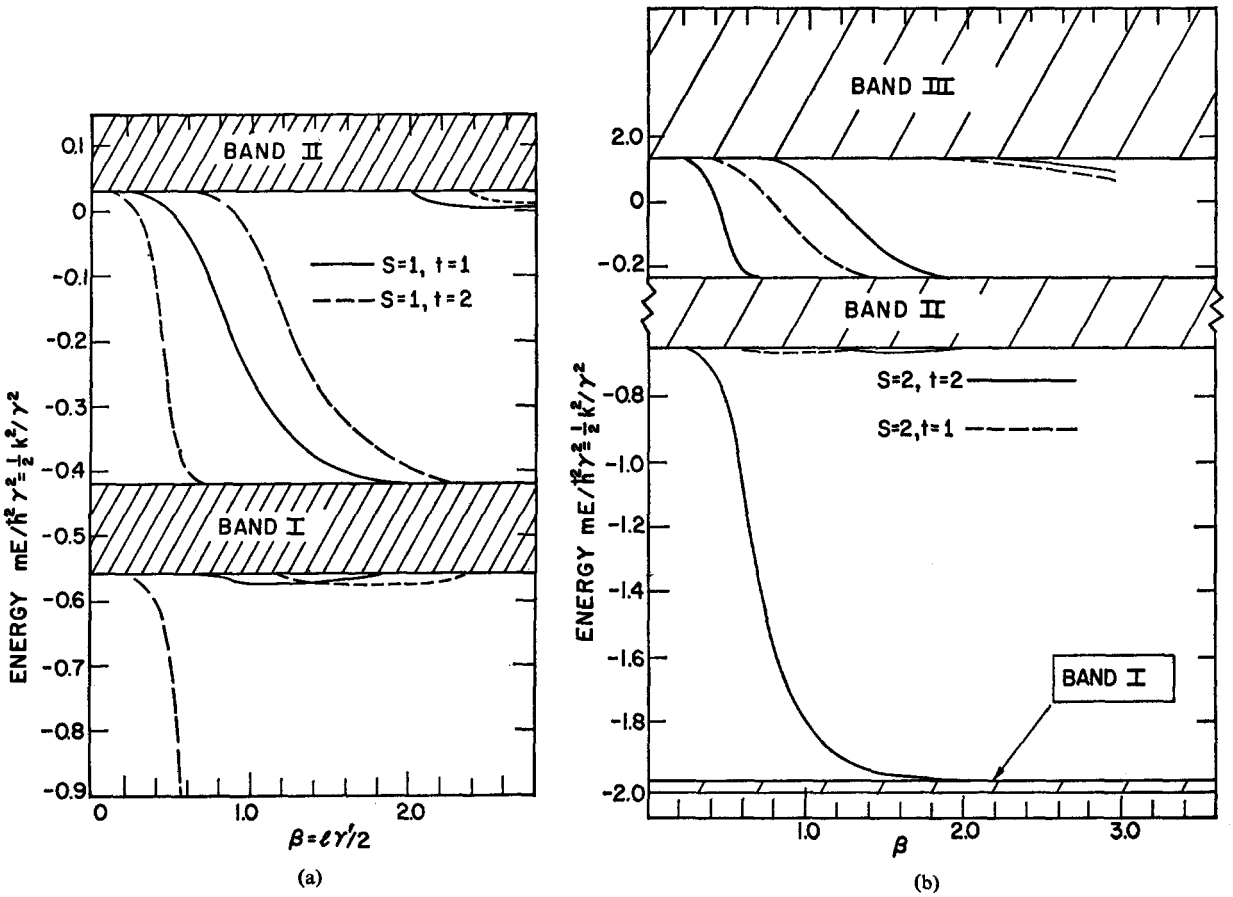


FIG. 11. (a) Variation of impurity energy levels with $\beta = \frac{1}{2}l\gamma'$, where $2(\gamma')^2$ is the well depth of the impurity potential, when $\alpha = \frac{1}{2}\gamma l = 2$. The case $s = 1$, $t = 1$ corresponds to one bound state per defect atom and one bound state per normal atom. The case $s = 1$, $t = 2$ corresponds to a normal atom with one bound state and an impurity atom with two bound states. When β is small, the defect potential is shallow and broad. The energy level associated with it falls in or close to the free electron range (band II). However, as β increases, the well deepens and narrows so that, if a localized electron is identified with it, the electron decreases until $\beta = \alpha$ (= 2 in the special case plotted, when it goes into band I). The solid line which drops from band II to band I in the figure exhibits this process when $t = 1$. The two dotted lines which behave in the same way exhibit the process when $t = 2$. The levels which hug the bottom of band I reflect a somewhat different mechanism. When $\beta < 2$, the impurity potential is shallower and *broader* than that of the normal atoms. This gives a lowering of the connecting energy path between the two neighbors to the defect. When electrons are given more space to expand into, their energy decreases (for example, the lowest energy level of an electron in a box of length a is $E \sim 1/a^2$). The level which drops from band I in the $t = 2$ is merely the location of the lower bound state which does not exist in the normal atoms. This diagram corresponds to a 1D chain with a defect.

(b) Impurity levels in a 1-dimensional chain. As with (a), $\alpha = 2$ for host chain, but now we also choose the atoms of the host chain to have two bound states per atom. The effect of two types of defects presented those in which the defect has two bound states, $s = 2$, and those in which it has only one, $t = 1$.

respectively, with

$$g(1, 0; f) = g(-1, 0; f) = g(0, 1; f) = g(0, -1; f), \quad \text{etc.}, \tag{70}$$

and similarly for the 3D Green's function.

In the 2D case one can successively let (j_1, j_2) be $(-1, 0)$, $(1, 0)$, $(0, -1)$, $(0, 1)$, and $(0, 0)$, while in the 3D case one successively lets (j_1, j_2, j_3) be $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$, $(0, 0, \pm 1)$ and $(0, 0, 0)$. In both the 2D and the 3D cases, one obtains a set of homogeneous equations for the values of the wavefunctions at the node points listed above. Since the determinants of the coefficients of these wavefunctions must vanish in order for the set of equations to have a nonvanishing solution, these determinants can be factored, and one obtains three characteristic equations for a system of given dimensionality. The first set is

$$f = (Af^* - c)/f^* + [g(0)/g(1)] \quad \text{in 1D}, \tag{71a}$$

$$f = (Af^* - c)/f^* + [g(0, 0)/g(1, 0)] \quad \text{in 2D}, \tag{71b}$$

$$f = (Af^* - c)/f^* + [g(0, 0, 0)/g(1, 0, 0)] \quad \text{in 3D}. \tag{71c}$$

The 2D Green's functions can be expressed in terms of elliptic integrals.[14] While the 3D functions have no simple relation to more standard functions, they have been tabulated in Ref. 19 where their various properties have been discussed. The corresponding

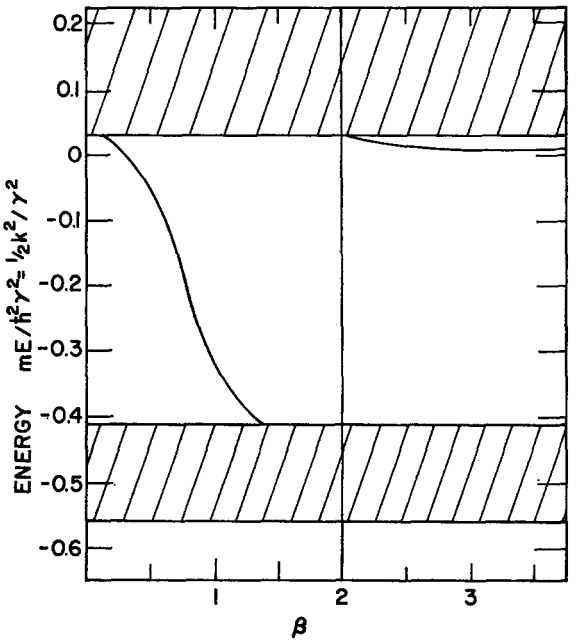


FIG. 12. Impurity levels in 3D network, again with $\alpha = 2$ for host atoms and $s = t = 1$. The main difference between the 1D and 3D cases is that, in the 1D case, any small change in a defect parameter is sufficient to give a defect level. In the 3D case, the difference between the parameter for the defect and for the perfect atom must exceed a critical value before the defect level appears. This situation is well known in the case of localized vibrational states in crystals.

body-centered and face-centered cubic lattice Green's functions have been tabulated in Ref. 20.

The second set of characteristic equations has the form

$$f = A + [g(0) - g(2)]^{-1} \quad \text{once in 1D,} \tag{72a}$$

$$f = A + [g(0,0) - g(0,2)]^{-1} \quad \text{twice in 2D,} \tag{72b}$$

$$f = A + [g(0,0,0) - g(0,0,2)]^{-1} \quad \text{thrice in 3D,} \tag{72c}$$

while the third set has the form

$$f = A + [g(0,0) + g(0,2) - 2g(1,1)]^{-1} \quad \text{once in 2D,} \tag{73a}$$

$$f = A + [g(0,0,0) + g(0,0,2) - 2g(1,1,0)]^{-1} \quad \text{twice in 3D.} \tag{73b}$$

There is no 1D characteristic equation of type (73). The words once, twice, and thrice represent the degree of degeneracy of the characteristic equations with which they are identified.

The 2D wavefunctions which correspond to the characteristic equations (71b), (72b), and (73a) are, respectively,

$$\psi[j_1,j_2] = 4[(fc - f^*) - f(f-A)T_2]g(j_1,j_2)\psi[0,0], \tag{74a}$$

with

$$T_2 = [4(cf - f^*)g(0,0) - c]g(2,0)/g(1,0), \tag{74b}$$

$$\psi(j_1,j_2) = (f-A)[g(j_1+1,j_2) + g(j_1-1,j_2) - g(j_1,j_2+1) - g(j_1,j_2-1)]\psi[1,0], \tag{75}$$

and

$$\psi[j_1,j_2] = (f-A)[g(j_1-1,j_2) - g(j_1+1,j_2] \times \psi[1,0] + (f-A)[g(j_1,j_2-1) - g(j_1,j_2+1)]\psi[0,1]. \tag{76}$$

In the 3D case, the corresponding equations for the wavefunctions, associated respectively with (71c), (72c), and (73c), are

$$\psi[j_1,j_2,j_3] = 6[(fc - f^*) - f(f-A)T_3] \times g(j_1,j_2,j_3)\psi[0,0,0] \tag{77a}$$

with

$$T_3 = [6(cf - f^*)g(0,0,0) - c]g(2,0,0)/g(1,0,0), \tag{77b}$$

$$\begin{aligned}\psi[j_1,j_2,j_3] = (f-A)\{&[g(j_1+1,j_2,j_3) + g(j_1-1,j_2,j_3)]\psi[1,0,0] \\ &+ [g(j_1,j_2+1,j_3) + g(j_1,j_2-1,j_3)]\psi[0,1,0] \\ &+ [g(j_1,j_2,j_3+1) + g(j_1,j_2,j_3-1)]\psi[0,0,1]\},\end{aligned} \tag{78}$$

and

$$\begin{aligned}\psi[j_1,j_2,j_3] = (f-A)\{&[g(j_1-1,j_2,j_3) - g(j_1+1,j_2,j_3)]\psi[1,0,0] \\ &+ [g(j_1,j_2-1,j_3) - g(j_1,j_2+1,j_3)]\psi[0,1,0] \\ &+ [g(j_1,j_2,j_3-1) - g(j_1,j_2,j_3+1)]\psi[0,0,1]\}.\end{aligned} \tag{79}$$

In the 3D case, the degree of localization of the impurity wavefunction follows from the asymptotic character of $g(j_1,j_2,j_3)$:

$$\begin{aligned}g(j_1,j_2,j_3) \sim{}& \frac{\exp(-AR)}{4\pi R} \\ &+ \frac{1}{768\pi(2\pi)^{\frac{1}{2}}}\left(\frac{16(j_1^4+j_2^4+j_3^4)}{R^7}(AR)^{\frac{7}{2}}K_{\frac{7}{2}}(AR)\right. \\ &- \frac{48(j_1^2+j_2^2+j_3^2)}{R^5}(AR)^{\frac{5}{2}}K_{\frac{5}{2}}(AR) \\ &\left.+ \frac{72}{R^3}(AR)^{\frac{3}{2}}K_{\frac{3}{2}}(AR)\right) + \cdots,\end{aligned} \tag{80}$$

where $K_n(x)$ is modified Bessel function of the second kind,

$$A^2 = 6(f-1), \quad \text{and} \quad R^2 = j_1^2 + j_2^2 + j_3^2.$$

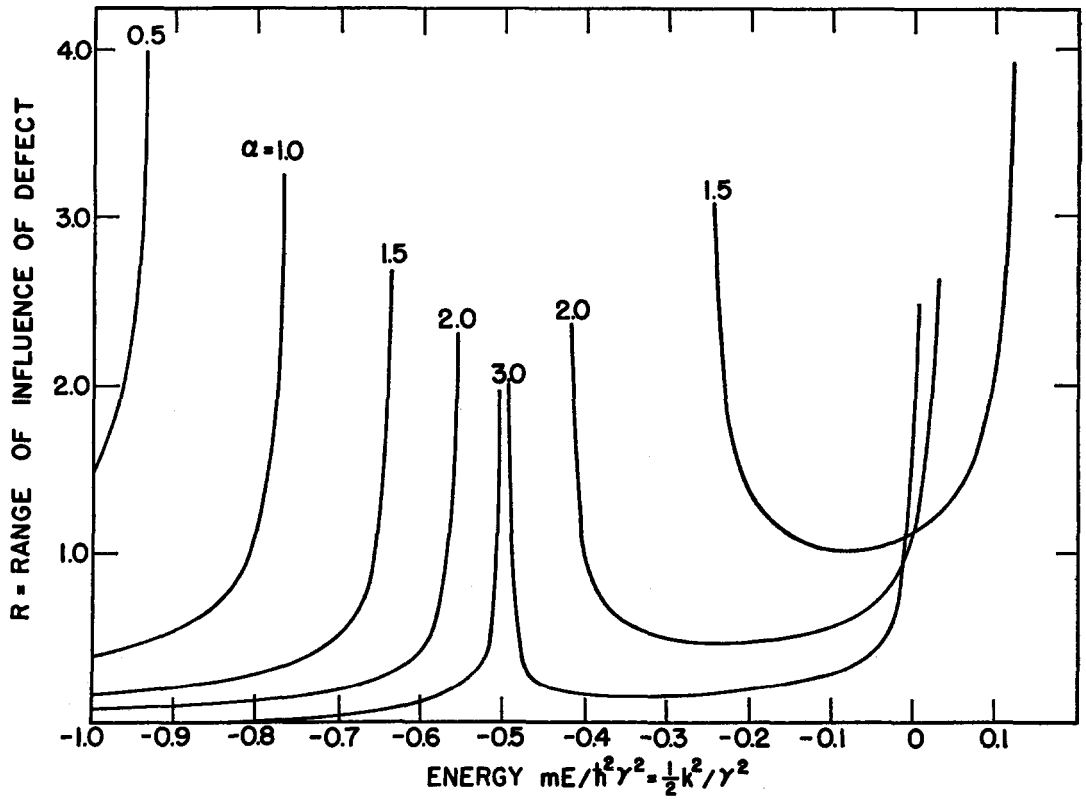


FIG. 13. The range of influence of a defect in a 3D network as a function of the location of the impurity energy level. The further the impurity level from band edges, the longer its range.

To a first approximation, the range of localization is obtained by setting $AR = 1$ or

$$R \sim [6(f-1)]^{\frac{1}{2}}. \tag{81}$$

This quantity is plotted in Fig. 13 as a function of energy when $s = 1$ for various α's. Notice that, as an impurity approaches the allowed band edge with $|F| \sim 1$, the range of localization tends to infinity.

Certain symmetries can be deduced from Eqs. (77a), (78), and (79). The wavefunctions (77a) [which correspond to characteristic equations (71)] are symmetrical with $\psi[j] = \psi[-j]$ and $\psi[0]$ finite. Wavefunctions (78) are symmetric with $\psi[0] = 0$, while (79) is antisymmetric with $\psi[0] = 0$.

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[1] E. W. Montroll, J. Math. Phys. **11**, 635 (1970).
[2] L. Pauling, J. Chem. Phys. **4**, 673 (1936).
[3] H. Kuhn, Helv. Chem. Acta **31**, 1441 (1948); J. Chem. Phys. **2**, 2098 (1954).
[4] J. Platt, J. Chem. Phys. **17**, 484 (1949); **21**, 1597 (1953).
[5] K. Ruedenberg and C. W. Scherr, J. Chem. Phys. **21**, 1565 (1953).
[6] T. S. Griffith, J. Chem. Phys. **21**, 174 (1953).
[7] C. A. Coulson, Proc. Phys. Soc. (London) **67**, 608 (1954); **68**, 1129 (1955).
[8] M. F. Manning, Phys. Rev. **38**, 161 (1935).
[9] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965).
[10] *Handbook of Mathematical Functions*, M. Abramowitz and I. Stegun, Eds. (Nat. Bur. Std., Washington, D.C., 1964).
[11] F. J. Dyson, Phys. Rev. **102**, 1217 (1956).
[12] G. F. Koster and J. C. Slater, Phys. Rev. **95**, 1167 (1954); **96**, 1208 (1964).
[13] E. W. Montroll and G. H. Weiss, J. Math. Phys. **6**, 167 (1965).
[14] E. W. Montroll, Proc. Berkeley Symp. Math. Statist. Probl. **3**, 209 (1956).
[15] E. M. Baroody, J. Math. Phys. **10**, 475 (1969).
[16] R. J. Jelitto, J. Phys. Chem. Solids **30**, 609 (1969).
[17] I. M. Lifshitz, Nuovo Cimento Suppl. **3**, 716 (1956).
[18] E. W. Montroll and R. B. Potts, Phys. Rev. **100**, 525 (1955); **102**, 72 (1956).
[19] A. Maradudin, E. Montroll, G. Weiss, R. Herman, and H. Milnes, Acad. Roy. Belg., Classe Sci., Mem.: Collection in 4°**14**, No. 1709 (1960).
[20] I. Mannari and C. Kawabata, "Extended Watson Integrals and their Derivatives," Dept. of Physics Okayama University, Research Note No. 15, Okayama, Japan, 1964.

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Theory of Formal Series with Applications to Quantum Field Theory

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The theory of formal series is developed in such a way that it includes conventional formal series as well as Volterra's series (generating functionals) as special cases. A method for expressing solutions of nonlinear equations is developed.

INTRODUCTION

In quantum field theory one encounters infinite sets of symmetric distributions,[1] "r and τ functions," satisfying complicated nonlinear integral equations such as Schwinger's[2] equations and the general unitarity equations.[3] These equations may be brought into a compact form by the introduction of formal "generating functionals" and formal functional differential operators.[2,4-6]

These generating functionals are formal Volterra's series

$$\mathcal{F}[J] = \sum_{n\geq 0} \int \cdots \int dx_1 \cdots dx_n \times \varphi_n(x_1, \cdots, x_n) J(x_1) \cdots J(x_n). \quad (1)$$

However, such a series is not a conventional one. Indeed, its coefficients should be the "values $\varphi_n(x_1, \cdots, x_n)$" of φ_n for given sets of points $(x_1, \cdots, x_n)$, expressions which are generally meaningless since the φ_n are not functions. This is because the defining property of the φ_n is such that they are symmetric multilinear mappings over some function's vector spaces.

Therefore, the "indeterminate function" J appearing in (1) must not be considered as an infinite family $(J(x))_x$ of indeterminates $J(x)$ but as *one* indeterminate.

The aim of this paper is a generalization of the theory of formal series such that it includes the formal Volterra's series considered in (1).

Let $\mathbb{K}[[X_1, \cdots, X_m]]$ denote the algebra of the formal series[7,8] with respect to the indeterminate $(X_1, \cdots, X_m)$, with coefficients in a field $\mathbb{K}$, and let

$$\sum_{q\geq 0} \left(\sum_{i_1=1}^{m} \sum_{i_q=1}^{m} a_{\lambda;i_1,\cdots,i_q} X_{i_1} \cdots X_{i_q} \right), \quad \lambda = 1, 2, \cdots, n, \quad (2)$$

be n formal series of $\mathbb{K}[[X_1, \cdots, X_m]]$.

The coefficients $a_{\lambda;i_1,\cdots,i_q}$ of the terms of degree q define a q-linear symmetric mapping which we shall denote by α_q with values into $\mathbb{K}^n$. Therefore, with the n series (2), we may associate the expression

$$\sum_{q\geq 0} \alpha_q X^q, \quad (3)$$

which will be called a formal series of $\mathbb{K}^m$ into $\mathbb{K}^n$ with respect to the indeterminate X. The α_q are, by definition, the kernels of this formal series. Conversely, there corresponds to (3) one and only one set of n elements of $\mathbb{K}[[X_1, \cdots, X_m]]$.

Suppose that E and F are two vector spaces over the field $\mathbb{K}$. A formal series of E into F with respect to the indeterminate X is an expression of the form $\sum_{q\geq 0} \tilde{\alpha}_q X^q$, where $\tilde{\alpha}_q$ is a q-linear symmetric mapping on E with values in F. We denote the set of these formal series by $\bar{F}[E, [X]]$.

If E and F are finite-dimensional spaces ($\dim E = m$ and $\dim F = n$), then E is isomorphic to $\mathbb{K}^m$ and F to $\mathbb{K}^n$. Therefore, the notion of a formal series of E into F is equivalent to the notion of formal series of $\mathbb{K}^m$ into $\mathbb{K}^n$ and hence to the notion of n formal series with respect to m indeterminates with coefficients in $\mathbb{K}$.

However, this is not the case for general vector spaces E and F. This is the reason why the concept of formal series of E into F is the generalization of the usual notion of formal series with coefficients in a field K. Roughly speaking, the idea of a kernel is more general than the idea of coefficient even if both concepts are equivalent for the finite-dimensional case. Clearly, the former concept includes the formal Volterra series.

In the first four sections of this paper, the conventional concepts which enter in the theory of formal series are generalized. In Sec. 5, differentials for such series are defined and a differential calculus developed. In Sec. 6, the existence and uniqueness of solutions for formal series equations are investigated, while in Sec. 7 we solve these equations in specific cases; as an example, we shall write down the perturbative solution of the classical (c-number) Yang–Feldmann equation in compact form.

1. MONOMIAL AND POLYNOMIAL MAPPINGS

Let I be a finite set of indices. Let F denote a vector space over a commutative field $\mathbb{K}$ and $(E_i)_{i\in I}$ denote a family of vector spaces over the same field $\mathbb{K}$. ($\mathbb{K}$ is supposed to have the characteristic zero.)

If $\mathbb{N}$ is the set of natural integers, then $\mathbb{N}^I$ denotes the set of families $(n_i)_{i\in I}$ with $n_i \in \mathbb{N}$, $i \in I$. We shall also write simply (n_i) for such a family when no confusion can arise.

Definition 1: A mapping $\tilde{\varphi}: \prod_{i\in I} E_i \to F$ is said to be a monomial of degree $(n_i)_{i\in I}$ if there is a linear mapping[9]

$$\Phi: \bigotimes_{i\in I} \left(\overset{n_i}{\otimes} E_i\right) \to F$$

such that

$$\tilde{\varphi}((j_i)) = \Phi\left(\bigotimes_{i\in I} \left(\overset{n_i}{\otimes} j_i\right)\right), \quad \forall (j_i)_{i\in I} \in \prod_{i\in I} E_i.$$

The integers n_i will be called partial degrees of $\tilde{\varphi}$ and the integer $|(n_i)| = \sum_{i\in I} n_i$ will be called the total degree of $\tilde{\varphi}$.

The set $M_{(n_i)}[\prod_{i\in I} E_i, F]$ of the monomial mappings of degree (n_i) of $\prod_{i\in I} E_i$ into F is a subspace of the vector space of the mappings of $\prod_{i\in I} E_i$ into F. $M_{(n_i)}[\prod_{i\in I} E_i, F]$ is isomorphic to the space

$$\mathfrak{L}\left(\bigotimes_{i\in I}\left(\overset{n_i}{\vee} E_i\right), F\right)$$

of the linear mappings of $\otimes_{i\in I} (\vee^{n_i} E_i)$ into F. In fact, for any

$$\tilde{\varphi} \in M_{(n_i)}\left[\prod_{i\in I} E_i, F\right]$$

there is one and only one $\varphi \in \mathfrak{L}(\otimes_{i\in I} (\vee^{n_i} E_i), F)$ such that

$$\tilde{\varphi}((j_i)) = \varphi\left(\bigotimes_{i\in I}\left(\overset{n_i}{\vee} j_i\right)\right), \quad \text{for all} \quad (j_i) \in \prod_{i\in I} E_i.$$

This one-to-one mapping $\tilde{\varphi} \rightsquigarrow \varphi$ is clearly linear. We shall write $\varphi(\otimes_{i\in I} (\vee^{n_i} j_i)) = \varphi \prod_{i\in I} j_i^{n_i}$ when no confusion can arise. Then $(j_i)_{i\in I} \rightsquigarrow \varphi \prod_{i\in I} j_i^{n_i}$ denotes the monomial mapping $\tilde{\varphi}$.

Definition 2: A mapping: $\varpi \prod_{i\in I} E_i \to F$ is said to be polynomial if it is a finite sum of monomial mappings. The supremum of the total degrees of these monomial mappings will be called the degree of ϖ, degree (ϖ).

The set $P[\prod_{i\in I} E_i, F]$ of the polynomial mappings is a subspace of the vector space of the mappings of $\prod_{i\in I} E_i$ into F. $P[\prod_{i\in I} E_i, F]$ is isomorphic with the space $\oplus_{(n_i)} \mathfrak{L}(\otimes_{i\in I} (\vee^{n_i} E_i), F)$.

We shall write $(j_i)_{i\in I} \rightsquigarrow \sum_{(n_i)} \varphi_{(n_i)} \prod_{i\in I} j_i^{n_i}$ for the polynomial mapping sum of the monomial mappings $(j_i)_{i\in I} \to \varphi_{(n_i)} \prod_{i\in I} j_i^{n_i}$ with *distinct* degrees (n_i); this decomposition is clearly unique.

2. FORMAL SERIES

Definition 3: A formal series of $(E_i)_{i\in I}$ into F with respect to the indeterminates J_i $(i \in I)$ is a pair $((J_i)_{i\in I}, (\tilde{\varphi}_{(n_i)})(n_i) \in \mathbb{N}^I)$, where $(J_i)_{i\in I}$ is a family whose terms are called indeterminates and where $(\tilde{\varphi}_{(n_i)})_{(n_i)\in\mathbb{N}^I}$ is a family of mappings of $\prod_{i\in I} E_i$ into F having $\mathbb{N}^I$ as the set of indices such that, for any $(n_i) \in \mathbb{N}^I$, $\tilde{\varphi}_{(n_i)}$ is a monomial mapping of degree (n_i). We write

$$\mathcal{F}[(J_i)_{i\in I}] = \sum_{(n_i)} \varphi_{(n_i)} \prod_{i\in I} J_i^{n_i} \quad (= \mathcal{F})$$

for such a formal series. The $\varphi_{(n_i)}$ are the kernels of $\mathcal{F}$, for $\varphi_{(n_i)} \in \mathfrak{L}(\otimes_{i\in I} (\vee^{n_i} E_i), F)$. We make the identification $\varphi_{(0)} \prod_{i\in I} J_i^0 \equiv \varphi_{(0)} \in F$.

The set $\bar{F}[E_i, [J_i]]_{i\in I}$ of these formal series is, by construction, in bijection with the vector space $\prod_{(n_i)\in\mathbb{N}^I} \mathfrak{L}(\otimes_{i\in I} (\vee^{n_i} E_i), F)$. We define a structure of vector space on $\bar{F}[E_i, [J_i]]_{i\in I}$ such that this bijection becomes an isomorphism of vector spaces.

Definition 4: A polynomial of $(E_i)_{i\in I}$ into F with respect to the indeterminates J_i $(i \in I)$ is a formal series $\sum_{(n_i)} \varphi_{(n_i)} \prod_{i\in I} J_i^{n_i}$ such that $\varphi_{(n_i)} = 0$ except for a finite number of (n_i). When there is only one $(n_i) \in \mathbb{N}^I$ such that $\varphi_{(n_i)} \neq 0$, this polynomial is called a monomial of degree (n_i) of $(E_i)_{i\in I}$ into F with respect to the indeterminates J_i $(i \in I)$.

The set $\bar{F}[E_i, J_i]_{i\in I}$ of these polynomials is a subspace of $\bar{F}[E_i, [J_i]]_{i\in I}$; this vector space is isomorphic to $P[\prod_{i\in I} E_i, F]$.

For the polynomials and the monomials we have also the notions of degree, partial degree, and total degree defined for the corresponding polynomial and monomial mappings.

Definition 5: The order $\omega(\mathcal{F})$ of a formal series

$$\mathcal{F} = \sum_{(n_i)} \varphi_{(n_i)} \prod_{i\in I} J_i^{n_i} \neq 0$$

is the lowest number

$$\omega(\mathcal{F}) = \sum_{i\in I} n_i = |(n_i)| \quad \text{with} \quad \varphi_{(n_i)} \neq 0.$$

If L is a set of indices, a family $(\mathcal{F}^\lambda)_{\lambda\in L}$ of formal series $\mathcal{F}^\lambda \in \bar{F}[E_i, [J_i]]_{i\in I}$ is said to be summable if, for any $n \in \mathbb{N}$, $\omega(\mathcal{F}^\lambda) > n$ except for a finite number of indices λ. If $(\mathcal{F}^\lambda)_{\lambda\in L}$ is such a family with

$$\mathcal{F}^\lambda[(J_i)] = \sum_{(n_i)} \varphi^\lambda_{(n_i)} \prod_{i\in I} J_i^{n_i},$$

then for each $(n_i) \in \mathbb{N}^I$ there is only a finite number of $\varphi^\lambda_{(n_i)} \neq 0$. Therefore,

$$\varphi_{(n_i)} = \sum_{\lambda \in L} \varphi^\lambda_{(n_i)}$$

has a meaning, and

$$\mathcal{F}[(J_i)] = \sum_{(n_i)} \varphi_{(n_i)} \prod_{i \in I} J_i^{n_i}$$

is a well-defined formal series. This formal series is called the sum of the family $(\mathcal{F}^\lambda)_{\lambda \in L}$, and we write

$$\mathcal{F}[(J_i)] = \sum_{\lambda \in L} \mathcal{F}^\lambda[(J_i)].$$

Let $\mathcal{F}[(J_i)]$ be a formal series whose kernels are $\varphi_{(n_i)}$ for $(n_i) \in \mathbb{N}^I$. The family

$$\left(\varphi_{(n_i)} \prod_{i \in I} J_i^{n_i}\right)_{(n_i) \in \mathbb{N}^I}$$

is clearly summable and its sum is just $\mathcal{F}[(J_i)]$. This is a justification of the notation

$$\mathcal{F}[(J_i)] = \sum_{(n_i)} \varphi_{(n_i)} \prod_{i \in I} J_i^{n_i}.$$

3. PRODUCTS OF FORMAL SERIES

A. Case of F an Algebra

Suppose now that F is an algebra over the field $\mathbb{K}$ and let us denote by fTf' the product of two elements f and f' of F.

Given two mappings u and u' of $\prod_{i \in I} E_i$ into F we define a new mapping uTu' of $\prod_{i \in I} E_i$ into F by

$$uTu'((j_i)) = u((j_i))Tu'((j_i)) \quad \text{for any} \quad (j_i) \in \prod_{i \in I} E_i.$$

With this product the vector space of the mappings of $\prod_{i \in I} E_i$ into F becomes an algebra over $\mathbb{K}$, and the space $P[\prod_{i \in I} E_i, F]$ of the polynomial mappings is a subalgebra of this algebra. If $\tilde{\varphi}$ is a monomial mapping of degree (n_i) and if $\tilde{\varphi}'$ is a monomial mapping of degree (n'_i), $\tilde{\varphi}T\tilde{\varphi}'$ is a monomial mapping of degree $(n_i + n'_i)$. We denote by $\varphi T\varphi'$ the element of

$$\mathcal{L}\left(\bigotimes_{i \in I} \left(\bigvee^{n_i} E_i\right), F\right)$$

corresponding to

$$\tilde{\varphi}T\tilde{\varphi}' \in M_{(n_i+n_{i'})}\left[\prod_{i \in I} E_i, F\right]$$

[therefore, $\tilde{\varphi}T\tilde{\varphi}' = (\varphi T\varphi')\tilde{}$].

Let

$$\mathcal{F}'[(J_i)] = \sum_{(n_i)} \varphi'_{(n_i)} \prod_{i \in I} J_i^{n_i}$$

and

$$\mathcal{F}''[(J_i)] = \sum_{(n_i)} \varphi''_{(n_i)} \prod_{i \in I} J_i^{n_i}$$

be two formal series of $\bar{F}[E_i, [J_i]]_{i \in I}$. The family

$$\left(\varphi'_{(n_{i'})} T \varphi''_{(n_{i''})} \prod_{i \in I} J_i^{n_{i'}+n_{i''}}\right)((n'_i), (n''_i)) \in \mathbb{N}^I \times \mathbb{N}^I$$

is summable. We denote its sum by $\mathcal{F}'T\mathcal{F}''[(J_i)]$, and we call it the product of the series $\mathcal{F}'$ and $\mathcal{F}''$.

We have

$$\mathcal{F}'T\mathcal{F}''[(J_i)] = \sum_{(n_i)} \varphi_{(n_i)} \prod_{i \in I} J_i^{n_i},$$

with

$$\varphi_{(n_i)} = \sum_{(n_{i'}+n_{i''})=(n_i)} \varphi'_{(n_{i'})} T \varphi''_{(n_{i''})}.$$

With this product, $\bar{F}[E_i, [J_i]]_{i \in I}$ becomes an algebra over the field $\mathbb{K}$. $\bar{F}[E_i, J_i]_{i \in I}$ is a subalgebra of this algebra (in fact, $\bar{F}[E_i, J_i]_{i \in I}$ is clearly isomorphic with the algebra $P[\prod_{i \in I} E_i, F]$).

B. Algebraic Inverse

We suppose now that there is an unit element in the algebra F; this element is denoted by u. If $f \in F$ has an inverse (for T), we denote it by f^{T-1} or $T^{-1}f$.

In the algebra $\bar{F}[E_i, [J_i]]_{i \in I}$ there is also a unit element, which is the formal series whose kernels are $\varphi_{(0)} = u$ and $\varphi_{(n_i)} = 0$ if $(n_i) \neq 0$. We denote it also by u. If $\mathcal{F} \in \bar{F}[E_i, [J_i]]_{i \in I}$ has an inverse, we shall write $T^{-1}\mathcal{F}$ for this inverse.

Let $\mathcal{F}$ be a formal series of $\bar{F}[E_i, [J_i]]_{i \in I}$; for any $n \in \mathbb{N}$ we define $T^n\mathcal{F}$ by $T^0\mathcal{F} = u$, $T^1\mathcal{F} = \mathcal{F}$, and $T^n\mathcal{F} = (T^{n-1}\mathcal{F})T\mathcal{F}$ for $n > 0$.

Proposition 1: For any $\mathcal{F}[(J_i)] \in \bar{F}[E_i, [J_i]]_{i \in I}$ such that $\omega(\mathcal{F}) \geq 1$, the family $(T^n\mathcal{F})_{n \in \mathbb{N}}$ is summable and

$$T^{-1}(u - \mathcal{F}) = \sum_{n \in \mathbb{N}} T^n\mathcal{F}.$$

Corollary: A formal series

$$\sum_{(n_i)} \varphi_{(n_i)} \prod_{i \in I} J_i^{n_i} \in \bar{F}[E_i, [J_i]]_{i \in I}$$

has an inverse if and only if $\varphi_{(0)} \in F$ has an inverse (in F).

C. Case of F a Vector Space

We come back now to the general case where F is an arbitrary vector space over the field $\mathbb{K}$. F may be considered as subspace of the tensor algebra $T(F)$ or as subspace of the exterior algebra $\bigwedge F$ or as subspace of the symmetric algebra $\bigvee F$:

$$T(F) = \bigoplus_{n \geq 0} \left(\bigotimes^n F\right),$$

$$\bigwedge F = \bigoplus_{n \geq 0} \left(\bigwedge^n F\right),$$

$$\bigvee F = \bigoplus_{n \geq 0} \left(\bigvee^n F\right).$$

As a result of this, any formal series of $\bar{F}[E_i, [J_i]]_{i\in I}$ may be considered as an element of $\overline{T(F)}[E_i, [J_i]]_{i\in I}$ or as an element of $\overline{\wedge F}[E_i, [J_i]]_{i\in I}$. Therefore, if $\mathcal{F}'$ and $\mathcal{F}\mathcal{F}''$ are two formal series of $\bar{F}[E_i, [J_i]]_{i\in I}$, we define as in Sec. 3A the tensor product $\mathcal{F}' \otimes \mathcal{F}''$, the exterior product $\mathcal{F}' \wedge \mathcal{F}''$, and the symmetric product $\mathcal{F}' \vee \mathcal{F}''$. We have the following inclusions:

$$\bar{F}[E_i, [J_i]]_{i\in I} \otimes \bar{F}[E_i, [J_i]]_{i\in I} \subset \overline{F\otimes F}[E_i, [J_i]]_{i\in I},$$

$$\bar{F}[E_i, [J_i]]_{i\in I} \wedge \bar{F}[E_i, [J_i]]_{i\in I} \subset \overline{F\wedge F}[E_i, [J_i]]_{i\in I},$$

$$\bar{F}[E_i, [J_i]]_{i\in I} \vee \bar{F}[E_i, [J_i]]_{i\in I} \subset \overline{F\vee F}[E_i, [J_i]]_{i\in I}.$$

D. Formal Series

More generally, let L be a finite set of indices and $(I_\lambda)_{\lambda\in L}$ a family of finite sets of indices. $(F_\lambda)_{\lambda\in L}$ and $(E_{i_\lambda})_{i_\lambda\in I_\lambda}$ for $\lambda \in L$ are families of vector spaces over $\mathbb{K}$.

The spaces $\bar{F}_\lambda[E_{i_\lambda}, [J_{i_\lambda}]]_{i_\lambda\in I_\lambda}$ for $\lambda \in L$ may be considered as subspaces of the algebra

$$\bigotimes_{\lambda\in L} \overline{T(F_\lambda)}[E_i, [J_i]]_{i\in \bigcup_{\lambda\in L} I_\lambda}.$$

Therefore, for any family $(\mathcal{F}^\lambda)_{\lambda\in L}$ of formal series $\mathcal{F}^\lambda \in \bar{F}_\lambda[E_{i_\lambda}, [J_{i_\lambda}]]_{i_\lambda\in I_\lambda}$ we define their tensor product $\otimes_{\lambda\in L}\mathcal{F}_\lambda$. This product is an element of

$$\overline{\bigotimes_{L\ni\lambda} F_\lambda}[E_i, [J_i]]_{i\in \bigcup_{\lambda\in L} I_\lambda}.$$

Remark: If, for any $\lambda \in L$, $F_\lambda = F$, this tensor product is obtained as a specific case of the tensor product defined in Sec. 3C because $\bar{F}[E_{i_\lambda}, [J_{i_\lambda}]]_{i_\lambda\in I_\lambda}$ may be considered as a subspace of $\bar{F}[E_i, [J_i]]_{i\in \bigcup_{\lambda\in L} I_\lambda}$.

4. SUBSTITUTIONS OF FORMAL SERIES

Let L be a finite set of indices and $(I_\lambda)_{\lambda\in L}$ a family of finite sets of indices. $(F_\lambda)_{\lambda\in L}$ and $(E_{i_\lambda})_{i_\lambda\in I_\lambda}$ for $\lambda \in L$ are families of vector spaces over the same field $\mathbb{K}$, and F is a vector space over $\mathbb{K}$. Let $(\mathcal{F}^\lambda[(J_{i_\lambda})])_{\lambda\in L}$ be a family of formal series

$$\mathcal{F}^\lambda[(J_{i_\lambda})] = \sum_{(n_{i_\lambda})} \varphi^\lambda_{(n_{i_\lambda})} \prod_{i_\lambda\in I_\lambda} J_i^{n_{i\lambda}} \in \bar{F}_\lambda[E_{i_\lambda}, [J_{i_\lambda}]]_{i_\lambda\in I_\lambda},$$

and let $\varphi_{(n_\lambda)} \prod_{\lambda\in L} J_\lambda^{n_\lambda}$ be a monomial of $\bar{F}[F_\lambda, J_\lambda]_{\lambda\in L}$. $\varphi_{(n_\lambda)}(\otimes_{\lambda\in L}(\vee^{n_\lambda}(\mathcal{F}^\lambda))$ denotes the formal series of $\bar{F}[E_i, [J_i]]_{i\in \cup_{\lambda\in L} I_\lambda}$ whose kernels are

$$\varphi_{(n_\lambda)} \circ \left\{ \bigotimes_{\lambda\in} \left(\vee^{n_\lambda} \varphi^\lambda_{(n_\lambda)} \right) \right\}.$$

More generally, if $\varpi[(J_\lambda)]$ is a polynomial of $\bar{F}[F_\lambda, J_\lambda]_{\lambda\in L}$ whose kernels are $(\varphi_{(n_\lambda)})$, we define $\varpi[(\mathcal{F}^\lambda)]$ by

$$\varpi[(\mathcal{F}^\lambda)_{\lambda\in L}] = \sum_{(n_\lambda)} \varphi_{(n_\lambda)} \left(\bigotimes_{\lambda\in L} \left(\vee^{n_\lambda} \mathcal{F}^\lambda \right) \right).$$

$\varpi[(\mathcal{F}^\lambda)]$ is a formal series of

$$\bar{F}[E_i, [J_i]]_{i\in \bigcup_{\lambda\in L} I_\lambda},$$

which is said to be obtained by substitution of the series $\mathcal{F}^\lambda$ to the indeterminates J_λ for $\lambda \in L$ in the polynomial $\varpi[(J_\lambda)]$.

Suppose now that, for any $\lambda \in L$, $\omega(\mathcal{F}^\lambda) \geq 1$, and let $\mathcal{F}[(J_\lambda)]$ be a formal series of $\bar{F}[F_\lambda, [J_\lambda]]_{\lambda\in L}$ whose kernels are the $\varphi_{(n_\lambda)}$ for $(n_\lambda) \in \mathbb{N}^L$. The family

$$\left(\varphi_{(n_\lambda)} \left(\bigotimes_{\lambda\in L} \left(\vee^{n_\lambda} \mathcal{F}^\lambda \right) \right) \right)_{(n_\lambda)\in\mathbb{N}}$$

is summable. We denote its sum by $\mathcal{F}[(\mathcal{F}^\lambda)]$. $\mathcal{F}[(\mathcal{F}^\lambda)_{\lambda\in L}]$ is a formal series of $\bar{F}[E_i, [J_i]]_{i\in \bigcup_{\lambda\in L} I_\lambda}$, which is said to be obtained by substitution of $\mathcal{F}^\lambda$ to the indeterminate J_λ for $\lambda \in L$ in the series $\mathcal{F}[(J_\lambda)]$.

The indeterminate J_λ may be considered as formal series of $\bar{F}_\lambda[F_\lambda[J_\lambda]]$. This justifies the notation $\mathcal{F}[(J_\lambda)]$.

Any element of $\bar{F}[E_i, [J_i]]_{i\in I}$ may be considered as an element of $\bar{F}[E_i, [J_i]]_{i\in C_I I'}[E_j, [J_j]]_{j\in I'}$ if $I' \subset I$ and $C_I I' = I - I'$ is its complement. A formal-series element of $\bar{F}[E_i, [J_i]]_{i\in I}$ is said to be polynomial in $J_j, j \in I'$, if it is a polynomial element of

$$\bar{F}[E_i, [J_i]]_{i\in I-I'}[E_j, J_j]_{j\in I'}.$$

If $\mathcal{F}[(J_\lambda)]$ is polynomial in $J_{\lambda'}$ $(\lambda' \in L')$ $(L' \subset L)$, we may substitute a series $\mathcal{F}^{\lambda'}$ of arbitrary order $\omega(\mathcal{F}^{\lambda'})$ for the indeterminate $J_{\lambda'}$, $\lambda' \in L'$, in $\mathcal{F}[(J_\lambda)]$.

5. TRANSLATIONS, DIFFERENTIALS, AND DERIVATIVES

Definition 6: Let $\mathcal{F}[(J_i)_{i\in I}]$ be an element of the space $\bar{F}[E_i, [J_i]]_{i\in I}$, and let $(J'_i)_{i\in I}$ be a family of indeterminates. The translation of indeterminates $(J'_i)_{i\in I}$ is by definition the mapping

$$t_{(J_{i'})i\in I}: \mathcal{F}[(J_i)] \rightsquigarrow t_{(J_{i'})}\mathcal{F}[(J_i)] = \mathcal{F}[(J_i + J'_i)],$$

where $J_i + J'_i$ is considered as being an element of $\bar{E}_i[E_i, E_i, [J_i, J'_i]]$.

Therefore,

$$t_{(J_{i'})}: \bar{F}[E_i, [J_i]]_{i\in I} \to \overline{F[E_i, [J_i]]}_{i\in I}[E_{i'}, [J'_i]]_{i\in I}.$$

The homogeneous part of degree p, $p \in \mathbb{N}$, of

$$\sum_{(n_i)} \varphi_{(n_i)} \prod_{i\in I} J_i^{n_i}$$

with respect to the $(J_{i'})_{i'\in I'}$, $I' \subset I$, is the formal series

$$\sum \varphi_{(n_i)} \prod_{i\in I} J_i^{n_i},$$

where

$$(n_i) \in \mathbb{N}^I \quad \text{and} \quad \sum_{i'\in I'} n'_i = p.$$

Definition 7: The differential of the formal series $\mathcal{F}[(J_i)_{i\in I}]$ is the homogeneous part of degree 1 of

$$\Delta\mathcal{F}[(J_i);(J'_i)] = \mathcal{F}[(J_i + J'_i)] - \mathcal{F}[(J_i)]$$

with respect to $(J'_i)_{i\in I}$. We denote it by $d\mathcal{F}$ or $d\mathcal{F}[(J_i);(J'_i)]$.

From this definition, we may write

$$d\mathcal{F} = \sum_{i\in I} \mathcal{F}_i J'_i,$$

with

$$\mathcal{F}_{i_0} \in \mathfrak{L}(E_{i_0}, \bar{F}[E_i, [J_i]]_{i\in I}), \quad i_0 \in I.$$

Definition 8: $\mathcal{F}_i$ is the functional derivative of $\mathcal{F}$ with respect to J_i. We write it $\mathcal{F}_i = \delta\mathcal{F}/\delta J_i$.

We also write

$$d\mathcal{F} = \sum_{i\in I} J'_i \frac{\delta\mathcal{F}}{\delta J_i}, \quad d\mathcal{F} = \left(\sum_{i\in I} J'_i \frac{\delta}{\delta J_i}\right)\mathcal{F},$$

or

$$d\mathcal{F} = \sum_{i\in I} \left\langle J'_i \frac{\delta\mathcal{F}}{\delta J_i} \right\rangle.$$

For $\mathcal{F}[(J_i)] = J_{i_0}$, $i_0 \in I$, we have $d\mathcal{F} = J'_{i_0}$. In view of this we write dJ_i for J'_i, and we write

$$d\mathcal{F} = \sum_{i\in I} dJ_i \frac{\delta\mathcal{F}}{\delta J_i} = d\mathcal{F}[(J_i);(dJ_i)].$$

Let $\mathcal{F}$ and $\mathcal{F}'$ be two elements of $\bar{F}[E_i, [J_i]]_{i\in I}$, and let λ and λ' be two elements of $\mathbb{K}$. We have

$$d(\lambda\mathcal{F} + \lambda'\mathcal{F}') = \lambda\, d\mathcal{F} + \lambda'\, d\mathcal{F}'.$$

If F is an algebra over $\mathbb{K}$, we have

$$d(\mathcal{F}T\mathcal{F}') = (d\mathcal{F})T\mathcal{F}' + \mathcal{F}T(d\mathcal{F}').$$

Let $(j_i)_{i\in I}$ be a family of $j_i \in E_i$, $i \in I$. The j_i may be considered as trivial formal series; if $\mathcal{F}[(J_i)] \in \bar{F}[E_i, [J_i]]_{i\in I}$, we have also

$$d\mathcal{F}[(J_i);(j_i)] \in \bar{F}[E_i, [J_i]]_{i\in I}.$$

The mapping

$$\sum_{i\in I} j_i \frac{\delta}{\delta J_i} : \bar{F}[E_i, [J_i]]_{i\in I} \to \bar{F}[E_i, [J_i]]_{i\in I},$$

defined by

$$\mathcal{F} \rightsquigarrow \left(\sum_{i\in I} j_i \frac{\delta}{\delta J_i}\right)\mathcal{F} = d\mathcal{F}[(J_i);(j_i)],$$

is linear; if F is an algebra over $\mathbb{K}$, then $\sum_{i\in I} j_i (\delta/\delta J_i)$ is a derivative of this algebra.

The mapping

$$(j_i)_{i\in I} \rightsquigarrow \left(\sum_{i\in I} j_i \frac{\delta}{\delta J_i}\right)^n \mathcal{F}[(J_i)]$$

is a polynomial mapping of $P[\prod_{i\in I} E_i, \bar{F}[E_i, [J_i]]_{i\in I}]$. Let

$$\left(\sum_{i\in I} \left\langle J' \frac{\delta}{i\delta J_i} \right\rangle\right)^n \mathcal{F}[(J_i)]$$

be the corresponding homogeneous polynomial of $\bar{F}[E_i, [J_i]]_{i\in I}[E_i, J'_i]_{i\in I}$

Let

$$f(X) = \sum_{n\geq 0} a_n X^n$$

be an element of the algebra $\mathbb{K}[[X]] = \overline{\mathbb{K}}[\mathbb{K}, [X]]$. The family

$$\left(a_n \left(\sum_{i\in I} \left\langle J'_i \frac{\delta}{\delta J_i} \right\rangle\right)^n \mathcal{F}[(J_i)]\right)_{n\in\mathbb{N}}$$

is summable; we denote its sum by

$$f\left(\sum_{i\in I} \left\langle J'_i, \frac{\delta}{\delta J_i} \right\rangle\right)\mathcal{F}[(J_i)].$$

Proposition 2: For any $\mathcal{F}[(J_i)] \in \bar{F}[E_i, [J_i]]_{i\in I}$, we have

$$\mathcal{F}[(J_i + J'_i)_{i\in I}] = \exp\left(\sum_{i\in I} \left\langle J'_i, \frac{\delta}{\delta J_i} \right\rangle\right)\mathcal{F}[(J_i)_{i\in I}].$$

This is Taylor's formula (or Volterra's formula) for the formal series we consider here.

Proposition 3: Let $\mathcal{F}[(J_\lambda)] \in \bar{F}[F_\lambda, [J_\lambda]]_{\lambda\in L}$, and let $(\mathcal{F}_\lambda)_{\lambda\in L}$ be a family of formal series which may be substituted for the J_λ ($\lambda \in L$) in the $\mathcal{F}[(J_\lambda)]$. We then have

$$d\mathcal{F}[(\mathcal{F}_\lambda)_{\lambda\in L}] = \sum_{\lambda\in L} \frac{\delta\mathcal{F}}{\delta J_\lambda}[(\mathcal{F}_\mu)_{\mu\in L}]\, d\mathcal{F}_\lambda.$$

Notations: (1) In view of Proposition 2, if $\mathcal{F}[(J_\lambda)] \in \bar{F}[F_\lambda, [J_\lambda]]_{\lambda\in L}$, we may write

$$\mathcal{F}[(J_\lambda)] = \sum_{(n_i)} \left(\prod_{j\in I} \frac{1}{n_j!}\left(\frac{\delta}{\delta J_j}\right)^{n_j}\right)\mathcal{F}[0] \prod_{i\in I} J_i^{n_i}.$$

Therefore,

$$\prod_{i\in I} \left(\frac{\delta}{\delta J_i}\right)^{n_i} \mathcal{F}[0] = \prod_{i\in I} n_i!\, \varphi_{(n_i)}.$$

(2) If $(\mathcal{F}_\lambda)_{\lambda\in L}$ is a family of formal series which may be substituted for the indeterminates J_λ in

$$f\left(\sum_{\lambda\in L} \left\langle J'_\lambda, \frac{\delta}{\delta J_\lambda} \right\rangle\right)\mathcal{F}[(J_\lambda)],$$

we denote the result of this substitution by

$$\mathrm{J}f\left(\sum_{\lambda\in L} \left\langle \mathcal{F}_\lambda, \frac{\delta}{\delta J_\lambda} \right\rangle\right)\mathcal{F}[(J_\lambda)].$$

6. FORMAL-SERIES EQUATIONS

Let E be a vector space over the field $\mathbb{K}$. If $\mathcal{F}[J] = \sum_{n\geq 0} \varphi_n J^n$ is a formal series of $\bar{E}[E, [J]]$, the kernel $\varphi_n = (1/n!)\delta^n\mathcal{F}[0]/\delta J^n$ is an n-linear symmetric mapping of E into E. Therefore, $\mathcal{F}[0] \in E$ and $\delta\mathcal{F}[0]/\delta J \in \mathfrak{L}(E, E)$, where $\mathfrak{L}(E, E)$ is the algebra of the linear mappings of E into E.

Theorem 1: Let $\mathcal{F}[J] \in \bar{E}[E, [J]]$. There is a formal series $\mathcal{E}[J] \in \bar{E}[E, [J]]$ such that $\mathcal{F}[\mathcal{E}[J]] = J$ and $\mathcal{E}[0] = 0$, if and only if $\mathcal{F}[0] = 0$ and $\delta\mathcal{F}[0]/\delta J$ has an inverse in $\mathfrak{L}(E, E)$. If these conditions are satisfied, there is only one such $\mathcal{E}[J]$ and $\mathcal{E}[\mathcal{F}[J]] = J$.

Proof: We must have $\mathcal{F}[\mathcal{E}[0]] = \mathcal{F}[0] = 0$ and

$$\frac{\delta\mathcal{F}[\mathcal{E}[0]]}{\delta J} = \frac{\delta\mathcal{F}[0]}{\delta J}\frac{\delta\mathcal{E}[0]}{\delta J} = I.$$

Therefore, the conditions that $\mathcal{F}[0] = 0$ and that $\delta\mathcal{F}[0]/\delta J$ have an inverse are necessary conditions. Suppose that these conditions are satisfied. We must also have

$$\left(\frac{\delta}{\delta J}\right)^n \mathcal{F}[\mathcal{E}[J]]|_{J=0} = 0$$

or

$$0 = \frac{\delta\mathcal{F}[0]}{\delta J}\left(\frac{\delta}{\delta J}\right)^n \mathcal{E}[0] + \Phi_n\left(\frac{\delta\mathcal{E}[0]}{\delta J}, \cdots, \left(\frac{\delta}{\delta J}\right)^{n-1}\mathcal{E}[0]\right).$$

This equation determines $(\delta/\delta J)^n\mathcal{E}[0]$ if the $(\delta/\delta J)^p\mathcal{E}[0]$ for $p < n$ are known and we have

$$\frac{\delta\mathcal{E}[0]}{\delta J} = \left(\frac{\delta\mathcal{F}[0]}{\delta J}\right)^{-1}.$$

Therefore, $\mathcal{E}[J]$ is uniquely defined by these equations. If $\mathcal{E}[0] = 0$ and if $\delta\mathcal{E}[0]/\delta J$ has an inverse, there is an $\mathcal{F}'[J] \in \bar{F}[E, [J]]$ such that $\mathcal{E}[\mathcal{F}'[J]] = J$, where

$$\mathcal{F}'[J] = \mathcal{F}[\mathcal{E}[\mathcal{F}'[J]]] = \mathcal{F}[J].$$

Therefore, $\mathcal{F}' \equiv \mathcal{F}$.

Suppose that $\mathcal{F}$ satisfies the conditions of Theorem 1. We can suppose (with a trivial substitution) without restriction that $\mathcal{F}$ is of the form $\mathcal{F}[J] = J + \mathcal{K}[J]$ with $\omega(\mathcal{K}) \geq 2$. Then the theorem says that there is one and only one solution $\mathcal{E}[J]$ of order $\omega(\mathcal{E}) \geq 1$ of the equation

$$\mathcal{E}[J] + \mathcal{K}[\mathcal{E}[J]] = J \tag{4}$$

and that this solution satisfies

$$\mathcal{E}[J + \mathcal{K}[J]] = J. \tag{5}$$

This last equation can be written

$$\lrcorner\exp\left(\left\langle \mathcal{K}[J], \frac{\delta}{\delta J}\right\rangle\right)\mathcal{E}[J] = J, \tag{5'}$$

where we have used Proposition 2 (Taylor's formula) and the notation (2) introduced in Sec. 5.

Therefore, in order to solve (4), we have only to find the inverse of the linear functional differential operator

$$\lrcorner\exp\left(\left\langle \mathcal{K}[J], \frac{\delta}{\delta J}\right\rangle\right) : \bar{E}[E, [J]] \to \bar{E}[E, [J]].$$

7. SPECIFIC CASES

A. Finite-dimensional Vector Space

Let $E = \mathbb{K}^n$ (or any n-dimensional space over $\mathbb{K}$ owing to the isomorphism between them). We identify canonically $\overline{\mathbb{K}^n}[\mathbb{K}^n, [J]]$ with $(\mathbb{K}[[J_1, \cdots, J_n]])^n$ and $\overline{\mathbb{K}}[\mathbb{K}^n, [J]]$ with $\mathbb{K}[[J_1, \cdots, J_n]]$. Then Eqs. (4) and (5) may be written

$$\mathcal{E}_\mu[J_1, \cdots, J_n] + \mathcal{K}_\mu[\mathcal{E}_1, \cdots, \mathcal{E}_n] = J_\mu, \quad \mu = 1, 2, \cdots, n, \tag{6}$$

$$\mathcal{E}_\mu[J_1 + \mathcal{K}_1, \cdots, J_n + \mathcal{K}_n] = J_\mu, \quad \mu = 1, \cdots, n, \tag{7}$$

and

$$\lrcorner\exp\left(\sum_{\lambda=1}^{\lambda=n}\mathcal{K}_\lambda\frac{\partial}{\partial J_\lambda}\right)\mathcal{E}_\mu[J_1, \cdots, J_n] = J_\mu, \quad \mu = 1, \cdots, n. \tag{7'}$$

We see here that the symbol $\lrcorner$ before the exponential means that, in each term of the expansion of this exponential, all derivatives have to be translated to the right; i.e., for any $\mathcal{F}[J_1, \cdots, J_n]$,

$$\lrcorner\left(\sum_{\lambda=1}^{n}\mathcal{K}_\lambda\frac{\partial}{\partial J_\lambda}\right)^p\mathcal{F} = \sum_{\lambda_1=1}^{n}\cdots\sum_{\lambda_p=1}^{n}\mathcal{K}_{\lambda_1}\cdots\mathcal{K}_{\lambda_p}\frac{\partial^p\mathcal{F}}{\partial J_{\lambda_1}\cdots\partial J_{\lambda_p}}.$$

Let us introduce, in the same way,

$$\Gamma\left(\sum_{\lambda=1}^{n}\frac{\partial\mathcal{K}_\lambda}{\partial J_\lambda}\right)^p\mathcal{F} = \sum_{\lambda_1=1}^{n}\cdots\sum_{\lambda_p=1}^{n}\frac{\partial^p\mathcal{K}_{\lambda_1}\cdots\mathcal{K}_{\lambda_p}\mathcal{F}}{\partial J_{\lambda_1}\cdots\partial J_{\lambda_p}},$$

and define the operator $\Gamma\exp(-\sum_{\lambda=1}^{n}\partial\mathcal{K}_\lambda/\partial J_\lambda)$ by

$$\Gamma\exp\left(-\sum_{\lambda=1}^{n}\frac{\partial\mathcal{K}_\lambda}{\partial J_\lambda}\right)\mathcal{F} = \sum_{p\geq 0}\frac{(-1)^p}{p!}\Gamma\left(\sum_{\lambda=1}^{n}\frac{\partial\mathcal{K}_\lambda}{\partial J_\lambda}\right)^p\mathcal{F}.$$

For $\omega(\mathcal{K}) \geq 2$, this is a well-defined operator. We have, for any $\mathcal{F}[J_1, \cdots, J_n]$,

$$\Gamma\exp\left(-\sum_{\lambda=1}^{\lambda=n}\frac{\partial\mathcal{K}_\lambda}{\partial J_\lambda}\right)\lrcorner\exp\left(\sum_{\mu=1}^{\mu=n}\mathcal{K}_\mu\frac{\partial}{\partial J_\mu}\right)\mathcal{F} = \mathcal{F}\cdot\Gamma\exp\left(-\sum_{\nu=1}^{\nu=n}\frac{\partial\mathcal{K}_\nu}{\partial J_\nu}\right)1.$$

Therefore, (6) is solved by

$$\mathcal{E}_\lambda[J_1, \cdots, J_n] = \frac{\Gamma \exp\left(-\sum_{\mu=1}^{\mu=n} \frac{\partial}{\partial J_\mu} \mathcal{K}_\mu[J_1, \cdots, J_n]\right) J_\lambda}{\Gamma \exp\left(-\sum_{\mu=1}^{\mu=n} \frac{\partial}{\partial J_\mu} \mathcal{K}_\mu[J_1, \cdots, J_n]\right) 1}.$$

B. Function Space

Let E be a space of functions. With the usual notations of Volterra's series, Eqs. (6) and (7) may be written

$$\mathcal{E}(x; J) + \mathcal{K}(x; \mathcal{E}(J)) = J(x), \tag{8}$$

$$\mathcal{E}(x; J + \mathcal{K}(J)) = J(x), \tag{9}$$

$$\text{J} \exp\left(\int \mathcal{K}(y; J) \frac{\delta}{\delta J(y)} dy\right) \mathcal{E}(x; J) = J(x). \tag{9'}$$

In analogy with Sec. 7A, we formally introduce

$$\Gamma\left(\int dx \frac{\delta}{\delta J(x)} \mathcal{K}(x; J)\right)^p \mathcal{F} = \int \cdots \int dx_1 \cdots dx_n \frac{\delta^n \mathcal{K}(x_1) \cdots \mathcal{K}(x_n) \mathcal{F}}{\delta J(x_1) \cdots \delta J(x_n)}$$

and the corresponding term

$$\Gamma \exp\left(-\int dy \frac{\delta}{\delta J(y)} \mathcal{K}(y; J)\right) \mathcal{F}.$$

Formally, we have

$$\Gamma \exp\left(-\int dy \frac{\delta}{\delta J(y)} \mathcal{K}(y)\right) \text{J} \exp\left(\int dz \mathcal{K}(z) \frac{\delta}{\delta J(z)}\right) \mathcal{F} = \mathcal{F} \cdot \Gamma \exp\left(-\int dx \frac{\delta}{\delta J(x)} \mathcal{K}(x)\right) 1.$$

Therefore, if $\mathcal{K}$ is such that, for any integer,

$$\int \cdots \int \frac{\delta^p \mathcal{K}(x_1; J) \cdots \mathcal{K}(x_p; J)}{\delta J(x_1) \cdots \delta J(x_p)}$$

exist, then the solution of (8) is

$$\mathcal{E}(x; J) = \frac{\Gamma \exp\left(-\int dy \delta \mathcal{K}(y; J)/\delta J(y)\right) J(x)}{\Gamma \exp\left(-\int dy \delta \mathcal{K}(y; J)/\delta J(y)\right) 1}.$$

As an example of the application of this formula, consider the classical (c-number) theory of a real scalar field $A(x)$ satisfying

$$(\Box_x + m^2) A(x) + \lambda (A(x)^k) = 0, \quad k \geq 2,$$

with $A(x) \to A_{i_n}(x)$ as $x^0 \to -\infty$, where $A_{i_n}(x)$ is solution of $(\Box + m^2) A_{i_n}$. As a consequence of the field equation and the asymptotic condition, $A(x)$ satisfies the Yang–Feldmann equation

$$A(x) + \lambda \int dy \Delta_{\text{R}}(x - y)[A(y)]^k = A_{i_n}(x),$$

where $\Delta_{\text{R}}(x)$ is the retarded solution of

$$(\Box_x + m^2) \Delta_{\text{R}}(x) = \delta(x).$$

The formal Volterra series or order ≥ 1 solution of

$$\mathcal{E}(x; J) + \lambda \int dy \Delta_{\text{R}}(x - y)[\mathcal{E}(y; J)]^k = J(x)$$

is

$$\mathcal{E}(x; J) = \Gamma \exp\left(-\lambda \int \cdots \int dy\, dz \frac{\delta \Delta_{\text{R}}(y - z)}{\delta J(y)} [J(z)]^k\right) J(x).$$

Note that

$$\Gamma \exp\left(-\lambda \int \cdots \int dy\, dz \frac{\delta \Delta_{\text{R}}(y - z)}{\delta J(y)} [J(z)]^k\right) 1 = 1$$

if closed loops of Δ_{R} vanish as usual. In order to obtain the formal solution of the Yang–Feldmann equation, which is also the perturbative solution here, we have only to substitute A_{i_n} for J in the formal Volterra series $\mathcal{E}(x; J)$.

C. Remarks on the General Case

In analogy with what has been done in Secs. 7A and 7B, we want now to study the general case of "abstract" spaces E; we thus have to introduce first a concept like $\sum_\mu \partial_\mu \mathcal{K}_\mu$ or $\int dx\, (\delta \mathcal{K}(x)/\delta J(x))$ very similar to the divergence of a vector in elementary vector analysis. This is indeed possible and we give the following definition of a generalized divergence.

Definition 9: A divergence on $\bar{E}[E, J]$ is a pair $\alpha = (D, \text{div})$, where

(1) D is a subspace of the space $\bar{E}[E, [J]]$ such that, for any $\mathcal{F} \in D$ and $\Phi \in \overline{\mathbb{K}}[E, [J]]$, $\Phi \mathcal{F} \in D$;

(2) div is a mapping of D into $\overline{\mathbb{K}}[E, [J]]$ such that, for any $\mathcal{F}$ and $\mathcal{F}'$ of D and for any $\Phi \in \overline{\mathbb{K}}[E, [J]]$,

$$\text{div}\,(\mathcal{F} + \mathcal{F}') = \text{div}\,\mathcal{F} + \text{div}\,\mathcal{F}', \tag{10}$$

$$\text{div}\,(\Phi \mathcal{F}) = \Phi\, \text{div}\,\mathcal{F} + \left\langle \mathcal{F}, \frac{\delta \Phi}{\delta J} \right\rangle. \tag{11}$$

Then, we may try to define recurrently $\Gamma_\alpha \langle \delta \mathcal{K}/\delta J \rangle^n$ operators. This is, however, formal because we cannot control the domains D_n to which $\mathcal{K}$ must belong for any n. This is the reason why we do not go further in this direction in the present paper.

8. CONCLUDING REMARKS

The theory we have been studying here may be extended in two ways: One may develop a topological generalization or an algebraic one.

(1) In the case of a topological extension, $(E_i)_{i\in I}$ and F are supposed to be topological vector spaces. We define then $\mathcal{F}$-continuous formal series of $(E_i)_{i\in I}$ into F as being formal series of $(E_i)_{i\in I}$ into F such that their kernels $\varphi_{(n_i)}$ define continuous monomial mappings of $\prod_{i\in I} E_i$ into F. For instance, in quantum field theory the "generating functional"

$$T[J] = \sum_{n\geq 0} \frac{i^n}{n!} \int \tau_n(x_1, \cdots, x_n) J(x_1) \cdots J(x_n)$$

$$= \sum_{n\geq 0} \frac{i^n}{n!} \tau_n J^n$$

is expected to be a continuous formal series of $\overline{\mathbb{C}}[\mathcal{S}, [J]]$, where $\overline{\mathbb{C}}$ is the field of complex numbers and $\mathcal{S}$ the space of rapidly decreasing functions.

(2) In the case of an algebraic extension, $(E_i)_{i\in I}$ and F are no longer supposed to be vector spaces, but they are modules over a ring A (or A-modules).

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[1] H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo Cimento **1**, 205 (1955); **6**, 319 (1957).
[2] J. Schwinger, Proc. Natl. Acad. Sci. (U.S.) **37**, 452 (1951).
[3] V. Glaser, H. Lehmann, and W. Zimmermann, Nuovo Cimento **6**, 1122 (1957).
[4] K. Symanzik, J. Math. Phys. **1**, 249 (1960).
[5] A. Visconti and J. Carmona, Nuovo Cimento **29**, 742 (1963).
[6] A. Visconti, *Théorie quantique des champs* (Gauthier-Villars, Paris, 1961), tome 2.
[7] N. Bourbaki, *Algèbre* (Hermann, Paris, 1959), Chap. 4.
[8] H. Cartan, *Théorie élementaire des fonctions analytiques d'une ou plusieurs variables complexes* (Hermann, Paris, 1961).
[9] For linear and multilinear algebra our notations are those of Ref. 7, Chaps. 2 and 3.

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Elastic Radiation in a Half-Space

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A Green's function for the elastic wave equation, which satisfies certain boundary conditions on the surface of a homogeneous half-space, is derived by means of the Fourier transformation. This half-space Green's function is then applied to the computation of radiative effects due to the earth's surface when a radiating source is located on or within that surface. The results obtained are to be taken as an extension of a previous and similar formulation for the infinite medium due to Case and Colwell.

1. INTRODUCTION

A method for computing the elastic radiation from a small source in the earth's interior has been presented by Case and Colwell.[1] This method, which assumes the earth to be an infinite medium, can be modified to include effects due to the earth's surface simply by replacing the (known) infinite-space Green's function, which is used, by an appropriate half-space Green's function. Our purpose here is, first of all, to obtain a representation for the half-space Green's function, and secondly, to demonstrate its applicability in computing corrections to the solution of Case and Colwell.

Our method is straightforward. To obtain the desired Green's function, we formulate the problem in terms of an integral equation, which equation is then solved by Fourier transforms. Our application of the Green's function then proceeds in a manner closely parallel to that of Ref. 1. The only complication lies in the fact that, once we choose a definite orientation for our half-space, the matrices which occur are not tensors, i.e., not rotation covariant. Hence tensor theory arguments, with the computational simplifications they often afford, are not available to us.

The notation to be used here differs in several minor

8. CONCLUDING REMARKS

The theory we have been studying here may be extended in two ways: One may develop a topological generalization or an algebraic one.

(1) In the case of a topological extension, $(E_i)_{i\in I}$ and F are supposed to be topological vector spaces. We define then $\mathcal{F}$-continuous formal series of $(E_i)_{i\in I}$ into F as being formal series of $(E_i)_{i\in I}$ into F such that their kernels $\varphi_{(n_i)}$ define continuous monomial mappings of $\prod_{i\in I} E_i$ into F. For instance, in quantum field theory the "generating functional"

$$T[J] = \sum_{n\geq 0} \frac{i^n}{n!} \int \tau_n(x_1, \cdots, x_n) J(x_1) \cdots J(x_n)$$

$$= \sum_{n\geq 0} \frac{i^n}{n!} \tau_n J^n$$

is expected to be a continuous formal series of $\overline{\mathbb{C}}[\mathcal{S}, [J]]$, where $\overline{\mathbb{C}}$ is the field of complex numbers and $\mathcal{S}$ the space of rapidly decreasing functions.

(2) In the case of an algebraic extension, $(E_i)_{i\in I}$ and F are no longer supposed to be vector spaces, but they are modules over a ring A (or A-modules).

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[1] H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo Cimento **1**, 205 (1955); **6**, 319 (1957).
[2] J. Schwinger, Proc. Natl. Acad. Sci. (U.S.) **37**, 452 (1951).
[3] V. Glaser, H. Lehmann, and W. Zimmermann, Nuovo Cimento **6**, 1122 (1957).
[4] K. Symanzik, J. Math. Phys. **1**, 249 (1960).
[5] A. Visconti and J. Carmona, Nuovo Cimento **29**, 742 (1963).
[6] A. Visconti, *Théorie quantique des champs* (Gauthier-Villars, Paris, 1961), tome 2.
[7] N. Bourbaki, *Algèbre* (Hermann, Paris, 1959), Chap. 4.
[8] H. Cartan, *Théorie élementaire des fonctions analytiques d'une ou plusieurs variables complexes* (Hermann, Paris, 1961).
[9] For linear and multilinear algebra our notations are those of Ref. 7, Chaps. 2 and 3.

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Elastic Radiation in a Half-Space

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A Green's function for the elastic wave equation, which satisfies certain boundary conditions on the surface of a homogeneous half-space, is derived by means of the Fourier transformation. This half-space Green's function is then applied to the computation of radiative effects due to the earth's surface when a radiating source is located on or within that surface. The results obtained are to be taken as an extension of a previous and similar formulation for the infinite medium due to Case and Colwell.

1. INTRODUCTION

A method for computing the elastic radiation from a small source in the earth's interior has been presented by Case and Colwell.[1] This method, which assumes the earth to be an infinite medium, can be modified to include effects due to the earth's surface simply by replacing the (known) infinite-space Green's function, which is used, by an appropriate half-space Green's function. Our purpose here is, first of all, to obtain a representation for the half-space Green's function, and secondly, to demonstrate its applicability in computing corrections to the solution of Case and Colwell.

Our method is straightforward. To obtain the desired Green's function, we formulate the problem in terms of an integral equation, which equation is then solved by Fourier transforms. Our application of the Green's function then proceeds in a manner closely parallel to that of Ref. 1. The only complication lies in the fact that, once we choose a definite orientation for our half-space, the matrices which occur are not tensors, i.e., not rotation covariant. Hence tensor theory arguments, with the computational simplifications they often afford, are not available to us.

The notation to be used here differs in several minor

respects from that of Case and Colwell. In particular, 2-dimensional vectors will be denoted by an arrow:

$$\vec{a} \equiv (a_1, a_2), \quad \mathbf{a} = (\vec{a}, a_3)$$

and we will use the convenient abbreviation

$$\partial_i \equiv \frac{\partial}{\partial x_i}, \quad \partial_i' \equiv \frac{\partial}{\partial x_i'}, \quad i = 1, 2, 3.$$

The Fourier transforms of a function $f(\mathbf{r})$ with respect to 2- and 3-dimensional space will be denoted by $\hat{f}$ and $\tilde{f}$, respectively, with the conventions

$$\hat{f}(\vec{k}, x_3) = \int \exp(i\vec{k} \cdot \vec{r}) f(\mathbf{r})\, d\vec{r},$$

$$\tilde{f}(\mathbf{k}) = \int \exp(i\mathbf{k} \cdot \mathbf{r}) f(\mathbf{r})\, d\mathbf{r}.$$

Note that we deal exclusively, and hence tacitly, with the Fourier transforms with respect to time. (It will become evident below that the inverse transform for the time variable is essentially as trivial here as it was in Ref. 1.) The summation convention is used throughout.

2. THE HALF-SPACE GREEN'S FUNCTION

Integral Formulation

We consider first a general region V of $\mathbf{r}$-space, and seek the solution $f_{ij}(\mathbf{r}, \mathbf{r}_0)$ to

$$-\omega^2 \rho f_{ij}(\mathbf{r}, \mathbf{r}_0) = \partial_k D_{ikm}(\partial) f_{mj}(\mathbf{r}, \mathbf{r}_0) + \delta_{ij}\delta(\mathbf{r} - \mathbf{r}_0), \quad \mathbf{r}, \mathbf{r}_0 \in V, \quad (2.1)$$

with the boundary condition

$$n_i D_{ikm}(\partial) f_{mj}(\mathbf{r}_s, \mathbf{r}_0) = 0, \quad \mathbf{r}_s \in S. \quad (2.2)$$

Here, n_i is (the ith component of) the inward normal to the region V with boundary S and

$$D_{ikm}(\partial) \equiv \lambda \delta_{ik}\partial_m + \mu(\delta_{im}\partial_k + \delta_{km}\partial_i). \quad (2.3)$$

The infinite-space Green's function G_{ij} satisfies Eq. (2.1) with V including all space:

$$-\omega^2 \rho G_{il}(\mathbf{r}, \mathbf{r}') = \partial_k D_{ikm}(\partial) G_{ml}(\mathbf{r}, \mathbf{r}') + \delta_{il}\delta(\mathbf{r} - \mathbf{r}'), \quad \text{all } \mathbf{r}, \mathbf{r}'. \quad (2.4)$$

We now proceed in a standard way to multiply Eq. (2.4) by f_{ij}, Eq. (2.1) by G_{il}, and subtract. Using the easily verified identity

$$G_{il}\partial_k D_{ikm} f_{mj} - f_{ij}\partial_k D_{ikm} G_{ml} = \partial_i [G_{kl} D_{ikm} f_{mj} - f_{kj} D_{ikm} G_{ml}], \quad (2.5)$$

we find

$$G_{il}(\mathbf{r}, \mathbf{r}')\delta_{ij}\delta(\mathbf{r} - \mathbf{r}_0) - f_{ij}(\mathbf{r}, \mathbf{r}_0)\delta_{il}\delta(\mathbf{r} - \mathbf{r}') + \partial_i [G_{kl}(\mathbf{r}, \mathbf{r}') D_{ikm}(\partial) f_{mj}(\mathbf{r}, \mathbf{r}_0) - f_{kj}(\mathbf{r}, \mathbf{r}_0) D_{ikm}(\partial) G_{ml}(\mathbf{r}, \mathbf{r}')] = 0. \quad (2.6)$$

We now integrate Eq. (2.6) over V, apply the divergence theorem, and note Eq. (2.2). Upon renaming variables (and indices) and using the facts that

$$G_{ij}(\mathbf{r}, \mathbf{r}_0) = G_{ij}(\mathbf{r}_0, \mathbf{r}) \quad (2.7)$$

and

$$D_{ikm}(\partial) G_{mj}(\mathbf{r}, \mathbf{r}') = -D_{ikm}(\partial') G_{mj}(\mathbf{r}', \mathbf{r}), \quad (2.8)$$

we obtain the desired equation

$$f_{ij}(\mathbf{r}, \mathbf{r}_0) = G_{ij}(\mathbf{r}, \mathbf{r}_0) + \int_S d^2 r' n_k(\mathbf{r}') f_{lj}(\mathbf{r}', \mathbf{r}_0) \times D_{klm}(\partial') G_{mi}(\mathbf{r}', \mathbf{r}). \quad (2.9)$$

A method for determining $f_{ij}(\mathbf{r}, \mathbf{r}_0)$ is clear from Eq. (2.9). Indeed, our problem clearly reduces to finding $f_{ij}(\mathbf{r}_s, \mathbf{r}_0)$; and, by taking the limit of Eq. (2.9) as $\mathbf{r} \to \mathbf{r}_s$, we obtain an integral equation which may be solved for $f_{ij}(\mathbf{r}_s, \mathbf{r}_0)$.

Specializing to the case in which V is the half-space $x_3 \geq 0$, we denote the half-space Green's function by g_{ij}:

$$g_{ij}(\mathbf{r}, \mathbf{r}_0) = G_{ij}(\mathbf{r}, \mathbf{r}_0) + \int d\vec{r}' g_{lj}(\vec{r}', 0; \mathbf{r}_0) \times [D_{3lm}(\partial') G_{mi}(\mathbf{r}', \mathbf{r})]_{x_3'=0}. \quad (2.10)$$

A certain amount of care is required in taking the limit $x_3 \to 0$ of Eq. (2.10), since the integrand is singular on S. In fact, if we define

$$\Sigma_{3li}(\mathbf{r}, \mathbf{r}') \equiv D_{3lm}(\partial) G_{mi}(\mathbf{r}, \mathbf{r}'), \quad (2.11)$$

then it easily follows from Eq. (2.4) that

$$\Sigma_{3li}(\vec{r}, 0+; \vec{r}', 0) - \Sigma_{3li}(\vec{r}, 0-; \vec{r}', 0) = -\delta_{li}\delta(\vec{r} - \vec{r}'). \quad (2.12)$$

Thus, we define the "principal value"

$$\Sigma^0_{3li}(\vec{r}, \vec{r}') \equiv \tfrac{1}{2}[\Sigma_{3li}(\vec{r}, 0+; \vec{r}', 0) + \Sigma_{3li}(\vec{r}, 0-; \vec{r}', 0)]. \quad (2.13)$$

Now let $x_3 \to 0$ in Eq. (2.10). Using Eqs. (2.12) and (2.13), the result may be written as

$$\tfrac{1}{2} g_{ij}(\vec{r}, 0; \mathbf{r}_0) = G_{ij}(\vec{r}, 0; \mathbf{r}_0) + S^0_{ij}(\vec{r}, \mathbf{r}_0), \quad (2.14)$$

where

$$S^0_{ij}(\vec{r}, \mathbf{r}_0) \equiv \int d\vec{r}' g_{lj}(\vec{r}', 0; \mathbf{r}_0) \Sigma^0_{3li}(\vec{r}', \vec{r}). \quad (2.15)$$

Equations (2.10) and (2.14) are the basic relations by means of which our problem is to be solved.

Solution of the Integral Equation

Because of the translation invariance of G_{ij}, $\Sigma^0_{3li}(\vec{r}', \vec{r})$ depends only on the difference $\vec{r}' - \vec{r}$. It

follows that the 2-dimensional Fourier transform of Eq. (2.14),

$$\tfrac{1}{2}\hat{g}_{ij}(\vec{k}, 0; \mathbf{r}_0) = \hat{G}_{ij}(\vec{k}, 0; \mathbf{r}_0) + \hat{S}^0_{ij}(\vec{k}, \mathbf{r}_0), \quad (2.16)$$

reduces to the purely algebraic equations

$$[\tfrac{1}{2}\delta_{il} + H^0_{il}(\vec{k})]\hat{g}_{lj}(\vec{k}, 0; \mathbf{r}_0) = \hat{G}_{ij}(\vec{k}, 0; \mathbf{r}_0). \quad (2.17)$$

Here, we have introduced a less cumbersome notation for $\hat{\Sigma}^0_{3li}(0; \vec{k})$:

$$H^0_{il}(\vec{k}) \equiv \tfrac{1}{2}[H_{il}(\vec{k}, 0+) + H_{il}(\vec{k}, 0-)], \quad (2.18)$$

where

$$H_{il}(\vec{k}, x_3) \equiv \frac{-1}{2\pi}\int_{-\infty}^{\infty} dk_3 e^{-ik_3x_3}\tilde{\Sigma}_{3li} \quad (\mathbf{k}; \mathbf{r}' = 0). \quad (2.19)$$

[The minus sign is occasioned by Eq. (2.8).] It is convenient to note here the identity

$$H_{il}(\vec{k}, 0+) = H^0_{il}(\vec{k}) - \tfrac{1}{2}\delta_{il}, \quad (2.20)$$

which follows from Eqs. (2.12) and (2.13) and which will be useful below.

Equation (2.17) has the solution

$$\hat{g}_{lj}(\vec{k}, 0; \mathbf{r}_0) = \|A^{-1}\|_{li}\hat{G}_{ij}(\vec{k}, 0; \mathbf{r}_0), \quad (2.21)$$

where $\|A^{-1}\|$ is the matrix inverse to

$$\|A\|_{il} = \tfrac{1}{2}\delta_{il} + H^0_{il}(\vec{k}). \quad (2.22)$$

We obtain H^0_{il} from the known[1] fact that

$$\tilde{G}_{ij}(\vec{k}, \mathbf{r}') = \frac{e^{i\mathbf{k}\cdot\mathbf{r}'}}{\omega^2\rho}\left(\frac{k_ik_j}{k^2 - k_l^2} + \frac{k_t^2\delta_{ij} - k_ik_j}{k^2 - k_t^2}\right), \quad (2.23)$$

where

$$k_l^2 = \omega^2\rho/(\lambda + 2\mu), \quad k_t^2 = \omega^2\rho/\mu \quad (2.24)$$

and from Eq. (2.13). A straightforward computation yields

$$\begin{aligned} 2\pi i\omega^2\rho H_{jk} = {} & \lambda k_l^2\delta_{3k}[(k_j - \delta_{3j}k_3)I_{0l} + \delta_{3j}I_{il}] \\ & + \mu\{2(k_l^2 - k_t^2) \\ & \times [(k_k - \delta_{3k}k_3)(k_j - \delta_{3j}k_3)I_2 \\ & + (k_j - \delta_{3j}k_3)\delta_{3k}I_3 + (k_k - \delta_{3k}k_3)\delta_{3j}I_3 \\ & + \delta_{3k}\delta_{3j}I_4] + k_t^2[\delta_{3j}(k_k - \delta_{3k}k_3)I_{0t} \\ & + \delta_{3k}\delta_{3j}I_{1t} + \delta_{kj}I_{1t}]\}, \end{aligned} \quad (2.25)$$

where[2]

$$\begin{aligned} I_{0l,t}(\vec{k}, x_3) &= \frac{\pi}{\kappa_{l,t}}e^{-\kappa_{l,t}|x_3|}, \\ I_{1l,t}(k, x_3) &= \mp i\pi e^{-\kappa_{l,t}|x_3|}, \quad x_3 \gtrless 0, \\ I_2(\vec{k}, x_3) &= [i\pi/(k_t^2 - k_l^2)](e^{-\kappa_l|x_3|} - e^{-\kappa_t|x_3|}), \\ I_3(\vec{k}, x_3) &= [\pi/(k_t^2 - k_l^2)](\kappa_te^{-\kappa_l|x_3|} - \kappa_te^{-\kappa_t|x_3|}), \\ I_4(\vec{k}, x_3) &= [\mp i\pi/(k_t^2 - k_l^2)](\kappa_l^2e^{-\kappa_l|x_3|} - \kappa_t^2e^{-\kappa_t|x_3|}), \\ & \qquad x_3 \gtrless 0. \end{aligned} \quad (2.26)$$

In Eqs. (2.26), we have introduced the abbreviations

$$\kappa_{l,t}^2 = \vec{k}^2 - k_{l,t}^2. \quad (2.27)$$

From Eqs. (2.18), (2.25), and (2.26), we have

$$H^0_{ij}(\vec{k}) = \tfrac{1}{2}a(\vec{k}^2)\delta_{3j}(k_i - \delta_{3i}k_3) + \tfrac{1}{2}b(\vec{k}^2)\delta_{3i}(k_j - \delta_{3j}k_3), \quad (2.28)$$

where

$$a(\vec{k}^2) = -i[\lambda\kappa_t - (\lambda + 2\mu)\kappa_l]/(\lambda + 2\mu)\kappa_l(\kappa_l + \kappa_t), \quad (2.29)$$

$$b(\vec{k}^2) = i[\lambda\kappa_t - (\lambda + 2\mu)\kappa_l]/(\lambda + 2\mu)\kappa_t(\kappa_l + \kappa_t), \quad (2.30)$$

whence

$$\|A\| = \frac{1}{2}\begin{bmatrix} 1 & 0 & ak_1 \\ 0 & 1 & ak_2 \\ bk_1 & bk_2 & 1 \end{bmatrix} \quad (2.31)$$

and we easily find

$$\|A^{-1}\| = \frac{2}{1 - ab\vec{k}^2}\begin{bmatrix} 1 - abk_2^2 & abk_1k_2 & -ak_1 \\ abk_1k_2 & 1 - abk_1^2 & -ak_2 \\ -bk_1 & -bk_2 & 1 \end{bmatrix}. \quad (2.32)$$

Equations (2.10), (2.21), and (2.32) provide the desired half-space Green's function. It is conveniently written in the form

$$g_{ij}(\mathbf{r}, \mathbf{r}_0) = G_{ij}(\mathbf{r}, \mathbf{r}_0) + S_{ij}(\mathbf{r}, \mathbf{r}_0), \quad (2.33)$$

where

$$\begin{aligned} S_{ij}(\mathbf{r}, \mathbf{r}_0) = {} & \frac{-1}{(2\pi)^2} \\ & \times \int d\vec{k} \exp(-i\vec{k}\cdot\vec{r})H_{il}(\vec{k}, x_3) \\ & \times \|A^{-1}\|_{lm}\hat{G}_{mj}(\vec{k}, 0; \mathbf{r}_0). \end{aligned} \quad (2.34)$$

3. APPLICATION OF THE HALF-SPACE GREEN'S FUNCTION

We demonstrate the usefulness of the Green's function obtained above by applying it to the solution of an idealized problem similar to that considered by Case and Colwell. That is, we provide an integral formulation by means of which the radiation field from a small radiating cavity may be computed. As in Ref. 1, the problem is simplified by assuming to be given certain quantities which could in theory be determined (by solving an integral equation). Our refinement here consists, of course, in taking the earth to be a homogeneous half-space, rather than an infinite medium. It is to the effect of this refinement, i.e., to the difference between the half-space solution and the solution of Case and Colwell, that we generally confine our attention.

General Formulation

Let V be the half-space as in Sec. 2, with the exclusion of a small cavity, located on or "above" S, with boundary B. Note that, if $\mathbf{r} = (x_1, x_2, x_3)$ is within B, then $x_3 \geq 0$. We wish to determine the functions $u_i(\mathbf{r})$ which satisfy

$$-\omega^2 \rho u_i(\mathbf{r}) = \partial_k D_{ikm} u_m(\mathbf{r}), \quad \mathbf{r} \in V, \tag{3.1}$$

with the boundary conditions

$$n_j D_{jkm} u_m(\mathbf{r}) = 0, \qquad \mathbf{r} \in S, \tag{3.2}$$

$$n_j D_{jkm} u_m(\mathbf{r}) = F_k(\mathbf{r}), \quad \mathbf{r} \in B \ (F_k \text{ given}). \tag{3.3}$$

That is, the normal component of the stress is to vanish on the surface of the earth and to be prescribed on the surface of the cavity.

Following a procedure closely analogous to that of Eqs. (2.1)–(2.9), it is a simple matter to show that Eqs. (3.1)–(3.3) may be restated in the form

$$u_j(\mathbf{r}) = \int_B d^2 r_B [g_{ij}(\mathbf{r}_B, \mathbf{r}) F_i(\mathbf{r}_B) - u_i(\mathbf{r}_B) n_k D_{kim} g_{mj}(\mathbf{r}_B, \mathbf{r})]. \tag{3.4}$$

Given the geometry of B, we could now, of course, let $\mathbf{r} \to \mathbf{r}_B$ and attempt to solve the resulting integral equation for $u_i(\mathbf{r}_B)$ (as in Sec. 2). Instead, we take a more practical approach, paralleling that of Case and Colwell, and assume the $u_i(\mathbf{r}_B)$ to be known. But first it is convenient to isolate the effects of the surface S, with which effects we are exclusively concerned below. Let $u_j^{(0)}(\mathbf{r})$ satisfy

$$u_j^{(0)}(\mathbf{r}) = \int_B d^2 r_B [G_{ij}(\mathbf{r}_B, \mathbf{r}) F_i(\mathbf{r}_B) - u_i(\mathbf{r}_B) n_k D_{ikm} G_{mj}(\mathbf{r}_B, \mathbf{r})]. \tag{3.5}$$

$u_j^{(0)}$ is precisely the solution investigated by Case and Colwell. Here, we are interested in the functions

$$v_j(\mathbf{r}) \equiv u_j(\mathbf{r}) - u_j^{(0)}(\mathbf{r}). \tag{3.6}$$

It is clear from Eqs. (2.33) and (3.5) that these are to be determined from

$$v_j(\mathbf{r}) = \int_B d^2 r_B [S_{ij}(\mathbf{r}_B, \mathbf{r}) F_i(\mathbf{r}_B) - u_i(\mathbf{r}_B) n_k D_{kim} S_{mj}(\mathbf{r}_B, \mathbf{r})], \tag{3.7}$$

where S_{ij} is given by Eq. (2.34).

Our problem is solved by Eq. (3.7). The remainder of this paper is concerned with bringing this equation into an explicit form directly suitable for evaluation.

The Case of a Source on the Surface

We consider first a situation in which the complexities of Eqs. (3.7) and (2.34) are considerably reduced: When the source cavity B is on the earth's surface S. That is,

$$\mathbf{r}_B = (x_{1B}, x_{2B}, 0+). \tag{3.8}$$

[The + sign is necessary because of the discontinuity of the integrand in Eq. (3.7) on S—cf. Eqs. (2.26). Note that our original differential Eq. (3.1) holds only for $x_3 \geq 0$.] Recalling the identity (2.20) and Eq. (2.22), we see that the integrand of Eq. (2.34) here takes the form

$$H_{il}(\vec{k}, 0+) \, \|A^{-1}\|_{lm} \, \hat{G}_{mj}(\vec{k}, 0; \mathbf{r}) = [\|A\|_{il} - \delta_{il}] \, \|A^{-1}\|_{lm} \, \hat{G}_{mj}(\vec{k}, 0; \mathbf{r}) \tag{3.9}$$

$$= -B_{im}(\vec{k}) \hat{G}_{mj}(\vec{k}, 0; \mathbf{r}), \tag{3.10}$$

where we have introduced the quantities

$$B_{im} = \|A^{-1}\|_{im} - \delta_{im}. \tag{3.11}$$

The B_{ij} are most conveniently given in matrix form:

$$\|B\| = \frac{2}{1 - ab\vec{k}^2} \begin{bmatrix} -abk_2^2 & abk_1k_2 & -ak_1 \\ abk_1k_2 & -abk_1^2 & -ak_2 \\ -bk_1 & -bk_2 & 0 \end{bmatrix}. \tag{3.12}$$

The "surface-effects Green's function" is now given by

$$S_{ij}(\mathbf{r}_B, \mathbf{r}) = \frac{1}{(2\pi)^2} \times \int d\vec{k} \exp(-i\vec{k} \cdot \vec{r}_B) B_{im}(\vec{k}) \hat{G}_{mj}(\vec{k}, 0; \mathbf{r}). \tag{3.13}$$

Heretofore, we have been dealing with the total elastic disturbance. We now wish to compute the effects of the radiation field only. This may be accomplished,[1] assuming the origin of coordinates to be within B, by replacing in our formulation the exact infinite-space Green's function

$$G_{ij}(\mathbf{r}', \mathbf{r}) = \frac{-1}{4\pi\omega^2\rho} \left(\partial_i \partial_j \frac{e^{ik_t|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} - (k_t^2 \delta_{ij} + \partial_i \partial_j) \frac{e^{ik_t|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \right) \tag{3.14}$$

by its asymptotic form for $|\mathbf{r}| \gg |\mathbf{r}'|$:

$$G_{ij}(\mathbf{r}', \mathbf{r}) = \frac{-1}{4\pi\omega^2\rho} \frac{1}{r} [\exp(ik_t \hat{\mathbf{r}} \cdot \mathbf{r}') \partial_i \partial_j e^{ik_t r} - \exp(-ik_t \hat{\mathbf{r}} \cdot \mathbf{r}')(k_t^2 \delta_{ij} + \partial_i \partial_j) e^{ik_t r}] + O\left(\frac{r'^2}{r^2}\right), \tag{3.15}$$

where $\hat{\mathbf{r}} \equiv \mathbf{r}/|\mathbf{r}|$. Because of the very simple dependence upon $\mathbf{r}'$ in Eq. (3.15), there is no difficulty in obtaining the Fourier transform needed for Eq. (3.13):

$$\hat{G}_{ij}(\vec{k}, 0; \mathbf{r}) = \frac{-(2\pi)^2}{4\pi\omega^2\rho}\frac{1}{r}\Big[\delta\Big(\vec{k} - k_l\frac{\vec{r}}{r}\Big)\partial_i\partial_j e^{ik_l r} - \delta\Big(\vec{k} - k_t\frac{\vec{r}}{r}\Big)(k_t^2\delta_{ij} + \partial_i\partial_j)e^{ik_t r}\Big]. \tag{3.16}$$

Here, of course,

$$\delta(\vec{k} - k_{l,t}(\vec{r}/r)) \equiv \delta(k_1 - k_{l,t}(x_1/r))\delta(k_2 - k_{l,t}(x_2/r)) \tag{3.17}$$

and, since Eq. (3.16) is exact with regard to the radiation field, we have omitted the error term.

From Eq. (3.16), we see that the integral of Eq. (3.13) is entirely trivial. The result is conveniently written as

$$S_{ij}(\mathbf{r}', \mathbf{r}) = S_{ij}^l(\mathbf{r})\exp(-ik_l\hat{\mathbf{r}}\cdot\mathbf{r}') + S_{ij}^t(\mathbf{r})\exp(-ik_t\hat{\mathbf{r}}\cdot\mathbf{r}'), \tag{3.18}$$

where

$$S_{ij}^l(\mathbf{r}) \equiv B_{im}\Big(k_l\frac{\vec{r}}{r}\Big)\Big(\frac{-1}{4\pi\omega^2\rho}\frac{1}{r}\partial_m\partial_j e^{ik_l r}\Big) \tag{3.19}$$

$$= \frac{k_l^2}{4\pi\omega^2\rho}\frac{e^{ik_l r}}{r}B_{im}\Big(k_l\frac{\vec{r}}{r}\Big)\hat{\mathbf{r}}_m\hat{\mathbf{r}}_j \tag{3.20}$$

and, similarly,

$$S_{ij}^t(\mathbf{r}) = \frac{k_t^2}{4\pi\omega^2\rho}\frac{e^{ik_t r}}{r}B_{im}\Big(k_t\frac{\vec{r}}{r}\Big)(\delta_{mj} - \hat{\mathbf{r}}_m\hat{\mathbf{r}}_j). \tag{3.21}$$

If we also define the (known) vector quantities

$$f_i^{t,l}(\hat{\mathbf{r}}) \equiv \int_B d^2r' F_i(\mathbf{r}')\exp(-ik_{t,l}\hat{\mathbf{r}}\cdot\mathbf{r}') \tag{3.22}$$

and the symmetrized tensors

$$T_{ij}^{t,l} \equiv \tfrac{1}{2}\int_B d^2r'[u_i(\mathbf{r}')n_j(\mathbf{r}') + n_i(\mathbf{r}')u_j(\mathbf{r}')] \times \exp(-ik_{t,l}\hat{\mathbf{r}}\cdot\mathbf{r}'), \tag{3.23}$$

then it requires only some elementary manipulations to write Eq. (3.7) in the form

$$\begin{aligned} v_j(\mathbf{r}) = {} & S_{ij}^l(\mathbf{r})f_i^l(\hat{\mathbf{r}}) \\ & + ik_l[\lambda\hat{\mathbf{r}}_m S_{mj}^l(\mathbf{r})T_{nn}^l(\hat{\mathbf{r}}) + 2\mu\hat{\mathbf{r}}_i T_{ik}^l(\hat{\mathbf{r}})S_{kj}^l(\hat{\mathbf{r}})] \\ & + S_{ij}^t(\mathbf{r})f_i^t(\hat{\mathbf{r}}) \\ & + ik_t[\lambda\hat{\mathbf{r}}_m S_{mj}^t(\mathbf{r})T_{nn}^t(\hat{\mathbf{r}}) + 2\mu\hat{\mathbf{r}}_i T_{ik}^t(\hat{\mathbf{r}})S_{kj}^t(\mathbf{r})]. \end{aligned} \tag{3.24}$$

Note, from Eqs. (3.20), (3.21), and (3.24) (which are exact for the radiation field), that the transverse and longitudinal waves are unmixed when the source is on the surface.

We could now proceed, as in Ref. 1, to make the small source approximation ($\mathbf{r}' \in B \Rightarrow k_{l,t}r' \ll 1$) and expand the exponentials in Eqs. (3.22) and (3.23):

$$\exp(-ik_{t,l}\hat{\mathbf{r}}\cdot\mathbf{r}') = 1 - ik_{t,l}\hat{\mathbf{r}}\cdot\mathbf{r}' + \cdots. \tag{3.25}$$

Since this calculation would proceed exactly as in Ref. 1, we omit it, and instead consider the explicit form of the matrices $S_{ij}^{l,t}$.

Consider first the longitudinal terms. According to Eq. (3.20), our first task is to substitute $k_l\vec{r}/r$ for $\vec{k}$ in the matrix B_{im}. This entails the substitution [cf. Eqs. (2.27)]

$$\kappa_l = ik_l\cos\theta, \quad \kappa_t = i(k_t^2 - k_l^2\sin^2\theta)^{\frac{1}{2}}, \tag{3.26}$$

where θ is the angle between $\mathbf{r}$ and the positive z axis, and we have chosen the signs in Eqs. (3.26) essentially by means of a radiation condition (that we have chosen them correctly will become clear below). Using Eqs. (3.26) we compute

$$\begin{aligned} a_l &\equiv a\Big(k_l^2\frac{\vec{r}^2}{r^2}\Big) \\ &= -\frac{C_l^2[(C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}} - C_t\cos\theta] - 2C_t^2(C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}}}{\omega C_l\cos\theta[C_t\cos\theta + (C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}}]}, \end{aligned} \tag{3.27}$$

where the C's are the velocities of the longitudinal and transverse modes:

$$C_l^2 = (\lambda + 2\mu)/\rho, \quad C_t^2 = \mu/\rho. \tag{3.28}$$

Similarly,

$$\begin{aligned} b_l &\equiv b\Big(k_l^2\frac{\vec{r}^2}{r^2}\Big) \\ &= \frac{C_l^2C_t[(C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}} - C_t\cos\theta] - 2C_t^3(C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}}}{\omega C_l(C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}}[(C_l^2 - C_t^2\sin^2\theta)^{\frac{1}{2}} + C_t\cos\theta]}. \end{aligned} \tag{3.29}$$

The matrix product in Eq. (3.20) is now easily computed and we find

$$\|S^l(\mathbf{r})\| = \frac{k_l^2}{4\pi\omega^2\rho}\frac{e^{ik_l r}}{r}\cdot\left(\frac{-2k_l}{1-a_l b_l k_l^2\sin^2\theta}\right)\begin{pmatrix} a_l\hat{\mathbf{r}}_1^2\hat{\mathbf{r}}_3 & a_l\hat{\mathbf{r}}_1\hat{\mathbf{r}}_2\hat{\mathbf{r}}_3 & a_l\hat{\mathbf{r}}_1\hat{\mathbf{r}}_3^2 \\ a_l\hat{\mathbf{r}}_1\hat{\mathbf{r}}_2\hat{\mathbf{r}}_3 & a_l\hat{\mathbf{r}}_2^2\hat{\mathbf{r}}_3 & a_l\hat{\mathbf{r}}_2\hat{\mathbf{r}}_3^2 \\ b_l\hat{\mathbf{r}}_1\sin^2\theta & b_l\hat{\mathbf{r}}_2\sin^2\theta & b_l\hat{\mathbf{r}}_3\sin^2\theta \end{pmatrix}. \tag{3.30}$$

In exactly the same way, for the transverse terms, we find

$$\|S^t(\mathbf{r})\| = \frac{k_t^2}{4\pi\omega^2\rho}\frac{e^{ik_t r}}{r}\left(\frac{-2k_t}{1-a_t b_t k_t^2\sin^2\theta}\right)\begin{pmatrix} a_t b_t k_t\hat{\mathbf{r}}_2^2 - a_t\hat{\mathbf{r}}_1^2\hat{\mathbf{r}}_3 & -a_t(b_t k_t\hat{\mathbf{r}}_1\hat{\mathbf{r}}_2 + \hat{\mathbf{r}}_1\hat{\mathbf{r}}_2\hat{\mathbf{r}}_3) & a_t(\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_1\hat{\mathbf{r}}_3^2) \\ -a_t(b_t k_t\hat{\mathbf{r}}_1\hat{\mathbf{r}}_2 + \hat{\mathbf{r}}_1\hat{\mathbf{r}}_2\hat{\mathbf{r}}_3) & a_t(b_t\hat{\mathbf{r}}_1^2 - \hat{\mathbf{r}}_2^2\hat{\mathbf{r}}_3) & a_t(\hat{\mathbf{r}}_2^2 - \hat{\mathbf{r}}_2\hat{\mathbf{r}}_3^2) \\ b_t\hat{\mathbf{r}}_1\hat{\mathbf{r}}_3^2 & b_t\hat{\mathbf{r}}_2\hat{\mathbf{r}}_3^2 & -b_t\hat{\mathbf{r}}_3\sin^2\theta \end{pmatrix}, \tag{3.31}$$

where

$$a_t = \frac{C_l C_t[(C_t^2 - C_l^2\sin^2\theta)^{\frac{1}{2}} - C_l\cos\theta] + 2C_t^3\cos\theta}{\omega(C_t^2 - C_l^2\sin^2\theta)^{\frac{1}{2}}[(C_t^2 - C_l^2\sin^2\theta)^{\frac{1}{2}} + C_l\cos\theta]}, \tag{3.32}$$

$$b_t = -\frac{C_l C_t[(C_t^2 - C_l^2\sin^2\theta)^{\frac{1}{2}} - C_l\cos\theta] + 2C_t^3\cos\theta}{\omega C_l\cos\theta[(C_t^2 - C_l^2\sin^2\theta)^{\frac{1}{2}} + C_l\cos\theta]}. \tag{3.33}$$

Actually, Eqs. (3.32) and (3.33) are correct only for $\theta < \theta_c$, where θ_c is the angle at which the radicand vanishes:

$$\sin^2\theta_c \equiv C_t^2/C_l^2 = \mu/(\lambda + 2\mu). \tag{3.34}$$

For $\theta > \theta_c$, we must modify (3.32) and (3.33) by the replacement

$$(C_t^2 - C_l^2\sin^2\theta)^{\frac{1}{2}} \to i(C_l^2\sin^2\theta - C_t^2)^{\frac{1}{2}}. \tag{3.35}$$

Equations (3.24) and (3.27)–(3.35) provide an exact description of the surface corrections at any point $\mathbf{r}$ to the radiation field from a surface source. We observe from (3.27)–(3.35) that

(i) the matrices $\|B(k_{l,t}\vec{r}/r)\|$ are independent of ω; thus, the inverse Fourier transform with respect to time is essentially as trivial here as it was[1] in the infinite medium case;

(ii) no radiation due to the surface appears (i.e., the radiation field of u_j coincides with that of $u_j^{(0)}$) on the axis $\vec{r} = 0$;

(iii) there may also occur, depending upon the relative magnitudes of λ and μ, cone-shaped regions on which either the longitudinal or the transverse parts of the radiation field due to the surface vanish. Specifically, we find from Eqs. (3.27) and (3.29) that $\|S^l\|$ is zero on the cone (which may or may not be physical)

$$\cos\theta = \lambda/2\mu \tag{3.36}$$

and, similarly, from Eqs. (3.32) and (3.33), that the transverse terms do not appear on

$$\cos\theta = (\lambda + 2\mu)/4\mu. \tag{3.37}$$

We conclude our discussion of the case of a source on the earth's surface by considering the effects observed at a point $\mathbf{r}$ which is also on that surface. (The result here is atypically simple.) Thus, we set

$$\mathbf{r} = (x_1, x_2, 0), \quad \theta = \tfrac{1}{2}\pi \tag{3.38}$$

and find, from Eqs. (3.27)–(3.33) that a_l and b_t are infinite. It follows immediately that

$$\|S^l\| = 0, \quad x_3 = 0, \tag{3.39}$$

and

$$\|S^t\| = \frac{2k_t^2}{4\pi\omega^2\rho}\frac{e^{ik_t r}}{r}\begin{pmatrix} \hat{\mathbf{r}}_2^2 & -\hat{\mathbf{r}}_1\hat{\mathbf{r}}_2 & 0 \\ -\hat{\mathbf{r}}_1\hat{\mathbf{r}}_2 & \hat{\mathbf{r}}_1^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.40}$$

Thus, the longitudinal waves on the surface are just as in the infinite medium case, while the transverse modes are modified by the correction term

$$v_j(x_1, x_2, 0) = \frac{k_t^2}{4\pi\omega^2\rho}\frac{e^{ik_t r}}{r}(2\delta_{kj} - \hat{\mathbf{r}}_k\hat{\mathbf{r}}_j) \times \{f_k^t(\hat{\mathbf{r}}) + ik_t[\lambda\hat{\mathbf{r}}_k T_{nn}^t(\hat{\mathbf{r}}) + 2\mu\hat{\mathbf{r}}_n T_{nk}^t(\hat{\mathbf{r}})]\}, \tag{3.41}$$

where $i, j, k = 1, 2$ only and $v_3 = 0$.

The Case of a Source in the Earth's Interior

While no serious difficulties occur in using Eq. (3.7) to determine the surface effects due to a source buried within the earth, it is not possible in the case to write the equation in any substantially simplified form. [This is because the identity (2.20) is no longer applicable.] Therefore, we confine our attention here mainly to isolating the radiation field.

In this regard, a minor difficulty is seen to occur. Equation (3.15), which we previously used to determine the radiation part of the field, is true for $r \gg r'$,

but no such inequality holds if the source is deeply buried and if, as we have stipulated in Sec. 2, our origin of coordinates is on the surface S. Hence, first of all, we affect on Eq. (3.7) a displacement of the origin by a distance R in the x_3 direction. Since the only relevant quantity which is not invariant under such a displacement is $H_{il}(\vec{k}, x_3)$, this modification is easily accomplished. We let [cf. Eq. (2.34)]

$$R_{ij}(\mathbf{r}', \mathbf{r}) \equiv \frac{-1}{(2\pi)^2} \int d\vec{k} \exp(-i\vec{k} \cdot \vec{r}') \times H_{il}(\vec{k}, x_3' + R) \|A^{-1}\|_{lm} \hat{G}_{mj}(\vec{k}, 0; \mathbf{r}). \tag{3.42}$$

Then we can conveniently compute the radiation due to the surface S from Eq. (3.7) with S_{ij} replaced by R_{ij}:

$$v_j(\mathbf{r}) = \int_B d^2r' [R_{ij}(\mathbf{r}', \mathbf{r}) F_i(\mathbf{r}') - u_i(\mathbf{r}') n_k D_{kim}(\partial') R_{mj}(\mathbf{r}', \mathbf{r})]. \tag{3.43}$$

Equation (3.16) is now directly applicable (i.e., we may again assume the origin is within B), and we find that for the radiation field, Eq. (3.42) reduces to

$$\begin{aligned} R_{ij}(\mathbf{r}', \mathbf{r}) = {} & \frac{-k_l^2}{4\pi\omega^2\rho} \frac{e^{ik_l r}}{r} \exp\left(-ik_l \frac{\vec{r} \cdot \vec{r}'}{r}\right) \hat{\mathbf{r}}_m \hat{\mathbf{r}}_j \\ & \times H_{il}\left(k_l \frac{\vec{r}}{r}, x_3' + R\right) \left\| A^{-1}\left(\vec{k} = k_l \frac{\vec{r}}{r}\right) \right\|_{lm} \\ & - \frac{k_t^2}{4\pi\omega^2\rho} \frac{e^{ik_t r}}{r} \exp\left(-ik_t \frac{\vec{r} \cdot \vec{r}'}{r}\right) (\delta_{mj} - \hat{\mathbf{r}}_m \hat{\mathbf{r}}_j) \\ & \times H_{il}\left(k_t \frac{\vec{r}}{r}, x_3' + R\right) \left\| A^{-1}\left(\vec{k} = k_t \frac{\vec{r}}{r}\right) \right\|_{lm}. \end{aligned} \tag{3.44}$$

Here we recall

$$\|A^{-1}(\vec{k} = k_{l,t}(\vec{r}/r))\|_{lm} = \delta_{lm} - \|B(k_{l,t}(\vec{r}/r))\|_{lm}, \tag{3.45}$$

where the $\|B\|$ matrices are given by Eq. (3.12), with Eqs. (3.27), (3.29), (3.32), and (3.33). The quantities H_{il} are obtained by making the appropriate substitution $(\vec{k} \to k_{l,t}(\vec{r}/r))$ in Eq. (2.25); for example, a fairly typical longitudinal matrix element is readily found to be

$$\begin{aligned} & H_{11}\left(k_l \frac{\vec{r}}{r}, x_3' + R\right) \\ & = \frac{-\mu}{\omega^2\rho}\left(k_l^2\left\{\exp\left[-ik_l \frac{x_3}{r}(x_3' + R)\right]\right.\right. \\ & \quad - \exp\left[-i\left(k_t^2 - k_l^2 \frac{\vec{r}^2}{r^2}\right)^{\frac{1}{2}}(x_3' + R)\right]\Bigg\} \frac{x_1^2}{r^2} \\ & \quad \left. + \frac{k_t^2}{2} \exp\left[-i\left(k_t^2 - k_l^2 \frac{\vec{r}^2}{r^2}\right)^{\frac{1}{2}}(x_3' + R)\right]\right). \end{aligned} \tag{3.46}$$

The other elements H_{ij} are similarly trivial to determine but lengthy to reproduce and it seems hardly worthwhile to exhibit them here. We leave our formulation of Eqs. (3.43)–(3.46) with the following remarks:

(i) for a small, deep source ($R \gg x_3'$), we might approximate by setting x_3' equal to zero in Eq. (3.46). Unfortunately, this does not yield any major computational simplification. In fact, the only apparent situation in which the complexities of R_{ij} are drastically reduced is that for which $\vec{r} = 0$, i.e., when the observation point is directly above the source (it is easily verified that, in this case, most of the quantities R_{ij} vanish);

(ii) unlike the case of a surface source, the surface correction to the radiation from an interior source cannot be separated into terms propagating purely at the velocities of Eqs. (3.28) [cf. the square-root exponents in Eq. (3.46)];

(iii) finally, it is clear from Eq. (3.46) that we chose the signs properly in Eqs. (3.26).

4. CONCLUSION

Equation (3.7) gives a prescription, based on the half-space Green's function presented by Eqs. (2.33) and (2.34), for calculating the elastic disturbance due to the earth's surface when an arbitrary source is embedded on or within that surface. (The earth is idealized as a homogeneous half-space.) We have examined the consequences of Eq. (3.7) in some detail, especially in the case of a source on the surface, and shown in general how the radiation part of the field is to be distinguished. In the combination of our results with those of Ref. 1, a fairly complete prescription for the elastic half-space problem is obtained.

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[1] K. M. Case and J. F. Colwell, Geophysics 32, 52 (1967). This reference includes a fairly extensive bibliography.

In addition, the authors are indebted to the referee for pointing out the following useful reference: C. C. Chao, J. Appl. Mech. 3, 559 (1960).

[2] The correspondence between the $(\mp)$ signs and the (l, t) subscripts in Eqs. (2.26) is such that the l goes with the upper $(-)$ sign. Note also that the subscripts on k_l^2 and k_t^2 are not coordinate subscripts [cf. Eq. (2.24)] and therefore are not summed over.

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Some Aspects of the Relationship between Mathematical Logic and Physics. I*

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Quantum mechanics has several deficiencies as a complete theoretical description of the measurement process. Among them is the fact that the quantum mechanical description of correlations between the single measurements of a sequence is quite problematic. A single measurement is defined to be a preparation followed by an observation. In particular, one feels that an infinite sequence of such single measurements which corresponds to the measurement of a question O on a state η where η does not lie entirely in an eigenspace of O should generate a random output sequence. However, quantum mechanics seems to say nothing about this. In this paper, physical theories are defined in such a manner that correlations between single measurements are explicitly included. In particular, a physical theory is considered to be a mapping U, with domain in the set $[Qs\tau]$ of infinite instruction strings for carrying out infinite sequences of single measurements and range in the set of probability measures defined on A, the usual σ algebra of subsets of Ω. Ω is the set of all infinite sequences of natural numbers. A fundamental property which any valid physical theory must satisfy is that it agrees with experiment. It is proposed and discussed here that much of the intuitive meaning of agreement between a theory U and experiment with respect to H is given by the statement

$$\forall Qs\tau\ [U(Qs\tau) \text{ defined} \Rightarrow E(H, U(Qs\tau), \psi_{Qs\tau})],$$

where $U(Qs\tau)$ is the probability measure U associates with the infinite instruction string $Qs\tau$ and $\psi_{Qs\tau}$ is the outcome sequence obtained by carrying out $Qs\tau$. $E(H, U(Qs\tau), \psi_{Qs\tau})$ is the statement that all formulas in H with one free sequence variable which are true on Ω almost everywhere with respect to $U(Qs\tau)$ are true for $\psi_{Qs\tau}$. H is a subclass of the class of all formulas in a formal language L. A theorem is proved which states that, if $U(Qs\tau)$ corresponds to a nontrivial product probability measure and U H-agrees with experiment, then the outcome sequence $\psi_{Qs\tau}$ is H-random. H-randomness is defined here in terms of the statement $E(H, P, \phi)$. Another property of a valid physical theory, which is defined here, is that, for some $Qs\tau$, $U(Qs\tau)$ must be determinable on much of A_H from $\psi_{Qs\tau}$. Sufficient conditions for this property to hold are given. A_H is the class of all H definable subsets of Ω. Some properties of the statement $E(H, P, \phi)$ are given. Among other things, it is proved that, if $E(H, P, \phi)$ holds and P is a nontrivial probability measure on A, then ϕ is not definable in H.

I. INTRODUCTION

The success of quantum mechanics in explaining many features of the physical world is remarkable indeed; yet there are continuing problems. In particular, quantum mechanics seems to be incomplete when it is used to describe the measuring process. For example, quantum mechanics, in its present form, does not define the class of Hermitian operators to be associated with laboratory procedures. Thus, no one knows what procedure, if any, corresponds[1] to the Hermitian operator xyp_z. Furthermore, the superselection rules which state the nonexistence of certain observables, and thus the nonexistence of certain measurement procedures,[2,3] cannot be derived within quantum mechanics.

Another difficulty is that there are many properties of sequences of single measurements which are clearly empirical, but whose description within quantum mechanics is quite problematic. For example, it appears impossible to describe the statistical properties of different single measurements in a sequence[4] where each single measurement consists of a preparation procedure followed by an observation procedure.

It is necessary here to distinguish clearly between the statistical properties among different single measurements in a sequence and those of the different parts of a compound single measurement. For example, consider the expression

$$\begin{aligned}\text{Tr}\,[\rho(1, 2, \cdots, n)P^n_{\lambda_1}(1) &\\ \times e^{iH'(t_2-t_1)}P^n_{\lambda_2}(2)\cdots e^{iH'(t_n-t_{n-1})}P^n_{\lambda_n}(n) &\\ \times e^{-iH'(t_n-t_{n-1})}\cdots P^n_{\lambda_1}(1)], &\qquad (1)\end{aligned}$$

where, for $i = 1, 2, \cdots, n$, $P^n_{\lambda_i}(i)$ is the projection operator given by

$$P^n_{\lambda_i}(i) = 1_1 \times \cdots \times 1_{i-1} \times P_{\lambda_i}(i) \times 1_{i+1} \times \cdots \times 1_n$$

and H' is an n-body Hamiltonian. If one assumes some postulate,[5] such as the problematic[6,7] projection postulate of von Neuman,[8] then Eq. (1) gives the probability, within a compound single measurement, that eigenvalue λ_1 is observed at time t_1 and $\cdots$ and eigenvalue λ_n is observed at time t_n on state $\rho(1\cdots n)$ with $t_1 \leq t_2 \leq \cdots \leq t_n$. On the other hand, even if one assumes the validity of the projection postulate, the use of expressions like Eq. (1) to describe the statistical properties between different single measurements (compound or not) in a sequence is quite

problematic. One reason is that each single measurement consists of a preparation followed by an observation whereas Eq. (1) describes a single n-body preparation at time t_1 and a single n-body compound observation.

It is to be noted that we are *not* saying that the usual intuitive assumption that each single measurement in a sequence is independent of the surroundings (including the other single measurements) is wrong. This assumption is very likely correct. Rather, the point is that the precise statement of this independence does not seem to be possible within quantum mechanics. To make such a statement within quantum mechanics requires, among other things, the assignment of a quantum mechanical state to the universe including the conscious observer as these are the surroundings of any single measurement.

An example of this deficiency in quantum mechanics, which is a motivation for the present work, is given by the following statement (a single measurement is a preparation followed by an observation): If an infinite sequence of single measurements corresponds to the measurement of a question, O, on a pure state η where η does not lie entirely within an eigenspace of O, then the associated outcome sequence is random. Now, offhand, one feels that this statement should be provable. However, in spite of the fact that one can give crude arguments to support the validity of this statement, it seems impossible to find a proof. Among the problems is the fact that the concept of randomness is so far not defined in quantum mechanical terms.

Another problem with quantum mechanics arises from the association of eigenvalues of an observable with a set of possible single measurement outcomes. The problem arises from the fact that, in general, eigenvalues are real numbers whereas the outcomes of single measurements are basically natural numbers and never real numbers.[9] In essence, a pointer reading is (a symbol for) a natural number which states between which marks on the dial the pointer lies. [Acceptance of this aspect of experiment does not mean that the mathematics of physics must give up real numbers (see the Appendix).]

One cannot avoid this problem by assuming that a single measurement outcome is some real number in an interval $[r, s]$ of the real line. One reason is that this requires that one be able to determine, as single-measurement outcomes, the real numbers r and s. Allowing r and s to be rational numbers does not help as these end points have meaning only as replacements for particular real numbers.

These and other aspects of quantum mechanics (see the Appendix) suggest that quantum mechanics is a part of some underlying structure or process. Clearly, the process must describe in detail the basic aspects of the construction of a physical theory from experiment. In essence, this process is the epistemological process, the importance of which to physics was suggested by Wigner[1,10] and others.[3,11] It is this author's belief that, besides clarifying the above and other problems, a precise description of this process will not only aid the understanding of the relation between the observer and the physical world, but will shed light on "the limits of explanation" of the physical world by any physical theory and may even yield new physics. This latter possibility arises from the circumstance that, at the most basic level, physical reality may not be independent of this process but may be essentially defined by it.

That mathematical logic may play a role in resolving these problems has received little attention. The literature includes discussion on the relation between the measurement process, physics, and logic,[12–14] discussions and attempts to axiomatize physical theories as formal systems and models,[15,16] and other papers.[17] Of special interest are the attempts[18,19] to bring explicitly into physics some properties of actual measurement procedures.

Among other reasons, the close relation between mathematical logic, physics, and the epistemological process arises from the fact that the basic aim of the process is to construct a physical theory which "explains" the empirical world. A physical theory includes a formal system of symbols, formulas, axioms, etc., which is the subject of mathematical logic.

Another reason which is more important for our purpose is that, for infinite sequences of natural numbers, the concept of randomness appears to be definable in mathematical logical terms only. Extensions of these definitions into classical mathematical definitions fail. Because of the importance of this fact, the literature definitions of randomness are reviewed in Sec. II and a definition of H-randomness is given in Sec. III.

This limitation on the definition of random sequences does not become relevant to physics until one notes that infinite sequences of single measurements are a very large part of the total contact (in the rigorous sense) between physical theory and experiment. Furthermore, it requires an infinite amount of time for an observer to carry out an infinite sequence of steps, be they computing steps or sequences of single measurements. These two basic facts of the epistemological process are given in slightly different

form as P1 and P2 in the Appendix. There, we briefly discuss why P1 and P2 are required by quantum mechanics and an upper limit to signal velocities. P2 and its consequences, which also apply to infinite sequences of computing steps, mean that the result of a single measurement cannot be a real number since an infinite number of steps in general are needed to record or read a real number. This fact applied to the epistemological process is also given in the Appendix as P3, which says that counting is basically the only operation by which one obtains numbers from the real world.

Clearly, if one is to understand the epistemological process and its relevance to physics, one must understand exactly what is meant by a physical theory "explaining" the empirical world. This paper takes steps in this direction by defining a class of mappings and considering a physical theory to be an element of the class. Then some necessary conditions are given and discussed for a mapping to be a valid physical theory.

One of the main results of this paper is an exact statement which includes much of the intuitive meaning of agreement between theory and experiment. To give a brief review of this result, let the triple $(Qs\tau)$ denote an infinite string of instructions for carrying out an infinite sequence of single measurements. Q is a function from N, the set of natural numbers to the class of instructions for carrying out single measurements. s and τ are functions from N to N which denote the space position and calendar times at which each single measurement is to be carried out. The jth single measurement in a sequence is described by $Q(j)$, $s(j)$, $\tau(j)$. Let $[Qs\tau]$ denote the class of all instruction strings which can be carried out by an observer. Let $\psi_{Qs\tau}$ be the outcome sequence of natural numbers obtained by carrying out $Qs\tau$.

Let H denote a subclass of formulas over N, Ω (the set of all functions from N to N), and R (the real numbers) of those of a formal language L. Define a physical theory to be a mapping U with domain in $[Qs\tau]$ and range in the class of probability measures defined on A, the classical σ algebra of all subsets of Ω. Then much of the intuitive meaning of agreement of theory U with experiment with respect to H is given in the statement (12)

$$\forall(Qs\tau)\ [U(Qs\tau)\text{ defined} \Rightarrow E(H, U(Qs\tau), \psi_{Qs\tau})],$$

where $E(H, P, \phi)$ is the statement (8) that every relation in H which is true P almost everywhere on Ω is true at ϕ. In words, Eqs. (12) and (8) say that, for all triples $(Qs\tau)$ for which $U(Qs\tau)$ is defined, every relation which is true almost everywhere with respect to the measure $U(Qs\tau)$ is true for $\psi_{Qs\tau}$.

This statement is discussed in detail in Sec. IV. There it is shown that, for a particular definition of H, much of the intuitive meaning of agreement between theory and experiment is included. If some probability-theoretic statements are added [Eqs. (14)–(18)], then some other properties of H-agreement between theory and experiment are included.

Another requirement on U is that there exists a U with a "large" domain of definition which satisfies Eq. (12). At present, not much can be said about this requirement as not much is known about the relation between $[Qs\tau]$, H, and $E(H, P, \phi)$.

A third requirement on U which is discussed in Sec. IV is that, for some $Qs\tau$ for which $U(Qs\tau)$ is defined, the measure $U(Qs\tau)$ should be determinable from $\psi_{Qs\tau}$ on much of A_H. A_H is the class of H-definable subsets of Ω. This requirement is given by Eq. (22), which is

$$\forall F\ [F \in A_H \wedge \gamma_F \in L_0 \Rightarrow \bar{M}\gamma_F\psi_{Qs\tau}\text{ exists} \wedge \bar{M}\gamma_F\psi_{Qs\tau} = U(Qs\tau)F],$$

where the mapping γ_F with domain and range in Ω is defined by Eq. (19). Equation (22) says that, for each F in A_H for which γ_F is in L_0, the computed probability $U(Qs\tau)F$ of F is obtained from the outcome sequence as $\bar{M}\gamma_F\psi_{Qs\tau}$. $\bar{M}\psi$ denotes the limit mean of ψ. It is shown, among other things, that a sufficient condition for this requirement to be satisfied is that the one-sided shift operator is measure preserving and ergodic with respect to $U(Qs\tau)$ (Theorem 5).

In Sec. III, definitions of $E(H, P, \phi)$ and H are given and discussed. In particular, an existence theorem for $E(H, P, \phi)$ is given. It is also proved that, if the class of formulas in H is closed under negation and P is nontrivial (that is, $PS = 0$ for any single element subset, S, of Ω), then $E(H, P, \phi)$ implies ϕ is not definable in H (Theorem 3).

Finally, it is to be emphasized that a physical theory, as defined here, shares with quantum mechanics the correspondence between expectation values and empirical limit means obtained from infinite sequences of single measurements (Appendix). The fact that it requires an infinite amount of time to carry out an infinite sequence of single measurements (Appendix) and that these numbers cannot be rigorously obtained by any finite time is felt by many to be a difficulty with this interpretation of quantum mechanics. Thus, to the extent that this is a deficiency in the above interpretation of quantum mechanics, it

will also be a corresponding deficiency in the theories discussed here.

II. REVIEW OF DEFINITIONS OF RANDOMNESS

Before reviewing the literature definitions of randomness, it is worthwhile to set out some definitions. Let Ω denote the set of all total (everywhere defined) functions from N to N, A the usual σ-algebra of subsets of Ω and P a probability measure defined on A. Define a mapping $\mathfrak{J}_g$ with domain and range in Ω by

$$(\mathfrak{J}_g\phi)(j) \simeq \phi(g(\phi,j)), \tag{2}$$

where g is a function with domain in $\Omega \times N$ and range in N and $\simeq$ means that both sides of Eq. (2) are simultaneously defined or undefined and, when defined, are equal.

Clearly, the mapping defined by Eq. (2) is a subsequence selection procedure with $\mathfrak{J}_g\phi$ the subsequence of ϕ selected by g. The term subsequence selection procedure includes those mappings such that $\mathfrak{J}_g\phi$ is a proper subsequence of ϕ, as well as those for which $\mathfrak{J}_g\phi$ is a permutation of ϕ. The set transformation T_g induced by $\mathfrak{J}_g$ is defined by

$$T_gE = [\phi \mid \mathfrak{J}_g\phi \in E] \tag{3}$$

for each $E \in A$.

Define a mapping F_n from Ω to $\Omega_{0,1}$ by

$$(F_n\phi)(j) = f_n(\phi(j)), \tag{4}$$

for each j, where

$$f_n(l) = \delta_{n,l}. \tag{5}$$

F_n is a mapping which projects ϕ onto a 0–1 sequence such that $(F_n\phi)(j) = 1(0)$ if $\phi(j) = n$ ($\phi(i) \neq n$). $\Omega_{0,1}$ denotes the set of all infinite sequences of 0's and 1's. Finally, let $\bar{M}\psi$ denote the limit mean of ϕ given by

$$\bar{M}\phi = \lim_{i\to\infty} \frac{1}{i} \sum_{j=0}^{i-1} \phi(j),$$

if it exists. $\bar{M}F_n\phi$ gives the limit relative frequency of occurrence of n in ϕ.

One of the first definitions of random sequences was that given by von Mises.[20] He defined a sequence ϕ to be random if each component limit mean $\bar{M}F_n\phi$ exists and has the same value under the operation of subsequence selection. A subsequence selection procedure was defined as any rule whereby the selection or rejection of $\phi(l)$ can depend at most on $\phi(0)\cdots\phi(l-1)$ but not on $\phi(l)$. Examples of selection procedures are "select in the natural order all even numbered elements" or "select in the natural order all elements following the occurrence of a 3 by 2 places," etc.

This definition, with some minor alterations, may be given in the form [$\forall$ (for all), $\exists$ (there exists), $\wedge$ (and) $\vee$ (or), $\Rightarrow$ (implies), and $\neg$ (not)]

$$R_S(\phi) \equiv \forall n \forall g\, [\bar{M}F_n\phi \text{ exists} \wedge g \in S \Rightarrow \bar{M}F_n\mathfrak{J}_g\phi = \bar{M}F_n\phi] \wedge \exists a \exists b\, [a \neq b \wedge \bar{M}F_a\phi > 0 \wedge \bar{M}F_b\phi > 0]. \tag{6}$$

The requirement $\exists a \exists b[\ ]$ removes trivial sequences which, except for a finite number of terms, are constant. The mathematical definition given by von Mises of a selection rule corresponds to defining S to be the set of *all* monotonic increasing functions g from $\Omega \times N$ to N such that $g(\phi,j)$ depends at most on $\phi(0)\cdots\phi(g(\phi,j)-1)$ and not on $\phi(g(\phi,j))$. (The form of von Mises' original definition differs inessentially from this.)

It was soon shown that, for this classical mathematical definition of allowed subsequence selection procedures, no random sequences exist. To see this, restrict S to be the set of all monotonic increasing functions from N to N independent of Ω. Then, for each sequence $\phi \in \Omega$ which assumes the values m and n an infinite number of times, there exist a g and a $g' \in S$ such that $\mathfrak{J}_g\phi$ and $\mathfrak{J}_{g'}\phi$ are constant sequences of m's and n's, respectively.

Ways out of this difficulty were suggested by Wald[21] and Church.[22] Wald proposed that S be restricted to be a denumerable set such that each selection rule in S was definable in some given logic. The monotonicity and ϕ-dependence requirements on elements of ϕ were kept the same as in von Mises' definition. Wald also proved that, under his definition, random sequences exist.

Church[22] defines random sequences by restricting S in Eq. 6 to be the set of all functions g such that (1) as a function of j, $g(\phi,j)$ is monotonic increasing, (2) $g(\phi,j)$ depends at most on $\phi(0)\cdots\phi(g(\phi,j)-1)$ (these are the same as in von Mises' definition), and (3) g is ϕ-effectively calculable. Church's original definition was given for 0–1 sequences but is easily extended [Eq. (6)] to sequences with range in N. In brief, a ϕ-effectively calculable function from N to N is one for which there exists a precisely defined computation procedure which, given any argument j, outputs the value of the function in an arbitrary but finite number of steps. Among the allowed steps are questions of the form, "does $\phi(m) = n$?" The yes or no answers are to be supplied by an external agent or oracle.[23,24]

The existence of random sequences satisfying Church's definition is a consequence of a theorem of Doob.[25] This theorem states that any selection rule

[Eq. (2)] of a type which includes those defined by Church generates a set transformation [Eq. (3)] which is measure preserving with respect to any product probability measure defined on A.

A product probability measure P is a measure with respect to which PE_{nl} is independent of n for each l and for all intersections $\bigcap_{i=1}^{m} E_{f(i),h(i)}$, where h is any one-to-one function from N to N,

$$\left(P \bigcap_{i=1}^{m} E_{f(i),h(i)} = \prod_{i=1}^{m} PE_{f(i),h(i)}\right).$$

E_{nl} is the subset of Ω defined for each $n, l \in N$ by $E_{nl} = [\theta \mid \theta(l) = n]$.

Loveland[26] has extended Church's definition by allowing g to be one-to-one instead of monotonic increasing. He limits g to be ϕ-effectively calculable and requires, for each j, that $\phi(g(\phi, j))$ need not have been examined by the computation procedure for $g(\phi, k)$ for all $k \leq j$. Doob's theorem[25] is also used in this case to prove the existence of random sequences.

It can be shown constructively[27] that there are a denumerable infinity of effectively calculable selection procedures which are excluded by Church's and Loveland's definition and which still satisfy Doob's theorem. In particular, the requirement that the computation procedure not examine an element of ϕ prior to its selection can be relaxed. A set of conditions on S in Eq. (6), which are sufficient as far as the existence requirement is concerned are (1) that S be denumerable and (2) that each g in S generate a measure preserving transformation T_g on A with respect to all product probability measures defined on A.[27]

The difficulty with using subsequence selection procedures only, to define randomness, as in Eq. (6), was noted some time ago by Ville.[28] He showed (nonconstructively) that for any denumerable set of selection procedures there exists a 0–1 sequence ϕ whose limit mean is the same for all subsequences selected by the procedures in the set. Yet ϕ has the property that

$$M_m\phi \geq \bar{M}\phi,$$

for each m, where $M_m\phi$ is the mean of the outcomes of the first m single measurements. Obviously, such a sequence where the mean sequence approaches the limit from one side only is not random.

Definitions of random sequences which avoid Ville's objection have been given by Martin Löf[29] and Kruse.[30] Martin Löf's definition is given for 0–1 sequences where the product measure P is such that $PE_{1l} = PE_{0l} = \frac{1}{2}$ for all l. Martin Löf defines a class of tests for randomness to be those given by the set of all hyperarithmetic relations with one free function variable which are true almost everywhere with respect to P. He then defines the class of random sequences as the intersection of all hyperarithmetic subsets of 0–1 sequences of P measure 1. Since there is only a denumerable infinity of such sets, the existence of random sequences follows immediately.

This definition, which is an extension of an earlier definition,[31] can be easily extended to sequences in Ω and arbitrary product measures. Martin Löf further notes that, if the class of tests for randomness is extended to include the classical totality of all subsets of Ω of P measure 1, the set of sequences passing these tests is empty.

In brief, the hyperarithmetic relations are those which are "just beyond" the arithmetic relations. The arithmetic relations are those relations which are made up from the usual logical symbols, the "equality," "plus," and "times" symbols, variables for natural numbers and functions in Ω, and the numerals $0, 1, \cdots$. The quantifiers $\forall$ and $\exists$ act only on number variables and not on function variables.

If one now allows $\forall$ and $\exists$ to act on the function variables as well, an extended class of relations, the analytical relations, are obtained. These can be converted into a standard form with the quantifiers in front and the function quantifiers ahead of number quantifiers. Then the hyperarithmetic relations are those which can be written in both one function quantifier forms. That is, $R(\cdots)$ is hyperarithmetic if and only if $\forall f S(f \cdots) = R(\cdots) = \exists f T(f \cdots)$, where $S(f \cdots)$ and $T(f \cdots)$ are arithmetic relations and f is a function variable. A hyperarithmetic subset of Ω is a set defined by $[\theta \mid R(\theta)$ true$]$, where $R(\theta)$ is hyperarithmetic.[23,32]

The definition of random sequences given by Kruse[30] is of the same type but more general. He first defines a collection of all "mixed" relations formed using the logical symbols of a set theory and objects from a model for the set theory. Then, for each product probability measure P such that $PE_{nl} > 0$ for each n and l, the class of tests for Z-randomness is defined to be the class of all such "mixed" relations where the model objects are in a class Z and the relations are true, P almost everywhere on Ω. Each test in the class defines a "Z-nameable" subset of Ω of P measure 1. A sequence φ is Z-random if, for some product measure P of the type described, φ is contained in the intersection of all "Z-nameable" sets of P measure 1. Kruse proves that if Z is countable, then Z-random sequences exist. This definition applies directly to sequences with range in N. Kruse gives his

definition in a different form and proves it to be equivalent to the above description.

One reason for studying these definitions of random sequences is that one intuitively feels that, for many infinite sequences of single measurements in physics, the associated outcome sequences are random. In particular, for certain sequences such as the example given in the introduction, one should be able to prove the randomness of the outcome sequence. Because this appears hard to carry out for quantum mechanics, a physical theory is defined in such a way that various properties of outcome sequences, including randomness, can be discussed. Such a discussion first requires a framework for discussing mathematical properties of the outcome sequence.

III. FRAMEWORK

To begin with, a formal language L is needed, relative to which the various concepts can be described. In order to make the discussion explicit and to clarify certain points, a particular L and set of formulas H in L will be chosen. At this point, it is neither necessary nor desirable to make a final choice for L or H and, with the exception of Theorem 1, none of the theorems which follow are dependent on such a choice. It is also clear from the discussion in Sec. IV that the L chosen here must ultimately be changed, as it is too simple in many respects.

Here, L is chosen to be a language somewhat more extended than that used for second-order arithmetic.[23] That is, L has a denumerable supply of variables $i, j, i', j', \cdots ; \phi, \theta, \phi', \theta', \cdots ; \alpha, \beta, \alpha', \beta' \cdots$ which range over N, Ω, and R (the class of real numbers), respectively. Besides these symbols, L contains the names $0, \cdots, n, l, m, \cdots ; \psi, \cdots$ and $r, s \cdots$ of all the elements of N, Ω, and R, respectively. Thus, L contains nondenumerably many constant symbols as names of elements in Ω and R.

The only primitive nonlogical predicate and operation symbols in L are the equality symbol $(=)$ and the symbols $+$ (plus) and $\times$ (times) defined on Ω, R, and N $[(\phi + \theta)(j) = \phi(j) + \theta(j)$ and $(\phi \times \theta)(j) = \phi(j) \times \theta(j)$ for all $j]$. Terms which designate individuals of Ω, R, or N are built up in the usual inductive manner: (1) Variables and names are terms; (2) if ϕ is a sequence variable and Y is an N-term, $\phi(Y)$ is an N-term; (3) $Y + Z$ and $Y \times Z$ are terms if Y and Z are terms of the same type (i.e., both N-terms or both Ω-terms or both R-terms). Similarly, by use of the nonlogical symbols $\neg$ (not), $\wedge$ (and), $\vee$ (or), $\Rightarrow$ (implies), $\forall$ (for all), and $\exists$ (there exists), formulas are built up inductively as follows: (1) $Y = Z$ is a formula if Y and Z are terms of the same type; (2) $\neg Y$, $Y \wedge Z$, $Y \vee Z$, $Y \Rightarrow Z$ are formulas if Y and Z are formulas; (3) $\exists x Y$ and $\forall x Y$ are formulas if Y is a formula and x is a variable of Ω, R, or N.

The reference class of formulas H used here is defined as follows: Let H_0 be the class of formulas in L_0, where L_0 is the sublanguage of L obtained by removing from L the names of elements of R and Ω. Define a class of formulas H' in L as follows:

For each L_0-definable operation $O:\Omega \to \Omega$, define the class of formulas, H^O, as follows: (1) for each real number r and sequence variable ϕ, the formula $\bar{M}O\phi = r$ is in H^O and (2) $\neg Y$, $Y \vee Z$, $Y \wedge Z$, $Y \Rightarrow Z$ are in H^O if Y and Z are formulas in H^O. Then H' is defined by $H' = \bigcup H^O$, where the union is taken over all L_0-definable operations O. The L_0-definability of O means that there exists a formula q' in H_0 such that for all ϕ and θ, $O(\phi) = \theta \Leftrightarrow q'(\phi, \theta)$. Finally, H is defined as $H = H_0 \cup H'$. Clearly H is a subset of the class of formulas of L. The reason for defining H in such a manner becomes clear later on.

From the definitions of L_0 and H, it is clear that statements about many operations are included in H. For example, the projection mappings of Eqs. (4) and (5) are definable in L_0 as are all subsequence selection mappings of Eq. (2) where g is definable in L_0. That is, there must exist a formula q in H_0 such that for, all ϕ, j, and k, $g(\phi, j) = k \Leftrightarrow q(\phi, j, k)$ holds. In particular, the one-sided shift operator $\mathfrak{z}:\Omega \to \Omega$ defined by

$$(\mathfrak{z}\phi)(j) = \phi(j + 1) \tag{7}$$

is included. For example, H includes the formulas $\bar{M}O\phi$ exists and $\bar{M}O\phi = \bar{M}O'\phi$ for all L_0-definable O and O' as these formulas are equivalent to the Cauchy limit statements $\exists\alpha\forall i\exists j\forall i'(2^i |M_{j+i'}O\phi - \alpha| < 1)$ and $\forall i\exists j\forall i'\forall j'(2^i |M_{j+i'}O\phi - M_{j+j'}O'\phi| < 1)$, respectively, where the indicated operations and relations are obviously L_0-definable.

Let A denote, as before, the usual classical σ algebra of subsets of Ω and $[P]$, the class of all probability measures defined on A. Let A_H denote the class of all H-definable subsets of Ω. A subset of Ω is H-definable if it is given by $[\theta \mid q(\theta)$ true$]$, where q is some formula of H with exactly one free sequence variable. Clearly, any measure P in $[P]$ is defined on A_H as $A_H \subset A$.

Finally, it should be noted that the discussion of this and the next section are all in a metalanguage which is not part of L. This includes expressions such as Eqs. (8), (9), etc., and the theorems which are all metatheorems. In this connection, the symbols Y and Z are syntactic variables which range over terms and formulas of L. Also, expressions such as $\bar{M}O\phi$ exists,

$\bar{M}O\phi = \bar{M}O'\phi$, etc., are syntactic names for formulas in H. Clearly, these expressions and symbols are all part of the metalanguage and are not in L.[32]

Define $E(H, P, \phi)$ by

$$E(H, P, \phi) \equiv \forall q\,[q \in H \wedge q \text{ has exactly one free sequence variable} \wedge P\,[\theta \mid q(\theta)] = 1 \Rightarrow q(\phi)]. \quad (8)$$

Here, q is a syntactic variable which ranges over all formulas of L. $E(H, P, \phi)$ says that all formulas in H which contain exactly one free sequence variable and are true P almost everywhere are true at ϕ. Equivalently, $E(H, P, \phi)$ says ϕ is contained in the intersection of all H-definable subsets of P measure 1. The requirement that q have exactly one free sequence variable excludes formulas with free number variables.

The following theorem, which shows that the above definition is not empty, requires that P be nontrivial or

$$\forall\theta\,(P[\theta] = 0). \quad (9)$$

This excludes pathological measures which are nonzero on any single element subset of Ω. The proof of the theorem is quite long.

Theorem 1: If P is nontrivial, then there exist sequences ϕ such that $E(H, P, \phi)$.

Proof: The goal of the proof is to show that $P[\phi \mid E(H, P, \phi)] = 1$. By the definition of H, one has

$$[\phi \mid E(H, P, \phi)] = [\phi \mid E(H_0, P, \phi)] \cap [\phi \mid E(H', P, \phi)].$$

Since H_0 is denumerable, Eq. (8) yields immediately that $P[\phi \mid E(H_0, P, \phi)] = 1$. It remains to show that $P[\varphi \mid E(H', P, \varphi)] = 1$.

Suppose that it can be shown that, for each sequence variable ϕ, some formula $B(L_0, P, \phi)$ exists such that (1) $P[\phi \mid B(L_0, P, \phi)] = 1$ and, for each formula $q(\phi)$ in H' with one free sequence variable, (2) if $P[\theta \mid q(\theta)] = 1$, then $B(L_0, P, \phi)$ implies $q(\phi)$, and (3) if $P[\theta \mid q(\theta)] = 0$, then $q(\phi)$ implies $\neg B(L_0, P, \phi)$. Then, for each $q(\phi)$ in H' for which $P[\phi \mid q(\phi)] = 1$, one has $[\phi \mid B(L_0, P, \phi)] \subseteq [\phi \mid q(\phi)]$. From this and Eq. (8), one obtains immediately the result that

$$[\phi \mid B(L_0, P, \phi)] \subseteq \bigcap_{q \in H'}{}' [\phi \mid q(\phi)] = [\phi \mid E(H', P, \phi)],$$

where $\bigcap'$ means the intersection is taken over all H'-definable subsets of P measure 1. Since

$$P[\phi \mid B(L_0, P, \phi)] = 1,$$

one has the desired result that $P[\phi \mid E(H', P, \phi)] = 1$.

In order to show that a formula $B(L_0, P, \phi)$ exists with the desired properties, one proceeds as follows: For each L_0-definable operation O, define the set A_O of real numbers by $r \in A_O$ if and only if

$$P\,[\phi \mid \bar{M}O\phi = r] > 0.$$

Either A_O is empty, in which case $P\,[\phi \mid \bar{M}O\phi$ does not exist$] = 1$, or A_O is not empty, in which case $P\,[\phi \mid \bar{M}O\phi$ does not exist$] < 1$.

Let $F_P(-, -)$ denote the choice function such that, for each L_0-definable operation O and each sequence variable ϕ,

(1) $F_P(O, \phi) = \bar{M}O\phi$ does not exist if $P\,[\phi \mid \bar{M}O\phi$ does not exist$] = 1$.

(2) $F_P(O, \phi) = \bigvee_{r \in A_O} \bar{M}O\phi = r$ if

$$P\,[\phi \mid \bigvee_{r \in A_O} \bar{M}O\phi = r] = 1.$$

In this case, $P\,[\phi \mid \bar{M}O\phi$ does not exist$] = 0$.

(3) $F_P(O, \phi) = \bigvee_{r \in A_O} \bar{M}O\phi = r \vee \bar{M}O\phi$ does not exist if $0 < P\,[\phi \mid \bar{M}O\phi$ does not exist$] < 1$. These cases are clearly exhaustive. Define $B(L_0, P, \phi)$ by

$$B(L_0, P, \phi) = \bigwedge_{O \in L_0} F_P(O, \phi).$$

By this definition, it is clear that $P[\phi \mid B(L_0, P, \phi)] = 1$ as there is, at most, a denumerable number of L_0-definable operations O and, for each such O,

$$P[\phi \mid F_P(O, \phi)] = 1.$$

To show that $B(L_0, P, \phi)$ has the other desired properties, one proceeds by induction on the length of the formulas in H'. It is necessary to consider the logical connectives $\neg$ and $\wedge$ only as $\vee$ and $\Rightarrow$ can be defined in terms of these two. The following statements, with $R(\phi)$ and $S(\phi)$ denoting formulas of H, are easily seen to be true.

(a) If $P[\phi \mid R(\phi)] = 1$ and $P[\phi \mid S(\phi)] = 1$ and $B(L_0, P, \phi)$ implies $R(\phi)$ and $B(L_0, P, \phi)$ implies $S(\phi)$, then $P\,[\phi \mid R(\phi) \wedge S(\phi)] = 1$ and $B(L_0, P, \phi)$ implies $R(\phi) \wedge S(\phi)$.

(b) If $P[\phi \mid R(\phi)] = 1$ and $P[\phi \mid S(\phi)] = 0$ and $B(L_0, P, \phi)$ implies $R(\phi)$ and $S(\phi)$ implies $\neg B(L_0, P, \phi)$, then $P\,[\phi \mid R(\phi) \wedge S(\phi)] = 0$ and $R(\phi) \wedge S(\phi)$ implies $\neg B(L_0, P, \phi)$. This latter implication follows from the proof, by truth-table construction, that the formula $((B \Rightarrow R) \wedge (S \Rightarrow \neg B)) \Rightarrow (R \wedge S \Rightarrow \neg B)$ is a tautology.[32] The argument for the case in which the roles of R and S are reversed is the same.

(c) If $P[\phi \mid R(\phi)] = 0$ and $P[\phi \mid S(\phi)] = 0$ and $R(\phi)$ implies $\neg B(L_0, P, \phi)$ and $S(\phi)$ implies $\neg B(L_0, P, \phi)$, then $P[\phi \mid R(\phi) \wedge S(\phi)] = 0$ and $R(\phi) \wedge S(\phi)$ implies $\neg B(L_0, P, \phi)$. Again, the latter implication follows

from the fact that

$$((R \Rightarrow \neg B) \wedge (S \Rightarrow \neg B)) \Rightarrow (R \wedge S \Rightarrow \neg B)$$

is a tautology.

(d) If $P[\phi \mid R(\phi)] = 1$ and $B(L_0, P, \phi)$ implies $R(\phi)$, then $P[\phi \mid \neg R(\phi)] = 0$ and $\neg R(\phi)$ implies $\neg B(L_0, P, \phi)$.

(e) If $P[\phi \mid R(\phi)] = 0$ and $R(\phi)$ implies $\neg B(L_0, P, \phi)$, then $P[\phi \mid \neg R(\phi)] = 1$ and $B(L_0, P, \phi)$ implies $\neg R(\phi)$.

The induction begins with the following two statements.

(f) For any L_0-definable O for which A_O is finite and $P[\phi \bigvee_{r \in A_O} \bar{M}O\phi = r] = 1$, $B(L_0, P, \phi)$ implies

$$\bigvee_{r \in A_O} \bar{M}O\phi = r.$$

[This follows directly from the definition of $B(L_0, P, \phi)$.]

(g) For any L_0-definable O and s for which $P[\phi \mid \bar{M}O\phi = s] = 0$, $\bar{M}O\phi = s$ implies $\neg B(L_0, P, \phi)$. The truth of this statement can be easily seen by considering separately the three cases in the definition of $F_P(O, \phi)$ with $s \notin A_O$.

The formulas $\bigvee_{r \in A_O} \bar{M}O\phi = r$ with A_O infinite and $\bigvee_{r \in A_O} \bar{M}O\phi = r \vee (\bar{M}O\phi$ does not exist) with A_O finite need not be considered in the initial statements of the induction since neither formula is in H'. [$B(L_0, P, \phi)$ is also not in H'.]

Comparison of the above seven statements with the definition of H' shows that the above induction includes all formulas of H' which are true P almost everywhere on Ω. Thus, the $B(L_0, P, \phi)$ constructed has the desired properties. QED

The following theorem about H and $E(H, P, \phi)$ is almost self-evident.

Theorem 2: Let H be closed under negation, let q be any formula in H with one free function variable, and suppose $E(H, P, \phi)$ holds. Then $P[\theta \mid q(\theta)] = 0 \Rightarrow q(\phi)$ false.

Proof: For any $q \in H$, one has $\neg q \in H$. Because $E(H, P, \phi)$ holds, one has

$$P[\theta \mid q(\theta)] = 0 \Rightarrow P[\theta \mid \neg q(\theta)] = 1 \Rightarrow \neg q(\phi) \text{ true} \Rightarrow q(\phi) \text{ false.}$$

QED

A more important property of H and $E(H, P, \phi)$ is given by the next theorem. The condition that H be closed under negation is clearly satisfied by the H as defined here.

Theorem 3: Let H be closed under negation and P be any nontrivial probability measure defined on A. Then, for any sequence ϕ, $E(H, P, \phi)$ implies that ϕ is not definable in H.

Proof: Assume the converse, that $E(H, P, \phi)$ holds and ϕ is definable in H. If ϕ is definable in H, then the formula $q_g(\theta)$ defined by $\forall j\,(g(j) = \theta(j))$ is in H where $g = \phi$ and g is definable in L_0. Since H is closed under negation, the relation $\neg q_g(\theta)$ defined by $\exists j\,(g(j) \neq \theta(j))$ is also in H. Consider the set $[\theta \mid \neg q_g(\theta)$ true]. Since this is the complement of the one point set $[\phi]$ and P is nontrivial, one has $P[\theta \mid \neg q_g(\theta)$ true$] = 1$. However, since $\neg q_g(\phi)$ is false, one has, by Eq. (8), that $E(H, P, \phi)$ is false. Thus, a contradiction is reached and ϕ must not be definable in H. QED

It should be stressed that this theorem holds for any nontrivial measure P, not just for product measures. Thus, there are many sequences ϕ which are not H-random [Eq. (10)] for which $E(H, P, \phi)$ is true. By this theorem, these sequences are not definable in H. Conversely, this theorem implies that there are many ϕ such that $E(H, P, \phi)$ is false for all nontrivial measures P. This includes any ϕ which is H-definable or is computable by a mathematical computation procedure. Computable functions are included in the definition of L_0 given here.

It is also clear that this theorem holds for many languages, not just the one defined here. This arises from the fact that the proof does not depend on any detailed properties of H. The only requirements are closure under negation and the containment of relations of the types $\forall j\,(g(j) = \theta(j))$.

Theorems 1 and 3 are the reason that formulas which contain the names of elements of Ω are excluded from H. For, if H contained all formulas of L which include the names of elements of Ω, then, for any sequence name ψ, the formula $\psi \neq \phi$ is in H and has exactly one free sequence variable. By the proof of the above theorem, $E(H, P, \psi)$ would be false, giving $E(H, P, \phi)$ false for all ϕ. Similarly, if H contains all formulas of L which include the names of elements of R and any one-to-one mapping from R to Ω (or from the irrationals to Ω) is L-definable, then H would again contain all formulas of L which contain the names of the elements of Ω.

H-randomness is defined by the expression

$$R_H(\phi) \equiv \exists P\,[P \text{ is a nontrivial product measure defined on } A \wedge E(H, P, \phi)]. \quad (10)$$

The existence of H-random sequences is an immediate consequence of Theorem 1.

This definition of H-randomness, with suitable modification of H, includes the definitions discussed

before. If one replaces H by H_1, where H_1 is the class of hyperarithmetic relations ($H_1 \subset H_0$ as defined here), then Eq. (10) gives Martin Löf's definition[29] (generalized to sequences in Ω and arbitrary product measures). If L is redefined to be the language of a set theory to which a denumerable collection Z of names of sets have added and H is the class of formulas of L, then one has Kruse's definition.[30]

With respect to subsequence selection tests $\mathfrak{F}_g$, Eq. (2), the formula $q_n(\theta)$, defined by

$$q_n(\theta) \equiv \bar{M}F_n\theta \text{ exists} \wedge \bar{M}F_n\mathfrak{F}_g\theta = \bar{M}F_n\theta,$$

is in H if $\mathfrak{F}_g$ is L_0-definable. Furthermore, $q_n(\theta)$ is true P almost everywhere for any product probability measure P if T_g [Eq. (3)] is measure preserving with respect to all such P.[25,27] Thus, Church's,[22] Loveland's,[26] and Wald's[21] definitions are included as each allowed $\mathfrak{F}_g$ is L_0-definable (or, in Wald's case, L-definable, where H is the class of formulas of some logic L) and T_g is measure preserving.

So far, infinite sequences ϕ and the measure P have been considered in the abstract. In order to relate the foregoing to the empirical world and use it to define properties of physical theories, one must relate ϕ and P to empirical procedures and their outcomes.

IV. PROPERTIES OF PHYSICAL THEORIES

A. Preliminaries

To begin, one notes that, in order for an observer to construct an infinite sequence of single measurements, he must at least (1) decide for each single measurement what preparation and observation procedures to use, and (2) decide the space position and calendar time at which each single measurement is to be carried out. To this end, let C and D denote respectively the classes of all instruction sets, written in some informal language, for preparation and observation procedures. Any $c \in C$ or $d \in D$ denotes a set of instructions for carrying out some preparation or observation procedure, respectively. It is to be noted that C and D contain all such sets of instructions, not just those which are applicable to physics.

Define the mappings $Q: N \to C \times D$, $s: N \to N$, and $\tau: N \to N$, where N is the set of natural numbers. Clearly, the triple $(Qs\tau)$ represents an infinite set of instructions for carrying out an infinite sequence of single measurements. For each j, the ordered pair $Q(j)$ denotes the preparation and observation instructions to be followed for the jth single measurement. $s(j)$ and $\tau(j)$ denote, respectively, the space position and calendar time (relative to some space and time measuring procedures) at which the jth single measurement is to be carried out. The fact that the orientation must also be given for each single measurement is ignored here. Also, each $d \in D$ is assumed to include instructions for the space–time positioning of the observation procedure *relative* to any preparation procedure in C.

By P1, the domains of Q, s, and τ must be N and not some initial segment of N. By P2, it takes forever to actually complete the carrying out of $(Qs\tau)$. Let $\psi_{Qs\tau}$ denote the infinite outcome sequence of natural numbers[33] obtained upon the carrying out of $(Qs\tau)$ and let $[Qs\tau]$ denote the class of all infinite sequences of instructions and space–time positions which an observer can carry out. Let $[Q]$ denote the set of all mappings from N to $C \times D$ and Ω, the set of all functions from N to N. Then $[Qs\tau]$ is a subclass of $[Q] \times \Omega \times \Omega$, as there are many sequences that cannot be carried out by any observer. For example, a necessary restriction is that τ be a nondecreasing function, as the $(n+1)$th single measurement obviously cannot be performed before the nth.

At this point, it may be helpful, especially to those not familiar with mathematical logic, to briefly discuss the definitions given so far. N, Ω, and R, the respective sets of natural numbers, infinite sequences of natural numbers, and real numbers and the many mathematical properties of these sets, are part of intuitive, or informal, mathematics. As such, they form a structure within which the otherwise meaningless symbol sequences of L and H are given meaning.

Each element of the class $[Qs\tau]$ is an ideal, informal element. It is ideal in that it cannot be carried out by an observer in any finite time [see the Appendix]. It is informal in that, for each j, $Q(j)$ is written in an informal language intuitively understandable to an observer and which is not part of L. Let Do denote a mapping with domain $[Qs\tau]$ and range in Ω. Then $Do(Qs\tau) = \psi_{Qs\tau}$ is the infinite sequence of natural numbers asymptotically obtainable by doing $Qs\tau$. Strictly speaking, $\psi_{Qs\tau}$ is an infinite sequence of symbols, each symbol of which is a name of a natural number. This distinction will be ignored here, as it is unimportant for this work.

It might be wondered why this work is not based instead on the class of all *finite* initial segments of the elements of $[Qs\tau]$ rather than on $[Qs\tau]$, since each finite segment can be completed by an observer by a finite time. One reason is that probability theoretic relations between a mean obtained by carrying out a finite initial segment of an element of $[Qs\tau]$ and an expectation value are given an exact, well-defined meaning in terms of infinite sequences *only* of single measurements (See the Appendix).

Let U denote a mapping with domain in $[Qs\tau]$ and

range in $[P]$ the class of probability measures defined on A. Here, a valid physical theory is defined to be some mapping U. Now, clearly, not all mappings U are valid physical theories. For example, $[Qs\tau]$ can include nonsense sequences or single measurements such as "Scratch your ear; if it hurts, output 1, if it does not, output 0," etc. Thus, if U is to represent a valid physical theory, it cannot be defined on all elements of $[Qs\tau]$. However, there are other restrictions on U which must be satisfied if U is to be a valid physical theory.

B. H-Agreement Between Theory and Experiment

One very important restriction on U is that it agree with experiment. Intuitively, this means that, for any infinite sequence $Qs\tau$ of physical measurements, there are many properties of the outcome sequence $\psi_{Qs\tau}$ which must be given by the theory. For example, if the theory states that the limit mean $\bar{M}\psi_{Qs\tau}$ exists (does not exist), then $\bar{M}\psi_{Qs\tau}$ should exist (not exist). If $\bar{M}\psi_{Qs\tau}$ exists, then the theory should give the value of $\bar{M}\psi_{Qs\tau}$. The theory should also give the value of $\bar{M}F_n\psi_{Qs\tau}$ [Eq. (4)] for each n. This is the limit relative frequency of occurrence of n in $\psi_{Qs\tau}$.

Besides these, there are many other properties of $\psi_{Qs\tau}$ which should be given by the theory. For example, let $\mathfrak{I}_g$ denote the subsequence selection procedure "select all and only the even numbered elements of $\psi_{Qs\tau}$ in the natural order" [$\mathfrak{I}_g\psi_{Qs\tau}$ is given by Eq. (2) with $g(\phi, j) = 2j$]. Then the theory should tell one whether $\bar{M}\mathfrak{I}_g\psi_{Qs\tau} = \bar{M}\psi_{Qs\tau}$ is true or not, and give the value of $\bar{M}\mathfrak{I}_g\psi_{Qs\tau}$, if it exists. Also, the theory should give the value of $\bar{M}(F_m\psi_{Qs\tau} \times F_n\mathfrak{I}^l\psi_{Qs\tau})$, if it exists. $\mathfrak{I}$ is the shift operator defined by Eq. 7. This expression gives the limit relative frequency of occurrence of n and then n, l places further on, in $\psi_{Qs\tau}$. Clearly, the value of this expression, or whether the statement

$$\bar{M}(F_m\psi_{Qs\tau} \times F_n\mathfrak{I}^l\psi_{Qs\tau}) = \bar{M}F_m\psi_{Qs\tau} \times \bar{M}F_n\mathfrak{I}^l\psi_{Qs\tau} \tag{11}$$

is true or not, is related to the question of whether or not $Qs\tau$ is a correlated sequence of single measurements.

Besides making predictions about properties of single sequences, a physical theory also compares different sequences of single measurements. For example, the theory may state that, for sufficiently well-isolated preparation and observation procedures, the space–time positions, at which sequences using these procedures are carried out, are irrelevant variables. (This is part of the statement of homogeneity of space–time.) This implies that, for some Q, the instruction sets $Qs\tau$ and $Qs'\tau'$ with $s'(j) = s(j) + m$ and $\tau'(j) = \tau(j) + n$ for all j and m, n independent of j and arbitrary, are "equivalent" experiments. This is empirically testable by carrying out $Qs\tau$ and $Qs'\tau'$ and seeing whether or not all empirically predictable properties of $\psi_{Qs\tau}$ are the same as those of $\psi_{Qs'\tau'}$.

From these examples, it is clear that, for each $Qs\tau$ for which $U(Qs\tau)$ is defined, there is a large class of statements which one requires to be true for $\psi_{Qs\tau}$ as part of the intuitive meaning of agreement between theory and experiment. Furthermore, the class depends on $Qs\tau$. For example, a physical theory may well give the prediction that the statement "$\bar{M}\mathfrak{I}_g\psi_{Qs\tau} = \bar{M}\psi_{Qs\tau}$" is true for some $Qs\tau$, false for others, and for still others it may not be predictable whether the statement is true or false. Thus, any acceptable definition of agreement between theory and experiment must define such a class for each physical $Qs\tau$ and contain the dependence of the class on $Qs\tau$.

To this end, we submit that much of the intuitive meaning of the agreement, with respect to H, of theory U with experiment is given by the statement $R_1(U, H)$ defined by

$$R_1(U, H) \equiv \forall(Qs\tau)\ [U(Qs\tau) \text{ defined} \Rightarrow E(H, U(Qs\tau), \psi_{Qs\tau})], \tag{12}$$

with $E(H, U(Qs\tau), \psi_{Qs\tau})$ given by Eq. (8). That is, if the theory U is to H-agree with experiment, then for any $Qs\tau$ for which $U(Qs\tau)$ is defined, the class of statements which must be true for $\psi_{Qs\tau}$ are those which are in H and are true almost everywhere with respect to $U(Qs\tau)$.

To see that this statement satisfies many intuitive aspects of the meaning of H-agreement between theory and experiment, some examples are considered. Let $q_{nl}(\theta)$ be the formula in H defined by $\theta(l) = n$. By the definition [Eq. (8)] of $E(H, P, \psi)$, Eq. (12) says that if U and $Qs\tau$ are such that

$$0 < U(Qs\tau)\ [\theta \mid \theta(l) = n] < 1$$

then one cannot predict from the theory U whether $\psi_{Qs\tau}(l) = n$ or not. However, if $U(Qs\tau)\ [\theta \mid \theta(l) = n] = 1(0)$, then Eq. (12) states that the theory predicts that $\psi_{Qs\tau}(l) = n$ is true (false).

This is in accord with intuition. For example, let U be a statistical theory of coin tossing. That is, U takes as input the properties of the coin and tossing procedures for each toss in a sequence and outputs the probabilities of various events. If U gives the probability of heads on the lth toss as a number between 0 and 1, one does not require the theory to give a prediction of the outcome of the lth toss. Such

a prediction is not part of the meaning of agreement between theory and experiment. However, if U and $Qs\tau$ are such that the probability of heads on the lth toss = 1(0) [e.g., a two-headed (two-tailed) coin with no edge effects was used for the lth toss], then the theory does predict heads (tails) for the lth toss. In this case, agreement of theory and experiment requires that heads (tails) occur on the lth toss.

Other examples which are in accord with intuition include any finite string of the formulas $q_{nl}(\theta)$ and $\neg q_{mk}(\theta)$ connected by $\vee$ or $\wedge$, as well as the formulas discussed previously. For example, for each $\mathfrak{F}_g$ which is definable in L_0, the formulas $q_{ng}(\theta)$ defined by $\bar{M}F_n\mathfrak{F}_g\theta = \bar{M}F_n\theta$ are in H. If $U(Qs\tau)$ is such that $q_{ng}(\theta)$ is true $U(Qs\tau)$ almost everywhere, then Eq. (12) requires, as a necessary condition of agreement between theory and experiment, that $\bar{M}F_n\mathfrak{F}_g\psi_{Qs\tau} = \bar{M}F_n\psi_{Qs\tau}$. However, if $0 < U(Qs\tau)\ [\theta \mid q_{ng}(\theta) \text{ true}] < 1$, then Eq. (12) says nothing about whether $q_{ng}(\psi_{Qs\tau})$ is true or not. In this case, one cannot predict from the theory U whether $q_{ng}(\psi_{Qs\tau})$ is true or not and this formula does not give a test, at $Qs\tau$, for agreement between experiment and theory U. Similar arguments hold for other formulas such as "$\bar{M}F_n\theta$ exists," Eq. (11), etc.

Furthermore, suppose that the theory predicts that $Qs\tau$ and $Qs'\tau'$, where s' and τ' are constant shifts of s and τ respectively, are "equivalent" experiments. For a theory U, this prediction is obtained by determining from computation that $U(Qs\tau) = U(Qs'\tau')$.

Now intuitively, the verification of this prediction of empirical equivalence means (1) that the class of statements about properties of the outcome sequences by which one tests for agreement between theory and experiment is the same for $\psi_{Qs\tau}$ as for $\psi_{Qs'\tau'}$ and (2) that each statement in this class is true (false) for $\psi_{Qs\tau}$ if and only if it is true [false] for $\psi_{Qs'\tau'}$. That is, by no statement in the class can one distinguish between $\psi_{Qs\tau}$ and $\psi_{Qs'\tau'}$.

These intuitive requirements are satisfied by Eq. (12). For clearly, if $U(Qs\tau) = U(Qs'\tau')$ on A_H, the class of formulas in H with one free function variable which are true (false) $U(Qs\tau)$ almost everywhere is the same as the class which are true (false) $U(Qs'\tau')$ almost everywhere. Furthermore, by Eq. (8) and Theorem 2, each relation in the class is true (false) for $\psi_{Qs\tau}$ if and only if it is true (false) for $\psi_{Qs'\tau'}$.

Perhaps the most important part of the meaning of comparison between theory and experiment is the comparison of the empirical limit means with the expectation values computed from theory. To this end, we consider the formulas $\bar{M}O\theta = r$. For any operation O defined in L_0 and any real number r, these formulas are in H. (This is the reason why H was defined by $H_0 \cup H'$ rather than by the simpler $H = H_0$.) If the theory U H-agrees with experiment, then Eq. (12) gives the result that, for each $Qs\tau$ for which $U(Qs\tau)$ is defined and for each O in L_0 and r, $U(Qs\tau)\ [\theta \mid \bar{M}O\theta = r] = 1$ requires that $\bar{M}O\psi_{Qs\tau} = r$. Also, for each O in L_0, there is at most one r such that Eq. (12) requires that $\bar{M}O\psi_{Qs\tau} = r$ hold. (*Proof:* Assume the converse, i.e., that for some measure P, $P\ [\theta \mid \bar{M}\theta = r] = 1$ and $P\ [\theta \mid \bar{M}\theta = r'] = 1$ with $r \neq r'$. Since the intersection of two sets of measure one is a set of measure one, there is some ϕ such that $\bar{M}\phi = r$ and $\bar{M}\phi = r'$, which is impossible.)

Although there is, at most, one r for which $U(Qs\tau)\ [\theta \mid \bar{M}O\theta = r] = 1$, Eq. (12) does not tell one how to find such an r or relate it to an expectation value computed from theory. To this end, probability theory is of value as it gives a relation between r and $U(Qs\tau)$. To obtain the relation, one first considers $\bar{M}F_mO\phi$, where

$$\bar{M}O\phi = \sum_m m\bar{M}F_mO\phi \tag{13}$$

and F_m is given by Eq. (4). Let X_F denote the characteristic function for any set F in A_H. That is,

$$\begin{aligned} X_F(\phi) &= 1, \quad \text{if} \quad \phi \in F, \\ &= 0, \quad \text{if} \quad \phi \notin F. \end{aligned} \tag{14}$$

Now set $F = O'E_{mj}$ where O' is the set transformation [Eq. (3)] generated by O and $E_{mj} = [\theta \mid \theta(j) = m]$. One has the result that $(F_mO\phi)(j) = 1(0)$ if and only if $X_{O'E_{mj}}(\phi) = 1(0)$. Thus, by the definition of the limit mean, one has

$$\bar{M}F_mO\phi = \lim_{i\to\infty} \frac{1}{i} \sum_{j=0}^{i-1} X_{O'E_{mj}}(\phi) = \bar{X}_{O'E_{m0}}(\phi). \tag{15}$$

The expectation value of the limit random variable $\bar{X}_{O'E_{m0}}$ for a measure P is given by[34,35]

$$\langle \bar{X}_{O'E_{m0}} \rangle = \lim_{i\to\infty} \frac{1}{i} \sum_{j=0}^{i-1} PO'T^jE_{m0}, \tag{16}$$

where the relation $T^jE_{m0} = E_{mj}$ with T, the one-sided shift operator [Eqs. (3) and (7)], has been used. Furthermore, if a random variable X is constant almost everywhere, then

$$X = \langle X \rangle \tag{17}$$

holds almost everywhere.[34,35]

Thus, the following result is obtained. Suppose that a theory U H-agrees with experiment. Then $R_1(U, H)$ [given by Eq. (12)] holds, and for any O in L_0 and $r \in R$ such that $U(Qs\tau)\ [\phi \mid \bar{M}O\phi = r] = 1$, one has that $\bar{M}O\psi_{Qs\tau} = r$. By Eqs. (13)–(17), one has that

$$\bar{M}O\psi_{Qs\tau} = \sum_m m \lim_{i\to\infty} \frac{1}{i} \sum_{j=0}^{i-1} U(Qs\tau)O'T^jE_{m0} \tag{18}$$

as the final relation between the limit mean of the sequence obtained by the operation O on the outcome sequence $\psi_{Qs\tau}$ and the theoretical expectation value computed from U, $Qs\tau$, and O. Clearly, the right-hand side of Eq. (18) is equal to r. The complexity of the right-hand side of Eq. (18) is treated in the next section.

It should be noted that Eqs. (13)–(18) hold for all operations in L_0, including those by means of which correlations among single measurements are determined. For example, let O denote the operation of Eq. (11) where $O\phi = F_l\phi \times F_k\mathfrak{F}^n\phi$. In this case, O maps every sequence of ϕ onto a 0–1 sequence. Then the only nonzero term of Eq. (13) is for $m = 1$. Equation (18) becomes

$$\bar{M}(F_l\psi_{Qs\tau} \times F_k\mathfrak{F}^n\psi_{Qs\tau}) = \lim_{i\to\infty} \frac{1}{i} \sum_{j=0}^{i-1} U(Qs\tau)T^j(E_{l0} \cap E_{kn}),$$

where the facts that O commutes with $\mathfrak{F}$ and thus O' commutes with T and $0'E_{10} = E_{l0} \cap E_{kn}$ with $E_{nl} = [\theta \mid \theta(l) = n]$ have been used.

From this discussion, one sees that the validity of $R_1(U, H)$ is a necessary but not sufficient condition for the theory U to agree with experiment with respect to H. The reason that $R_1(U, H)$ is not sufficient is that Eqs. (14)–(18) are also necessary conditions and they have not been included in H. Whether or not one can find an H which includes these statements, so that H-agreement between theory and experiment can be defined by Eqs. (12) and (8) only, is a question left to future work.

For a slightly different perspective on Eq. (12), suppose an observer is considering a physical theory which is new to him. After some study, he finds that the theory suggests entirely new experiments which he has never done and predicts their outcomes. On carrying them out, he finds that the results do indeed agree with the new prediction and thus, the empirical support for the theory is broadened.

This characteristic of a theory giving new testable predictions is included in the description given here. In terms of Eq. (12), it means that for a new theory U, one must discover the domain of definition of U. At first, one knows that a certain class of empirical procedures is in the domain of U. By a study of the theory, he finds that another $Qs\tau$ not previously carried out is in the domain of definition of U. The predictions U makes about the new experiment are given by all statements in H which are true almost everywhere with respect to $U(Qs\tau)$. By Eq. (12), if U is to H-agree with experiment at $Qs\tau$, all these predictions must be true for $\psi_{Qs\tau}$.

With respect to randomness, one has the following easy theorem.

Theorem 4: Let U be any map with domain in $[Qs\tau]$ and range in $[P]$ such that U agrees with experiment with respect to H. Then, for each $Qs\tau$ for which $U(Qs\tau)$ is defined and is a nontrivial product measure on A, $\psi_{Qs\tau}$ is H-random.

Proof: Since $R_1(U, H)$ is a necessary condition for H-agreement of U with experiment, one has by hypothesis that $R_1(U, H)$ holds. This means that $E(H, U(Qs\tau), \psi_{Qs\tau})$ is true for every $Qs\tau$ for which $U(Qs\tau)$ is defined. This includes any $Qs\tau$ for which $U(Qs\tau)$ is a nontrivial product measure. Thus, any such $U(Qs\tau)$ satisfies the conditions of Eq. (10) and $\psi_{Qs\tau}$ is H-random. QED

It is clear from this theorem that the problem of the relation between quantum mechanics and randomness, mentioned in the introduction, is solved for a physical theory as defined here. All one has to know for any $Qs\tau$ is whether or not $U(Qs\tau)$ is a nontrivial product measure. If it is such a measure, and if U H-agrees with experiment, then $\psi_{Qs\tau}$ is H-random.

In order to apply the foregoing directly to quantum mechanics and prove the statement given in the introduction, one would have to show that quantum mechanics is a physical theory of the type discussed here. That is, one would have to show that (1) each $Qs\tau$ which is a sequence of measurements in quantum mechanics defines a probability measure on A, and (2) in particular, if $Qs\tau$ corresponds to measuring a question valued observable O on a pure state η, then the associated probability measure is a product measure. Suppose this could be shown *and* one could demonstrate that quantum mechanics H-agrees with experiment as defined by Eqs. (8) and (12); then the above theorem allows one to prove that, if $Qs\tau$ corresponds to the measurement of a question O on a pure state η with η not lying entirely within an eigenspace of O, then the outcome sequence $\psi_{Qs\tau}$ is H-random.

The main difficulty seems to be in showing that quantum mechanics is a physical theory of the type discussed here, for, as was noted earlier, quantum mechanics seems to say nothing about the statistical relations between single measurements in a sequence. Yet, clearly, such information is given by any theory U and is also intuitively assumed whenever one actually carries out physical measurements.

C. Existence

From the previous discussion, $R_1(U, H)$ is clearly a necessary condition for U to be a valid physical theory. However, there are other conditions. Of great importance is the requirement that there exist a U whose domain is not empty. In fact, the domain of U must be large in some sense if U is to be a comprehensive physical theory.

At present, not much can be said about this requirement except to emphasize that it is nontrivial. For, by Eq. (12), it has the consequence that $E(H, U(Qs\tau), \psi_{Qs\tau})$ holds for each $(Qs\tau)$ for which $U(Qs\tau)$ is defined. If $U(Qs\tau)$ is nontrivial [Eq. (9)] this places the restrictions of Theorems 1 and 3 on H. As was noted before, these restrictions first arose in the existence problem for random sequences.[21,22,29,30] Thus, H cannot be too large if a U which H-agrees with experiment is to exist. On the other hand, H cannot be too small if $R_1(U, H)$ with Eqs. (14)–(18) are to be a reasonable statement of H-agreement between theory and experiment.

D. Empirical Determinability of $U(Qs\tau)$

Another property which, intuitively, a valid physical theory should have, is that, for some sequences of single measurements, the probabilities of single measurement events should be determinable from the sequences of outcomes. For example, if the probability of heads occurring in the fifth flip of a sequence of coin flips is determined to be $\frac{1}{2}$, one feels that, at least for some sequences, this number should be determinable from the infinite sequence of outcomes. For the class of theories considered here, this is equivalent to the requirement that, if U H-agrees with experiment, then, at least for some $Qs\tau$, $U(Qs\tau)F$ should be determinable from $\psi_{Qs\tau}$ for many F in A_H. This requirement is related[34] to the problem in quantum mechanics of whether or not a state represents a single system or an infinite ensemble of systems.[36]

Now it is clear from Eq. (18) that this requirement is not satisfied in general. If O' commutes with T, Eq. (18) simplifies to

$$\bar{M}O\psi_{Qs\tau} = \sum_m m\overline{U(Qs\tau)}O'E_{m0},$$

where $\overline{U(Qs\tau)}$ is the limit ensemble probability measure defined for each F in A_H by

$$\overline{U(Qs\tau)}F = \lim_{i\to\infty}\frac{1}{i}\sum_{j=0}^{i-1}U(Qs\tau)T^jF.$$

However, even in this case, one determines $\overline{U(Qs\tau)}$ from experiment and not $U(Qs\tau)$, the measure associated with individual events.[34]

In order to formulate this requirement and give sufficient conditions for it to be satisfied, some definitions are needed. For each F in A_H, let $\mathfrak{d}_F: \Omega \to \Omega_{0,1}$ be defined by

$$(\mathfrak{d}_F\phi)(j) = X_{T^jF}(\phi) = X_F(\mathfrak{d}^j\phi) \tag{19}$$

for each ϕ and j. X_{T^jF} is the characteristic function for T^jF [Eq. (14)] and T is the shift operator given by Eqs. (3) and (7). $\mathfrak{d}_F$ maps ϕ onto a 0–1 sequence such that $(\mathfrak{d}_F\phi)(j) = 1(0)$ if $\mathfrak{d}^j\phi \in F$ $(\mathfrak{d}^j\phi \notin F)$.

Let T_F denote the set transformation [Eq. (3)] generated by $\mathfrak{d}_F$. Then, repeating the development of Eqs. (14)–(16) with T_F replacing $0'$ and noting that

$$\begin{aligned} T_FE_{mj} &= \Phi, && \text{if } m > 1,\\ &= T^jF, && \text{if } m = 1,\\ &= \Omega - T^jF, && \text{if } m = 0, \end{aligned} \tag{20}$$

where Φ is the empty set, one obtains for any $F \in A_H$ with $m = 1$ and $T_FE_{10} = F$

$$\langle \bar{X}_F\rangle = \lim_{i\to\infty}\frac{1}{i}\sum_{j=0}^{i-1}PT^jF = \bar{P}F, \tag{21}$$

if the limit exists. [By Eq. (15) and the above, $\bar{M}\mathfrak{d}_F\phi = \bar{X}_F(\phi)$.]

The requirement that $U(Qs\tau)$ be determinable on A_H from $\psi_{Qs\tau}$, $R_2(H, U(Qs\tau), \psi_{Qs\tau})$, is defined by

$$\begin{aligned} &R_2(H, U(Qs\tau), \psi_{Qs\tau})\\ &\quad\equiv \forall F\,[F \in A_H \wedge \mathfrak{d}_F \text{ is in } L_0 \Rightarrow \bar{M}\mathfrak{d}_F\psi_{Qs\tau} \text{ exists}\\ &\qquad\qquad \wedge\, \bar{M}\mathfrak{d}_F\psi_{Qs\tau} = U(Qs\tau)F]. \end{aligned} \tag{22}$$

That is, for each F in A_H such that $\mathfrak{d}_F$ is an operation in L_0, the limit relative frequency that $\psi_{Qs\tau}, \mathfrak{d}\psi_{Qs\tau}\cdots$ are found in F, exists and equals the probability of F, as given by the theory U.

Theorem 5 gives sufficient conditions for

$$R_2(H, U(Qs\tau), \psi_{Qs\tau})$$

to hold.

Theorem 5: Let H be such that, for any real number r, and for each F in A_H for which $\mathfrak{d}_F$ is an operation in L_0, the formula $\bar{M}\mathfrak{d}_F\phi = r$ is in H. Let U be a theory which agrees with experiment with respect to H.

Then, for each $Qs\tau$ for which $U(Qs\tau)$ is defined and nontrivial, sufficient conditions for $U(Qs\tau)$ to be determinable from $\psi_{Qs\tau}$ are (1) that the shift operator T [Eqs. (3) and (7)] be $U(Qs\tau)$ measure preserving and (2) that T be an ergodic transformation.

The first condition means that, for all $F \in A_H$, $U(Qs\tau)TF = U(Qs\tau)F$ and the ergodicity of T means that, for each F in A_H for which $\mathfrak{d}_F$ is in L_0, the limit $\overline{U(Qs\tau)}F$ [Eq. (21)] exists, and $\bar{M}\mathfrak{d}_F\phi$ exists and is a constant $U(Qs\tau)$ almost everywhere.[34,35]

Proof: By the ergodic conditions, one has that, for each F in A_H for which $\mathfrak{I}_F$ is an operation in L_0, Eqs. (17) and (21) hold, and thus,[34,35]

$$\bar{M}\mathfrak{I}_F\phi = \overline{U(Qs\tau)}F$$

$U(Qs\tau)$ almost everywhere. Since T is measure preserving, $\overline{U(Qs\tau)}F = U(Qs\tau)F$ [Eq. (21)] and, thus,

$$\bar{M}\mathfrak{I}_F\phi = U(Qs\tau)F \tag{23}$$

almost everywhere.

Let $Qs\tau$ be such that $U(Qs\tau)$ is defined and nontrivial. Then, since $U(Qs\tau)$ H-agrees with experiment, $R_1(U, H)$ holds and, by Eq. (12), $E(H, U(Qs\tau), \psi_{Qs\tau})$ holds. Thus, by Eq. (8), $\bar{M}\mathfrak{I}_F\psi_{Qs\tau}$ exists as $\bar{M}\mathfrak{I}_F\phi$ exists $U(Qs\tau)$ almost everywhere. For any F in A_H for which $\mathfrak{I}_F$ is in L_0, let r be the real number such that $U(Qs\tau)F = r$. By hypothesis and Eq. (23), $\bar{M}\mathfrak{I}_F\phi = r$ is in H and is true almost everywhere and, from Eq. (8), one has that $\bar{M}\mathfrak{I}_F\psi_{Qs\tau} = U(QFs\tau)$.

QED

As a consequence of the theorem, one has the following corollary.

Corollary 1: Let H and U satisfy the conditions of Theorem 5. Then, for each $Qs\tau$ for which $U(Qs\tau)$ is defined, a sufficient condition for $U(Qs\tau)$ to be determinable from $\psi_{Qs\tau}$ is that $U(Qs\tau)$ be a product measure on A_H.

Proof: Clearly, H contains all finite intersections, complements, and unions of the sets $E_{ml} = [\phi \mid \phi(l) = m]$ for m, $l = 0, 1 \cdots$ (beginning of Sec. III). Since $U(Qs\tau)$ is a product measure on these sets, it can be extended uniquely[37] to a product measure defined on A. Since, for any such measure, T is measure preserving and ergodic on A[34,35] and $A_H \subseteq A$, T is measure preserving and ergodic with respect to $U(Qs\tau)$ on A_H. By Theorem 5, $U(Qs\tau)$ is determinable from $\psi_{Qs\tau}$. QED

This corollary corresponds with intuition since one feels that, for any infinite sequence of independent, identically distributed single measurements, the probabilities of various individual events should be determinable from the outcome sequence. Thus consider, for example, an infinite sequence of spin projection measurements on protons where each single measurement consists of a preparation of a proton in some state and observation of the spin projection of the proton along some axis. If each single measurement is independent of the other single measurement then, for example, one feels that the probability of observing spin up on the nth measurement should be determinable from the infinite outcome sequence. This is just what the corollary states.

The next (and final) theorem shows that a potential difficulty for H and $E(H, P, \phi)$ raised by the operations $\mathfrak{I}_F$ does not arise. To illustrate the problem, one notes that, if $\mathfrak{I}_F$ is an operation in L_0, the set $F_r = [\phi \mid \bar{M}\mathfrak{I}_F\phi = r]$ is H-definable. If $\mathfrak{I}_{F_r}$ is an operation in L_0, then the set $F_{r,s} = [\phi \mid \bar{M}\mathfrak{I}_{F_r}\phi = s]$ is H-definable. If $\mathfrak{I}_{F_{r,s}}$ is in L_0, then . . . , etc. If the appropriate operation is in L_0 at each stage of this iterative process, then potentially this inductive process generates many new formulas in H which could conceivably cause $E(H, P, \phi)$ to be false for all ϕ.

That this cannot happen is shown by Theorem 6. This theorem says, in effect, that the only new sets added to A_H by the process are the F_r and their complements. (Of course, any union and intersection which is H-definable is also included.) It should be noted that, for the particular H defined here, none of the $\mathfrak{I}_{F_r}$, $\mathfrak{I}_{F_{r,s}}, \cdots$, are defined in L_0. However, this theorem shows that, for any more general H for which the sets $F_r, F_{r,s}, \cdots$, are H-definable, one does not add any new sets to A_H by this process.

Lemma 1: For any F in A_H and any j, $\mathfrak{I}_F\mathfrak{I}^j = \mathfrak{I}^j\mathfrak{I}_F$ where $\mathfrak{I}$ is given by Eq. (7).

Proof: It is sufficient to prove $\mathfrak{I}_F\mathfrak{I} = \mathfrak{I}\mathfrak{I}_F$. By Eqs. (7) and (19), for each ϕ and i,

$$(\mathfrak{I}\mathfrak{I}_F\phi)(i) = \mathfrak{I}_F\phi(i+1) = X_{T^{i+1}F}(\phi)$$
$$= X_{T^iF}(\mathfrak{I}\phi) = (\mathfrak{I}_F\mathfrak{I}\phi)(i). \quad \text{QED}$$

Theorem 6: Let r and s be any pair of real numbers in $[0, 1]$. Let $F_r = [\phi \mid \bar{M}\mathfrak{I}_F\phi = r]$ and

$$F_{r,s} = [\phi \mid \bar{M}\mathfrak{I}_{F_r}\phi = s].$$

Then

(1) $F_r = F_{r,1}$,

(2) $\Omega - F_r = F_{r,0}$,

(3) if $0 < s < 1$, $F_{r,s} = \Phi$.

Proof: (1.A) $F_r \subseteq F_{r,1}$.

Let ϕ be such that $\bar{M}\mathfrak{I}_F\phi = r$. By Eqs. (14) and (19),

$$(\mathfrak{I}_{F_r}\phi)(j) = 1, \quad \text{if} \quad \mathfrak{I}^j\phi \in F_r$$
$$= 0, \quad \text{if} \quad \mathfrak{I}^j\phi \notin F_r. \tag{24}$$

Since $\phi \in F_r$ and $\bar{M}\mathfrak{I}^l\phi = \bar{M}\phi$ for any l (this follows immediately from the fact that $\mathfrak{I}^l$ discards the first l terms of ϕ only and does not affect the limit mean),

one has (by Lemma 1), for each j,

$$r = \bar{M}\mathfrak{I}_F\phi = \bar{M}\mathfrak{I}^j\mathfrak{I}_F\phi = \bar{M}\mathfrak{I}_F\mathfrak{I}^j\phi \quad \text{or} \quad \mathfrak{I}^j\phi \in F_r.$$

Thus, $(\mathfrak{I}_{F_r}\phi)(j) = 1$ for each j and $\bar{M}\mathfrak{I}_{F_r}\phi = 1$ and $\phi \in F_{r,1}$.

(1.B) $F_{r,1} \subseteq F_r$.

If $\phi \in F_{r,1}$, there is some k such that $\mathfrak{I}^k\phi \in F_r$. By the definition of F_r, this means that $\bar{M}\mathfrak{I}_F\mathfrak{I}^k\phi = r$. By Lemma 1 and the fact that $\bar{M}\mathfrak{I}^l\phi = \bar{M}\phi$ for any l, one has that $\bar{M}\mathfrak{I}^l\mathfrak{I}_F\phi = r$ for any l. In particular, for $l = 0$ $\bar{M}\mathfrak{I}_F\phi = r$ and thus, $\phi \in F_r$.

(2.A) $\Omega - F_r \subseteq F_{r,0}$.

Let ϕ be such that $\bar{M}\mathfrak{I}_F\phi \neq r$. By the same use of Lemma 1 and the invariance of the limit mean under $\mathfrak{I}^j$ (this includes the case where $\bar{M}\mathfrak{I}_F\phi$ does not exist) as in case (1.A), one has that $\bar{M}\mathfrak{I}_F\mathfrak{I}^j\phi \neq r$ for each j. By Eq. (24), $(\mathfrak{I}F_r\phi)(j) = 0$ for each j, and thus, $\bar{M}\mathfrak{I}_{F_r}\phi = 0$ and $\phi \in F_{r,0}$.

(2.B) $F_{r,0} \subseteq \Omega - F_r$.

If $\phi \in F_{r,0}$, then $\mathfrak{I}^k\phi \notin F_r$ for some k. By Lemma 1 and the invariance of $\bar{M}$ under $\mathfrak{I}^j$ as in case (1.B), $\bar{M}\mathfrak{I}_F\phi \neq r$ and $\phi \in \Omega - F_r$.

(3) By the arguments of cases (1.B) and (2.B), $\mathfrak{I}_{F_r}\phi$ is either a constant sequence of 0's or a constant sequence of 1's for all ϕ. Let $F_{r,s}$ be nonempty for $0 < s < 1$. Then there is some $\theta \in F_{r,s}$, which means that $\bar{M}\mathfrak{I}_{F_r}\theta = s$. Since $0 < s < 1$, this means that $\mathfrak{I}_{F_r}\theta$ is not a constant sequence, which is a contradiction. Thus, $F_{r,s}$ is empty for $0 < s < 1$. QED

V. CONCLUSION

Although some steps have been taken here towards defining necessary conditions for a mapping U to be a valid physical theory, much work remains to be done. The open questions include: Can H be extended to include Eqs. (14)–(18) or their equivalents so Eqs. (8) and (12) are a complete statement of the meaning of H agreement between theory and experiment? How does one ensure that the existence condition on U is satisfied? Clearly, Theorems 1 and 3 are relevant here. What are sufficient conditions for U to be a physical theory and not a biological theory? What is the relation between this work and quantum mechanics?, etc. We hope to answer some of these questions in future work.

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APPENDIX

Two basic properties of the measurement process which are of relevance here are

(P1) A very large part of the total contact between theory and experiment is made by means of infinite sequences of single measurements only.

(P2) By any finite time, an observer can know the results of an arbitrary but, at most, finite number of single measurements.

By contact between theory and experiment is meant the actual having in hand, by an observer, the empirical numbers which are to be directly compared, in terms of mathematical equality or nonequality, with numbers computed from theory. It is to be noted that an immediate conclusion from P1 and P2 is that, by any finite time, an observer cannot make contact, in the precise sense defined, between theory and experiment. The fact that observers can and do make approximate contact between theory and experiment in a finite time is discussed later.

To see the relation of P1 to quantum mechanics, one first notes that the only empirical numbers which can be directly compared with an expectation value is a limit mean. If ψ represents the outcome sequence associated with an infinite sequence of single measurements and $M_n\psi$ represents the mean of the first n single measurements, then one has the relation

$$\lim_{n\to\infty} M_n\psi = \bar{M}\psi = \langle\ \rangle.$$

The right-hand equality holds only if ψ corresponds to measuring the expectation value $\langle\ \rangle$ in question.

In quantum mechanics, a very large part of the theory makes contact with experiment only through measurement of expectation values. This includes many statements about the physical properties of systems, expressed in terms of observables measured on states. Also, many mathematical properties can be defined in terms of corresponding properties of expectation values.[19,38] For example, equality between two states or two observables is defined in terms of equality within many pairs of expectation values. Also, any statement to the effect that a system is prepared in an eigenstate of an observable is included. For the meaning of this is that, with probability one, the system will be found in an eigenstate of the observable. This corresponds to the empirical statement that, in an appropriate infinite sequence of single measurements, the limit relative frequency for the occurrence of one and only one outcome is equal to 1. Whether or not this case can be given the stricter interpretation that the associated infinite sequence of

outcomes is a constant sequence is, at present, an open question.

In classical mechanics, the situation is quite different. There, if a system is prepared in a pure state one can, in principle, make one or more single measurements on the system and compare the results of each single measurement directly with the values computed from theory. Only for mixed states must one discuss their properties in terms of expectation values. This is in contrast to quantum mechanics, where one must discuss the physical properties of all states, pure or mixed, in terms of expectation values.

P2 is perhaps more immediate than P1, in that it is a basic fact of epistemology and of any observer's experience that he can know by any finite time an arbitrary but, at most, finite number of empirical facts. To see that P2 is required by quantum mechanics and an upper limit to signal velocities,[39] one first notes that, in quantum mechanics, any pair of single measurements must be separated by a finite space or finite time interval. (Again, each single measurement is to be carried out on a separate system.) To see this, one first notes that any state is described by a wavepacket which has a finite space extension. Thus any pair of single measurements carried out at the same time must be separated by a finite space interval. If one attempts to reduce this interval arbitrarily, the wavepackets will strongly overlap, giving a large interference between the single measurements. Similar arguments can be made against arbitrarily reducing the size of the measurement apparatus.[40]

If one now adds the finite signal velocity of relativity,[6] it is clear that it requires a finite time interval to complete any single measurement. The reason is that, as noted above, the wavepacket or measurement apparatus must be of finite size. It then takes a finite time for the packet to enter the apparatus or for a signal to cross the apparatus. Thus, any pair of single measurements which occur at the same space position must be separated by a finite time interval. The reason is that a necessary condition for noninterference is that one single measurement be completed before the next one is begun.

From the above, one concludes that for any space time arrangement of an infinite sequence of single measurements, an infinite time interval is needed for an observer to receive or know the infinite outcome sequence. If all the single measurements in a sequence occur at the same space position, then the above arguments give the immediate conclusion that an infinite time interval is necessary.

If each measurement in a sequence occurs at the same time but at different space positions, then the time interval for receipt of the outcome sequence is also infinite. This holds, even if one arranges an infinite set of single measurements so that those occurring in distant space regions occur earlier with respect to their local times than the close ones. For just to set up such an arrangement, including synchronization of the clocks involved, requires sending light signals over arbitrarily great distances.[41]

In classical mechanics, on the other hand, for any single particle state, one can, in principle, carry out one or more measurements on the particle at a point in space–time. Thus, even if such a state is a mixed state, the infinite sequences of one or more single measurements necessary for its determination can be carried out in an arbitrarily small space–time volume. This conclusion is independent of whether or not there is an upper limit to signal velocities.

An immediate consequence of P1 and P2 is that, by any finite time, an observer cannot obtain empirically the value of even one expectation value. As noted, an infinite sequence of single measurements must be performed to measure an expectation value as a limit mean and it requires an infinite time interval to carry out such a sequence. This is the reason why an observer cannot make contact, by an finite time, between theory and experiment in the precise sense defined.

It must be emphasized that this conclusion does not deny that one can make approximate contact between theory and experiment in a finite time in terms of means $M_n\psi$ of n single measurements. However, any comparison between an empirical mean $M_n\psi$ for n finite and an expectation value computed in a theory can only be made by some statistical statement. Now, all such probability theoretic statements are asymptotic. They state, in terms of real numbers, what will be found as limit relative frequencies, if either the sequences of n single measurements, considered as a single measurement, were repeated an infinite number of times, or if the sequence were extended to the limit of infinite n. Thus, it is clear that the use of probability theory or statistics to relate $M_n\psi$ to an expectation value does not remove the infinite sequences of P1. For the purposes of this work, then, we can dispense with such statistical comparisons and consider direct comparisons only between limit means and expectation values.

In essence, P2 states the constructive nature of the epistemological process. Since each step of a mathematical computation procedure is a process largely subject to the laws of physics, P2 (or quantum mechanics and the finite signal velocity of relativity) has the consequence that an infinite number of

computation or measurement steps cannot be completed in a finite time interval.

It is also well known that no single measurement completed in a finite time interval ever gives, as an outcome, a real number. One reason is that the recording and reading of a real number will, in general, take an infinite number of steps and thus require an infinite amount of time. This fact can be stated as a third basic property of the epistemological process, namely:

P3. The basic operation which generates numbers from basic sense data is that of counting.

An immediate consequence of P3 is that, since all arithmetic operations are effective, one can generate rational numbers immediately from sense data. However, the above arguments show that the outcomes of single measurements can be associated effectively with rational numbers, at most, and not real numbers.[9]

It is to be emphasized that this does not mean that the mathematics of physics must give up real numbers; for, by P1, a very large part of the contact between theory and experiment is through measurement of limit means. Now, one way of defining real numbers is by convergent Cauchy sequences of rational numbers. Each infinite sequence of single measurements generates, through the outcome sequence ψ, a sequence of means $M_n\psi$, $n = 0, 1, \cdots$, which, for the cases of interest, is a convergent Cauchy sequence. Thus, the operation of constructing the limit mean as an infinite sequence of effective arithmetic operations automatically introduces the needed real numbers. (Under P2, these are available only in the infinite future.)

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[1] E. P. Wigner, Am. J. Phys. **31**, 6 (1963).
[2] G.-C. Wick, A. S. Wightman, and E. P. Wigner, Phys. Rev. **88**, 101 (1952).
[3] M. M. Yanase, Am. J. Phys. **32**, 208 (1964).
[4] H. Margenau, Ann. Phys. (N.Y.) **23**, 469 (1963).
[5] M. Goldberger and K. Watson, Phys. Rev. **134** B919 (1964).
[6] W. C. Davidon and H. Ekstein, J. Math. Phys. **5**, 1588 (1964).
[7] H. Margenau, Phys. Rev. **49**, 240 (1936).
[8] J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, translated by R. T. Beyer (Princeton U.P., Princeton, N.J., 1955), p. 335.
[9] M. Born, Kgl. Danske Videnskab. Selskab. Mat-Fys. Medd. **30**, No. 2 (1955).
[10] E. P. Wigner, in *The Scientist Speculates*, I. Good, Ed. (W. Heinemann, London, 1962).
[11] A. Shimony, Am. J. Phys. **31**, 755 (1963); B. D'Espagnat, in *Logic, Methodology and Philosophy of Science III, Amsterdam 1967*, B. Van Rootselaar and J. F. Stool, Eds. (North-Holland, Amsterdam, 1968), pp. 377–84; P. A. Moldauer, Am. J. Phys. **32**, 172 (1964).
[12] M. N. Hack, Nuovo Cimento **54B**, 147 (1968).
[13] M. H. Stone, in *Symposia on Theoretical Physics, Vol. 4, Madras, India, 1965*, A. Ranakrishnan, Ed. (Plenum, New York, 1967).
[14] D. Finkelstein, I.C.T.P., Trieste, Report No. IC/68/35, 1968; Phys. Rev. **184**, 1261 (1969).
[15] M. Bunge, Rev. Mod, Phys. **39**, 463 (1967).
[16] J. Yates, Intern. J. Theoret. Phys. **1**, 171, 179 (1968).
[17] W. Yourgau, J. Symbolic Logic **32**, 572 (1967); S. A. Basri, *A Deductive Theory of Space and Time* (North-Holland, Amsterdam, Holland, 1966); E. W. Bastin and C. W. Kilmister, Proc. Cambridge Phil. Soc. **50**, 278 (1954); **51**, 454 (1955).
[18] C. H. Randall, Ph.D. Thesis, Rensselaer Polytechnic Institute, KAPL 3147, 1966; C. H. Randall and D. J. Foulis, "The Basic Concepts of Empirical Logic" (unpublished).
[19] H. Ekstein, Phys. Rev. **153**, 1397 (1967); **184**, 1315 (1969).
[20] R. von Mises, *Mathematical Theory of Probability and Statistics*, H. Geiringer, Ed. (Academic Press, New York, 1964), Chap. I.
[21] A. Wald, Ergeb. Math. Kolloquiums **8**, 38 (1937) [Reprinted in *Selected Papers in Statistics and Probability* (McGraw-Hill, New York, 1955), pp. 25–45].
[22] A. Church, Bull. Am. Math. Soc. **46**, 130 (1940).
[23] H. Rogers, Jr., *Theory of Recursive Functions and Effective Computability* (McGraw-Hill, New York, 1967).
[24] M. Davis, *Computability and Unsolvability* (McGraw-Hill, New York, 1958).
[25] J. Doob, Ann. Math. **37**, 363 (1936).
[26] D. W. Loveland, Trans. Am. Math. Soc. **125**, 497 (1966); Z. Math. Logik Grundlagen Math. **12**, 279 (1966).
[27] P. Benioff, unpublished work.
[28] J. Ville, *Etude critique de la notion de collectif* (Gauthier-Villars, Paris 1939).
[29] P. Martin Löf, Proceedings of Symposium on Proof Theory and Intuitionism, Summer Institute, State University at Buffalo, New York, 1968 (unpublished).
[30] A. H. Kruse, Z. Math. Logik Grundlagen Math. **13**, 299 (1967).
[31] P. Martin Löf, Inform. Control **9**, 602 (1966).
[32] J. Shoenfield, *Mathematical Logic* (Addison-Wesley, Reading, Mass., 1967).
[33] We here assume that $\psi_{Qs\tau}$, τ, and s take values in N rather than in the set of rational numbers. As is noted in the Appendix, this is an inessential restriction. However, by P3, they cannot have real numbers as values.
[34] P. Benioff, J. Math. Phys. **9**, 514 (1968).
[35] M. Loeve, *Probability Theory* (Von Nostrand, Princeton, N.J., 1963), 3rd ed., Chap. IX.
[36] G. Ludwig, "Solved and Unsolved Problems of the Measurement Process," translated by E. Wilip from *Werner Heisenberg and Contemporary Physics*, F. Bopp, Ed. (Vieweg, Braunschweig, Germany, 1961), pp. 150–181; D. Bohm and J. Bubb, Rev. Mod. Phys. **38**, 453 (1966); J. L. Park, Am. J. Phys. **36**, 211 (1968).
[37] P. Halmos, *Measure Theory* (Von Nostrand, Princeton, N.J., 1950), p. 157.
[38] See, for example, G. W. Mackey, *The Mathematical Foundations of Quantum Mechanics* (Benjamin, New York, 1963).
[39] P. Benioff, Z. Naturforsch. **24a**, 86 (1969).
[40] E. P. Wigner, Z. Physik **133**, 101 (1952); H. Araki and M. M. Yanase, Phys. Rev. **120**, 622 (1960); M. M. Yanase, Phys. Rev. **123**, 666 (1961).
[41] We thus come to the opposite conclusion from that reached by A. Grunbaum, Science **159**, 396 (1968).

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Electromagnetic Wave Propagation through Slowly Varying Plasma

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We solve the second-order linear inhomogeneous wave equation by the WKB method. Then a sequence of successive substitutions are developed, by the help of which solutions correct up to any higher order are reduced to the WKB solution of an equation like the original equation. This procedure is adopted to study propagation of electromagnetic wave obliquely through slowly but continuously varying plasma layers. Across a plane where N (the equilibrium plasma concentration) is continuous, but its first- and second-order space rate of variation along the normal are discontinuous, we have solved the boundary value problems for wave propagation. The characteristics of the reflected and transmitted fields depend on these derivatives of N such that the reflected wave vanishes in the limit of constancy of N. We find that the direction of flow of electromagnetic energy is deviated from its straight course in the uniform region. Expressions for relative shift of the wave vector along and perpendicular to the direction in the uniform medium, with respect to the distance of wave advancement in that medium in a given time, have been deduced. The deviation of the direction of propagation is slightly more for the field of transverse magnetic (TM) polarization than for the transverse electric (TE) polarization, but both these directions lie in the plane of incidence and are opposite to one another with respect to the direction in the uniform medium, where by transverse polarizations are meant those with respect to the plane of incidence. Hence, the original wave is split into two waves. Deflection is increased and, consequently, speed of propagation decreased for the TM field, whereas deflection is decreased and speed of propagation increased for the TE component if the wave propagates into a plasma of increasing concentrations; consequently, the TM field will be reflected back earlier than the TE part. Besides these results, it is hoped that our treatment may help in attacking problems of coupling of different types of plasma waves due to slow variation of equilibrium parameters occuring from more complete set of equations describing plasma behavior.

1. INTRODUCTION

The study of propagation of electromagnetic and electroacoustic waves through nonuniform plasmas and their mutual coupling due to various factors have found important applications in space research. Considerable work on wave propagation in ionized media and also in dielectrics is known to exist.[1–15] But actual progress towards understanding the phenomena is retarded by complications owing to the handling of several interrelated vector quantities and, besides, by both physical and theoretical difficulties coming from inhomogeneity of the equilibrium plasma. For this reason, approximation is essential, and it is the aim of the investigation that decides the nature of approximation to be followed.

In a uniform plasma in the absence of any external magnetic field, high-frequency waves propagate freely without reflection and mutual coupling.[16] In a nonuniform plasma the situation becomes complicated and the picture of wave propagation loses its clarity. But it is possible and also worthwhile to study the development of complications by considering a very slowly varying plasma. In the present work we have confined our study to electromagnetic wave propagation through a cold, slowly varying plasma medium in the absence of any external magnetic field. The works of Bremmer,[17–19] Tidman,[1] Wait,[8] and Budden[9] have shown that the method of WKB would be suitable for our purpose.

It may be mentioned that there are, in general, the following three types of problems associated with wave propagation in a slowly varying plasma in the linearized approximation: (1) analysis of the equation governing a primary longitudinal perturbation and the subsequent production of the scattered secondary transverse field; (2) the same for a transverse primary field and the scattered secondary longitudinal field and (3) analysis of coupling between the primary longitudinal and transverse fields.

Tidman[1] considered the influence of gradients of concentration and temperature on longitudinal wave and obtained expressions for the scattered transverse radiation field. Ignoring ion motion, Vlasov[2] obtained equations linking electron density propagation with the transverse electromagnetic field through the gradient of the equilibrium charge density ρ_0. Excitation of electron density wave by electromagnetic field was studied, assuming ρ_0 to be in the form grad $\rho_0 = \rho_0\delta(z)$, where $\delta(z)$ is the δ function and Oz is a coordinate direction. Dunphy *et al.*,[3] Kritz and Mintzer,[4] and Chakraborty[5] have also considered coupling between longitudinal and transverse waves. Their study, however, is confined to that at the plane of separation between two semi-infinite media of uniform but different concentrations and hence, in these cases, the density does not continuously change, but abruptly jumps from one value to another within the thickness of an infinitely thin region. This is just

opposite to the case we have considered in the present paper, namely the case of approximation of geometrical optics in which the equilibrium density changes slowly but continuously in such a way that the characteristic length of variation is much larger than the wavelength of the transmitted wave.

In Sec. 2 we solve the second-order linear inhomogeneous wave equation by the WKB method. We then proceed further and find out a sequence of successive substitutions by the help of which solutions correct up to any higher order are reduced to the WKB solution of an equation like the simple original equation. Section 3 contains the appropriate plasma equations for electromagnetic field in the cold plasma approximation in the absence of any external magnetic field. We consider the effect of an electromagnetic wave propagation obliquely with respect to the slowly but continuously varying plane layers of plasma. The plane containing the wave vector and the normal to the layers of inhomogeneity is called the plane of incidence. Then the electromagnetic field has one part with electric field transverse to the plane of incidence and hence, denoted simply by TE field, and another part whose magnetic field is perpendicular to this plane, called the TM field, In Sec. 4, we have obtained the WKB solution for the TE field and made initial steps for the theory of higher-order approximations, which is the subject matter of the next section. We have developed the sequence of the proper variables of substitution which makes study of approximations correct up to any higher order feasible. Across a plane, where N is continuous but its first- and second-order space gradients are discontinuous, we have solved the boundary-value problem for wave propagation using continuity of the tangential components of electric and magentic fields. We have verified that for our results the energy flow across the layer is conserved. The characteristics of the reflected and transmitted waves depend on the gradients and higher space derivatives of N, such that the reflected wave vanishes in the approximation of constancy of N. Expressions for the linear and angular deviations of the direction of flow of energy from its straight course in the uniform medium also depend on the gradient of N. We have obtained the values of relative shift of the wave vector along and perpendicular to the direction in the uniform medium, with respect to the distance of wave advancement in that medium in a given time. Higher-order coupling between the reflected and incident secondary waves show that the $(m+1)$th-order incident wave is scattered by both incident and reflected waves of the nth order. In Sec. 6, analogous results for the TM field have been determined. Quantitative comparison of the results for the two cases leads to interesting conclusions. We find that the derivation of the wave vector for the TE field is slightly different in magnitude and direction from that of the TM field, but both directions lie in the plane of incidence and are opposite to one another with respect to the direction in the uniform medium. This shows that a small ∇N splits up the wave into two waves propagating in slightly different directions. It is known that a wave deflects away from the normal in a denser medium more than in a rarefied medium. The existence of ∇N works in such a way that this deflection is increased and consequently, speed of propagation is decreased for the TM part, whereas deflection is decreased and speed of propagation increased for the TE component. Again, for the same reason, if the wave penetrates obliquely through a region of increasing N, the TM field will be reflected earlier than the TE part.

We believe that, besides obtaining these concrete and quantitative results, our approach and treatment would pave the way for attacking problems of coupling of different types of plasma waves due to slow variation of equilibrium parameters, occuring from more complete set of equations describing the behavior of plasmas.

2. THE PRELIMINARY ESSENTIAL MATHEMATICS

Let us consider the equation

$$\frac{d^2\psi(z)}{dz^2} + K^2(z)\psi(z) = 0, \tag{2.1}$$

where $\psi(z)$ and $K(z)$ are scalar quantities, K is slowly varying with z and takes up only large values. If K is independent of z, the solution is a wavefunction infinitely extended to both positive and negative directions of the z axis. If some properties of the medium slowly and continuously change perpendicular to Oz, then K comes out to be a slowly varying function z and the wavefunction solution of (2.1) is modified. We shall study this modification starting with the method of WKB.[20–22]

We seek solution of (2.1) in the form

$$\psi(z) = Ae^{i\varphi(Z)}, \tag{2.2}$$

where A is a constant and $\varphi(z)$ is the generalized phase. Wait[8] obtained solution of (2.1) in which A is also assumed to be a function of z. But (2.2) is also a general solution where all functional dependence on z can be included within $\varphi(z)$ by keeping constant.

Substituting (2.2) into (2.1), we get

$$\left(\frac{d\varphi}{dz}\right)^2 = K^2 + i\frac{d^2\varphi}{dz^2}. \tag{2.3}$$

If $\varphi(z)$ only slowly varies with z, then the nontrivial first approximation would be

$$\frac{d\varphi}{dz} = \pm K, \quad \frac{d^2\varphi}{dz^2} = \pm\frac{dK}{dz}. \tag{2.4}$$

The second derivative of φ with respect to z is a quantity of order smaller than K. Putting the value of $d^2\varphi/dz^2$ from (2.4) to (2.3), taking square roots and keeping up to first power of dK/dz, we get

$$\frac{d\varphi}{dz} = \pm\left(K + \frac{i}{2K}\frac{dK}{dz}\right). \tag{2.5}$$

Integrating (2.5) and putting in (2.2), the WKB solution of (2.1) is given in the form

$$\psi = \frac{A_0}{(K)^{\frac{1}{2}}}\exp\left(-i\int^z K\,dz\right) + \frac{B_0}{(K)^{\frac{1}{2}}}\exp\left(i\int^z K\,dz\right). \tag{2.6}$$

The lower limit of the integral in the phase can be set equal to zero or any other value z_0, since in effect, this alteration changes only the value of the arbitrary constants A_0 and B_0. The range of validity of K is obtained by putting this solution into the left-hand side of (2.1) dividing it by $K^2\psi$ to make the quantity dimensionless and making the modulus of it much less than unity. This gives

$$\left|\frac{3}{4K^4}\left(\frac{dK}{dz}\right)^2 - \frac{1}{2K^3}\frac{d^2K}{dz^2}\right| < 1, \tag{2.7}$$

showing that dK/dz and d^2K/dz^2 should be sufficiently small and K large.

If we now substitute

$$\xi = \int^z K\,dz \tag{2.8}$$

and

$$\psi_1 = (K)^{\frac{1}{2}}\psi, \tag{2.9}$$

we get

$$\frac{d^2\psi_1}{dz^2} + \left[1 - \frac{1}{2K}\frac{d^2K}{dz^2} + \frac{1}{4K^2}\left(\frac{dK}{dz}\right)^2\right]\psi_1 = 0. \tag{2.10}$$

The introduction of ξ in place of z means the transition to a new unit of length depending on the local value of the wavelength.

To contract Eq. (2.10) into shorter form, we substitute

$$R = -\frac{1}{4}\frac{d}{d\xi}(\log K). \tag{2.11}$$

The quantity R has a physical significance[23] because it can be written as

$$R = \frac{[1/(K)^{\frac{1}{2}}]_2 - [1/(K)^{\frac{1}{2}}]_1}{[1/(K)^{\frac{1}{2}}]_2 + [1/(K)^{\frac{1}{2}}]_1} \tag{2.12}$$

if the layers denoted by 1 and 2 are separated by the unit length of an infinitely thin stratum. Hence, up to the WKB order of solution, R is proportional to the ratio of the loss of amplitude to the total amplitude of the wave propagating through the unit length of an infinitely thin stratum of a nonuniform medium. Since the medium is assumed to be loss free, the loss of energy due to change of amplitude cannot be absorbed and so must be entirely reflected. For this reason, R can be called the reflected coefficient at the point.

Equation (2.10) can be written as

$$\frac{d^2\psi_1}{d\xi^2} + (1 + 2p)\psi_1 = 0, \tag{2.13}$$

where

$$p = \frac{dR}{d\xi} - 2R^2. \tag{2.14}$$

The value of p, obtained as derivatives if z, is

$$p = \frac{3}{8K^4}\left(\frac{dK}{dz}\right)^2 - \frac{1}{4K^3}\frac{d^2K}{dz^2} \tag{2.15}$$

and so, up to orders of first derivatives of K, the value of p is positive.

Following (2.6) the WKB solution of (2.13) is

$$\psi_1 = \frac{A_1}{(K_1)^{\frac{1}{2}}}\exp\left(-i\int^\xi K_1\,d\xi\right) + \frac{B_1}{(K_1)^{\frac{1}{2}}}\exp\left(i\int^\xi K_1\,d\xi\right), \tag{2.16}$$

where

$$K_1 = (1 + 2p)^{\frac{1}{2}}. \tag{2.17}$$

Again, if we put

$$\xi_1 = \int^\xi K_1\,d\xi, \tag{2.18}$$

$$R_1 = -\frac{1}{4}\frac{d}{d\xi}\log K_1, \tag{2.19}$$

$$p_1 = \frac{dR_1}{d\xi} - 2R_1, \tag{2.20}$$

we would get an equation like (2.13) correct up to quantities of the order of the third derivative of K with respect to z.

We can now proceed further and get an equation like (2.13) in terms of ψ_2 and ξ_2, where

$$\psi_2 = (K_1)^{\frac{1}{2}}\psi_1 = (KK_1)^{\frac{1}{2}}\psi, \tag{2.21}$$

$$K_2 = (1 + 2p_1)^{\frac{1}{2}}, \tag{2.22}$$

$$\xi_2 = \int^{\xi_1} K_2\, dz, \tag{2.23}$$

etc. Thus, we can form a set of successive variables of substitution and consequently, equations such as (2.13), containing the substitution (2.17), which are like the original equation (2.1), and whose solutions are better solutions of (2.1) than an earlier member of the set of solutions.

The inequality (2.7), written in terms of R and ξ, becomes

$$\left| 2\frac{dR}{d\xi} - 4R^2 \right| \ll 1. \tag{2.24}$$

The condition for the validity of the solution (2.16) can be obtained from (2.24), replacing R and ξ by R_1 and ξ_1, respectively. Similarly the condition of validity of the solution of (2.1) correct up to any order of derivatives of K with respect to z can be written down from (2.24) replacing R and ξ by the R and ξ associated with that order.

3. THE COLD PLASMA EQUATIONS FOR ELECTROMAGNETIC FIELD

We study the simple case of electromagnetic wave propagation in a cold plasma. The relevant equations are

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{H}}{\partial t}, \tag{3.1}$$

$$\nabla \times \mathbf{H} = \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c}\mathbf{j}, \tag{3.2}$$

where

$$\mathbf{j} = -Ne\mathbf{u}, \tag{3.3}$$

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{e}{m}\mathbf{E}. \tag{3.4}$$

$\mathbf{u}$ is the velocity of electrons in the field $\mathbf{E}$, $\mathbf{H}$ is the magnetic component of the field, N is the equilibrium electron-number density slowly varying in space, m is its mass, and other quantities have their usual meaning.

We assume that electron concentration varies along Oz, i.e., that the plasma is stratified continuously perpendicular to Oz and that the incident wave falls at a nonzero angle with Oz. Let the (z, X) plane be the plane of incidence. Then all physical quantities will be functions of x and z only, and their derivatives with respect to y will vanish. We take time dependence and x dependence of all perturbation variables to be contained in the expression $\exp(i\omega t - iK_0 x)$, where K_0 is a constant and ω is the frequency of oscillation. Then expanding the curls, and simplifying and replacing the partial differentiation sign $\partial/\partial z$ by the total differentiation d/dz, we get

$$\frac{i\omega}{c}H_x = \frac{dE_y}{dz}, \tag{3.5}$$

$$-\frac{i\omega}{c}H_y = \frac{dE_x}{dz} + iK_0E_z, \tag{3.6}$$

$$\frac{i\omega}{c}H_z = iK_0E_y, \tag{3.7}$$

$$\frac{iK^2c}{\omega}E_x = -\frac{dH_y}{dz}, \tag{3.8}$$

$$\frac{iK^2c}{\omega}E_y = iK_0H_y + \frac{dH_x}{dz}, \tag{3.9}$$

$$\frac{iK^2c}{\omega}E_z = -iK_0H_y, \tag{3.10}$$

where

$$K^2c^2 = \omega^2 - \omega_0^2, \tag{3.11}$$

$$\omega_0^2 = 4\pi Ne^2/m. \tag{3.12}$$

Equations (3.5), (3.7), and (3.9) mutually relate E_y, H_x, and H_z, and are independent of (3.6), (3.8), and (3.10), which connect H_y, E_x, and E_z among themselves. These are two sets of equations which can be solved independently of each other. In the first set, the electric field is perpendicular to the plane of incidence and is the TE field. In the second set, the electric field is situated in the plane of incidence and is the TM field. The equations governing the behavior of the TE field would be slightly different from, and also simpler than, those associated with the TM part. As a result, the solutions also differ quantitatively to a certain extent though the methods of solution do not differ significantly.

4. THE WKB SOLUTION FOR TE POLARIZATION

From the set of equations (3.5), (3.7), and (3.9) associated with the TE field, we eliminate H_z between the last two equations and get

$$\frac{dH_x}{dz} = \frac{iK_1^2c}{\omega}E_y, \tag{4.1}$$

where

$$K_1^2 = K^2 - K_0^2. \tag{4.2}$$

In (4.2), we should remember that $K^2 - K_1^2$, is a constant quantity for further evaluation of results.

Elimination of H_x between (4.1) and (3.5) gives

$$\frac{d^2E_y}{dz^2} + K_1^2E_y = 0. \tag{4.3}$$

Since this equation resembles (2.1), its WKB solution is

$$E_y = \frac{A}{(K_1)^{\frac{1}{2}}} \exp\left(-i\int^z K_1\,dz\right) + \frac{B}{(K_1)^{\frac{1}{2}}} \exp\left(i\int^z K_1\,dz\right), \tag{4.4}$$

where A and B are arbitrary quantities having constant values up to the WKB approximation; also, this K plays the role of K in (2.6) and so is different from K_1 in (2.17) in value and meaning. Hence, K_1 must satisfy the inequality (2.7) and for this

$$K_0^2 \ll |(\omega^2 - \omega_0^2)/c^2|, \tag{4.5}$$

which is true for very high frequences and large wavelengths.

Equations (3.9) or (4.1) show that $d\varphi/dz$ slowly varies with z since it contains ω_0 [see (3.11), (3.12), and (4.2)]; whereas (3.5) requires that $d\varphi/dz$ be a constant. Hence, as already remarked by Budden,[9] functional dependence of the perturbed quantities on z is not the same in all the linear equations involved and so progressive wave solution is not, rigorously speaking, possible in any slowly varying, electrically conducting medium. But we can take progressive waves to be approximately possible in a slowly varying medium also, because free propagation is possible in the limits of uniform medium.

Considering A and B in (4.4) as constants and using (3.5), we get for H_x the expression

$$H_x = \left(-\frac{K_1c}{\omega} + \frac{ic}{2K_1\omega}\frac{dK_1}{dz}\right)\frac{A\exp\left(-i\int^z K_1\,dz\right)}{(K_1)^{\frac{1}{2}}} + \left(\frac{K_1c}{\omega} + \frac{ic}{2K_1\omega}\frac{dK_1}{dz}\right)\frac{B}{(K_1)^{\frac{1}{2}}}\exp\left(i\int^z K_1\,dz\right). \tag{4.6}$$

We may note that, if K_1 is positive, the first term of (4.4) or (4.6) gives the wave progressing in a direction of increasing x and z both and the second term of these equations is associated with the wave progressing in a direction of increasing x and decreasing z. To keep our analysis and terminology close to the usual transmission and reflection of waves at the plane of separation of two media of different concentrations, we call the former the incident wave and the latter the reflected wave. The incident wave has field components whose mutual relations are given by

$$H_x^i = -\frac{K_1c}{\omega}\left(1 - \frac{i}{2K_1^2}\frac{dK_1}{dz}\right)E_y^i, \quad H_z^i = \frac{K_0c}{\omega}E_y^i, \tag{4.7}$$

and which are obtained from the first terms on the right-hand side of (4.4), (4.6), and (3.7). Similar relations can be obtained for the reflected field components by equating the second terms on the right-hand side of (4.4), (4.6), and (3.7). Besides this, we shall also use the connecting relations

$$E_y = E_y^i + E_y^r, \quad H_x = H_x^i + H_x^r, \quad \text{etc,} \tag{4.8}$$

in the next section.

5. HIGHER-ORDER APPROXIMATIONS FOR TE POLARIZATION

For higher-order approximations, we put the relations (4.7) and the corresponding ones for the reflected quantities in (4.8) and the resulting relations in (3.5), (3.7), and (3.9), solve for dE_y^i/dz and dE_y^r/dz, and get

$$\frac{dE_y^i}{dz} + \left[iK_1 + \frac{1}{2K_1}\frac{dK_1}{dz} + \frac{3i}{8K_1^3}\left(\frac{dK_1}{dz}\right)^2 - \frac{i}{4K_1^2}\frac{d^2K_1}{dz^2}\right]E_y^i = E_y^r\left[-\frac{3i}{8K_1^3}\left(\frac{dK_1}{dz}\right)^2 + \frac{i}{4K_1^2}\frac{d^2K_1}{dz^2}\right], \tag{5.1}$$

$$\frac{dE_y^r}{dz} + \left[-iK_1 + \frac{1}{2K_1}\frac{dK_1}{dz} - \frac{3i}{8K_1^3}\left(\frac{dK_1}{dz}\right)^2 + \frac{i}{4K_1^2}\frac{d^2K}{dz^2}\right]E_y^r = E_y^i\left[\frac{3i}{8K_1^3}\left(\frac{dK_1}{dz}\right)^2 - \frac{i}{4K_1^2}\frac{d^2K_1}{dz^2}\right]. \tag{5.2}$$

These are two linear first-order differential equations connecting E_y^i and E_y^r among themselves. Their right-hand sides are proportional to the squares of dK_1/dz and d^2K_1/dz^2, though the left-hand sides contain terms proportional to K_1 and dK_1/dz. This shows that coupling is weak and up to orders of first power of dK_1/dz is negligible. This is contrary to results which follow from the work of Bremmer[17] for slowly varying dielectric media if extended to our case. When transformed to the plasma field Eqs. (3.1)–(3.4), Bremmer's equations[5] show coupling even up to orders of dK_1/dz. The reason for this is that, if we

follow the treatment of Bremmer, then terms with coefficients dK_1/dz would be neglected in (4.6), but later on, terms of this very order would be used for calculating higher-order quantities. This mistake then gives terms proportional to dK_1/dz in the right-hand side of (5.1) and (5.2), but actually they exactly cancel with those gotten by including the full expression for H_x in (4.6), and so are absent.

The question at this stage arises whether in each successively higher-order calculation the immediately next-lower-order answer exactly cancels or not. To answer this question, more accurate solutions of (4.3) than (4.4) have to be constructed, say, correct up to $(2r)$th order of smallness in the sense of order of quantities adopted in the present work. Then equations should be constructed similar to (5.1) and (5.2), and the coefficients of E_y^i and E_y^r on the right side of these equations are to be studied. Exact behavior in this regard would be clear after finding out whether the $(2r-1)$th-order quantities exactly cancel out or not. This analysis is reserved for a subsequent investigation.

If we substitute

$$I_i = (K_1)^{\frac{1}{2}}E_y^i, \quad I_r = (K_1)^{\frac{1}{2}}E_y^r, \tag{5.3}$$

$$\xi = \int^z K_1\, dz \tag{5.4}$$

into Eqs. (5.1) and (5.2), then we obtain

$$\frac{dI_i}{d\xi} + i(1+p)I_i = -ipI_r, \tag{5.5}$$

$$\frac{dI_r}{d\xi} - i(1+p)I_r = ipI_i, \tag{5.6}$$

where p has the value given in (2.14) and (2.15) if K there is replaced by K_1. This change also gives the reflection coefficient R for the TE polarization.

The second-order differential equation for I_i, obtained by eliminating I_r from the above equations, can be written as

$$\frac{d^2}{d\xi^2}\left(\frac{I_i}{\sqrt{p}}\right) + \left(1 + 2p - i2S - S^2 + \frac{dS}{d\xi}\right)\left(\frac{I_i}{\sqrt{p}}\right) = 0, \tag{5.7}$$

where

$$2S = \frac{d}{d\xi}(\log p). \tag{5.8}$$

This equation contains both the solutions for the incident and reflected waves and is inhomogeneous, because p is a function of ξ. If, from the properties of the medium, the function determining the slow variation of N on z is given, then we can determine the dependence of p on z and so, ultimately, on ξ, and from that try to solve Eq. (5.7) exactly. But following the treatment in Sec. 2, we can solve (5.7) up to any order of accuracy desirable. We study below the simple case where p is a constant, because this restriction will also include within it considerably the effects of slow variation of the medium.

To study scattering of reflected waves, we assume uniform plasma in $z < z_0$ and slowly varying plasma in $z \geq z_0$. The concentration N continuously changes from the uniform to the nonuniform regions, but the derivatives of N discontinuously change from zero in $\xi < 0$ to nonzero quantities in $\xi \geq 0$. As a result, K and K_1 are continuous throughout, but their derivatives and, consequently, the function p are discontinuous, being zero in $\xi < 0$ and nonzero in $\xi \geq 0$. The primary incident wave enters obliquely from the homogeneous region $z < z_0$ into the inhomogeneous part. We can then define equations of I in the two regions in the way.

$$\frac{d^2I}{d\xi^2} + (1+2p)I = 0, \quad \xi \geq 0,$$

$$\frac{d^2I}{d\xi^2} + I = 0, \quad \xi < 0. \tag{5.9}$$

The solution necessary for our purpose is

$$I = I_0e^{-i\xi} + Te^{i\xi}, \quad \xi < 0,$$

$$= De^{-i\xi(1+2p)^{\frac{1}{2}}}, \quad \xi \geq 0, \tag{5.10}$$

where I_0 is the amplitude of the incident wave, T that of reflection, and D of transmission. If the square of dK_1/dz and not d^2K_1/dz^2 determines mainly the value of p, then p is positive. In that case, ∇N deflects the wave towards the normal as shown by the solution (5.10) in $\xi \geq 0$. This deflection, which is small in a slowly varying medium, thus slightly retards the deflection away from the normal as the wave enters from a rarefied to a denser region.

The constants T and D are determined from the usual two boundary conditions which are the continuity of the horizontal field components H_x and E_y. When transformed in terms of I and ξ, the boundary conditions turn out to be the continuity of $I/(K_1)^{\frac{1}{2}}$ and $K_1\, d[I/(K_1)^{\frac{1}{2}}]/d\xi$. The two conditions then give

$$I_0 + T = D, \tag{5.11}$$

$$I_0 - T = D[(1+2p)^{\frac{1}{2}} + 2iR]. \tag{5.12}$$

Solving for T and D, we get

$$D = \frac{2I_0}{1 + (1+2p)^{\frac{1}{2}} + i2R},$$
$$T = \frac{I_0[1 - (1+2p)^{\frac{1}{2}} - i2R]}{1 + (1+2p)^{\frac{1}{2}} + i2R} \tag{5.13}$$

We see that $T = 0$ and $D = 1$ when R and $dR/d\xi$ vanish, showing that there would be no reflection losses for transmission through uniform medium.

If the Poynting vector $(= (c/4\pi)[\mathbf{EH}])$ for the incident, reflected, and transmitted portions respectively are $\mathbf{S}^i$, $\mathbf{S}^r$, and $\mathbf{S}^t$, then their averages over one time period have the magnitudes

$$\langle S^i \rangle = I_0^2 K c^2/8\pi K_1 \omega,$$
$$\langle S^r \rangle = |T|^2 K c^2/8\pi K_1 \omega, \tag{5.14}$$
$$\langle S^t \rangle = |D|^2 c^2 (K^2 + 2pK_1^2)^{\frac{1}{2}}/8\pi K_1 \omega.$$

Conservation of flow of energy across the layers, namely the relation

$$\langle S_z^i \rangle = \langle S_z^r \rangle + \langle S_z^t \rangle, \tag{5.15}$$

which is an inevitable consequence of the boundary conditions in a loss free plasma, is also satisfied by our solutions (5.13) or (5.14).

If the direction of flow of energy as the wave enters the inhomogeneous region makes an angle $\varphi + \delta\varphi$ with Oz and φ with Oz in the uniform region or in vacuum so that $\delta\varphi$ is the deviation due to nonuniformity, then

$$\langle S_z^t \rangle / \langle S_z^t \rangle = \cot(\varphi + \delta\varphi) = K_1(1+2p)^{\frac{1}{2}}/K_0 \tag{5.16}$$

and

$$\cot\varphi = K_1/K_0.$$

It is evident that $\delta\varphi < 0$ when $p > 0$.

Expanding (5.16), neglecting squares and higher powers of p, and keeping terms which survive differentiation, we get

$$\delta\varphi = -\frac{c^2 \sin\alpha_0 \sec^2\alpha_0}{8(\omega^2 - \omega_0^2)^2}\left[\frac{5\sec^2\alpha_0}{4(\omega^2-\omega_0^2)}\left(\frac{d\omega_0^2}{dz}\right)^2 + \frac{d^2\omega_0^2}{dz^2}\right], \tag{5.17}$$

where α_0 is the inclination of the wave vector in the uniform region or in vacuum with Oz. This shows that $\delta\varphi$ is negative, if the second derivative of ω_0^2 with respect to z is positive, or if the second derivative of ω_0^2 is negative but does not become the dominant term in comparison with the other term. The sign of $\delta\varphi$ will be positive in the region where N is a maximum. We can also express (5.17) for practical purposes in terms of characteristic lengths l and l_1 given by

$$\frac{1}{l} = \frac{1}{N}\frac{dN}{dz} \equiv \frac{1}{\omega_0^2}\frac{d\omega_0^2}{dz}, \quad \frac{1}{ll_1} = \frac{1}{\omega_0^2}\frac{d^2\omega_0^2}{dz^2}. \tag{5.18}$$

The value of $\delta\varphi$ is cumulative if the nonuniformity is monotonic in a region. The formula for $\delta\varphi$ suggests that within astronomical order of distances angular derivation from an early initial direction would take on a sizable value.

We can also find out the shift in the position of the foot of the perpendicular from the origin O to the wave front. At a time t let A be that position for the uniform medium and B that in the slowly varying medium. Then the coordinates of B [say, $(\delta x, \delta z)$] with reference to axes through A parallel to the original axes are

$$(\delta x, \delta z) = \frac{-2\omega K_0 K_1^2 pt,\ \omega K_1 t\{K^2[(1+2p)^{\frac{1}{2}} - 1] - 2pK_1^2\}}{K^2(K^2 + 2pK_1^2)}. \tag{5.19}$$

With reference to perpendicular to OA and the direction of OA if these deviations are denoted by α and β, respectively, then

$$(\alpha, \beta) = \frac{\omega K_0 K_1 t[(1+2p)^{\frac{1}{2}} - 1],\ -\omega K_1^2 t(1+2p)^{\frac{1}{2}}[(1+2p)^{\frac{1}{2}} - 1]}{K(K^2 + 2pK_1^2)}. \tag{5.20}$$

The relative shift of β with respect to the distance OA of wave advancement in time t in the uniform region along the above mentioned directions have approximately the value

$$\frac{\alpha K}{\omega t} = \frac{c^2 \sin\alpha_0 \sec^3\alpha_0}{8(\omega^2 - \omega_0^2)^2}\left[\frac{5\sec^2\alpha_0}{4(\omega^2-\omega_0^2)}\left(\frac{d\omega_0^2}{dz}\right)^2 + \frac{d^2\omega_0^2}{dz^2}\right] \tag{5.21}$$

and

$$\frac{\beta K}{\omega t} = \left(\frac{\alpha K}{\omega t}\right)(-\cot\alpha_0).$$

The right-hand sides of the relations (5.17)–(5.21) vanish in the approximation of uniform medium. The negative value of β in (5.20) and (5.21) show that the propagation speed is retarded.

Following the procedure of Bremmer,[17] we have developed in Appendix A the series solution for A and B of (4.4) because it determines the mutual relation between the higher-order secondary waves of the types of incidence as well as reflection. The derivatives of a higher-order A or B become proportional to a linear relation of both A and B of one order less multiplied by the order-raising factor p.

Bremmer obtained the result that the $(m+1)$th-order incident wave can only be scattered by the mth-order reflected wave and is not related to the mth-order incident wave, and that similar conclusions hold for the $(m+1)$th-order reflected wave.[24] These results were deduced from the incorrect equations of coupling and from the consequent incorrect recurrence relations of Ref. 17. The equations (A7) and (A8) of Appendix A show that the $(m+1)$th-order incident wave can be scattered by both the mth-order reflected and mth-order incident waves, and similarly for the $(m+1)$th-order reflected wave.

6. PROPAGATION OF THE TM FIELD

To solve the set of equations (3.6), (3.8), and (3.10) we eliminate E_z between (3.6) and (3.8). Then, using (4.2) we get

$$-i\omega K_1^2 H_y = K^2 c \frac{dE_x}{dz}. \tag{6.1}$$

The second-order equation for H_y, which is simpler than those for E_x and E_z, obtained from this equation by eliminating E_x with the help of (3.8), is

$$\frac{d^2H_y}{dz^2} - \frac{2}{K}\frac{dK}{dz}\frac{dH_y}{dz} + K_1^2 H_y = 0. \tag{6.2}$$

Though this equation is different from (2.1) and (4.3), a suitable rearrangement, however, gives

$$\frac{d^2}{dz^2}\left(\frac{H_y}{K}\right) + \left[K_1^2 + \frac{1}{K}\frac{d^2K}{dz^2} - \frac{2}{K^2}\left(\frac{dK}{dz}\right)^2\right]\left(\frac{H_y}{K}\right) = 0. \tag{6.3}$$

Up to the order of squares of the first derivatives of K and K_1 and the order of the first power of their second derivatives, Eq. (6.3) can be solved straightforwardly by the WKB method. For this, we put

$$I' = \frac{(K)^{\frac{1}{2}} H_y}{K}, \tag{6.4}$$

$$\xi = \int^z K_1\, dz \tag{6.5}$$

in (6.3), and obtain

$$\frac{d^2I'}{d\xi^2} + (1+2p')I' = 0, \tag{6.6}$$

where

$$p' = -\left(2R'^2 + \frac{dR'}{d\xi}\right) \tag{6.7}$$

and

$$R' = -\frac{1}{2}\frac{d}{d\xi}\left(\log\frac{K}{(K_1)^{\frac{1}{2}}}\right). \tag{6.7'}$$

For normal incidence, R' becomes equal to R, but p' does not become equal to p because of additional contributions to p' from the middle term of (6.2). Also, R', like R, is proportional to the ratio of loss of amplitude to the total amplitude for TM polarization up to the WKB order of solution, and so may be similarly called the reflection coefficient of this field. It may be mentioned that the dimensions of I' is $1/K$ times that of I of (5.3) and (5.9).

We could also follow the treatment which gave Eq. (5.7) and obtain the analogous equation for this case. But, as we are content with orders of accuracy up to the constancy of p', we have avoided that procedure.

Starting with (6.6), we now formulate equations like (5.9) in the uniform and nonuniform parts and seek solutions of the form (5.10). To solve for T' and D', the boundary conditions are the continuity of E_x and H_y at $\xi = 0$. In terms of I' of (6.4), these conditions lead to the continuity of $I'K/(K_1)^{\frac{1}{2}}$ and

$$\frac{K_1}{K^2}\frac{d}{d\xi}\left(\frac{KI'}{(K_1)^{\frac{1}{2}}}\right)$$

at the same level. We should remember that K and K_1 are continuous, but that their derivatives with respect to ξ are discontinuous at $\xi = 0$. The values of T' and D' are

$$(D', T') = \frac{2I_0', I_0'[1 - (1+2p')^{\frac{1}{2}} - 2iR']}{1 + (1+2p')^{\frac{1}{2}} + 2iR'}. \tag{6.8}$$

The incident, reflected, and transmitted parts of the Poynting vector, averaged over one time period, give

$$\begin{aligned} \langle S^i\rangle &= I_0'^2 K\omega/8\pi K_1, \\ \langle S^r\rangle &= |T'|^2 K\omega/8\pi K_1, \\ \langle S^t\rangle &= |D'|^2 \omega(K^2 + 2p'K_1^2)^{\frac{1}{2}}/8\pi K_1. \end{aligned} \tag{6.9}$$

The conservation of energy flow relation (5.15) is satisfied by our solution (6.8).

The angular deflection $\delta\varphi'$ of the direction of energy flow has the value

$$\begin{aligned} \delta\varphi' &= -\frac{K_1 K_0}{K^2}[(1+2p')^{\frac{1}{2}} - 1] \\ &\approx \frac{c^2 \sin\alpha_0 \sec\alpha_0}{8(\omega^2 - \omega_0^2)^2}\left[\frac{(12 - 5\sec^4\alpha_0)}{4(\omega^2-\omega_0^2)}\left(\frac{d\omega_0^2}{dz}\right)^2\right. \\ &\quad \left. + (2 - \sec^2\alpha_0)\frac{d^2\omega_0^2}{dz^2}\right]. \end{aligned} \tag{6.10}$$

Comparison with (5.17) shows that $\delta\varphi'$ is quantitatively different from $\delta\varphi$. This indicates splitting of the single wave into two waves propagating in slightly different directions in the plane of incidence—the TM field is transmitted along one direction and the

TE along the other. For a wave almost normally incident from the uniform region we can take $\sin \alpha_0 \approx \alpha_0$ and $\sec \alpha_0 \approx 1$, getting (1) $|\delta\varphi'| > |\delta\varphi|$, and (2) $\delta\varphi' > 0$, while $\delta\varphi < 0$. The first result shows that the TM field is bent more by ∇N than the TE field. As a result, when a wave propagates into a region of increasing concentration the TM field will be reflected back earlier than the TE part and so will not reach levels as far as the latter. The second result indicates that bifurcation of the wave is in opposite direction for the two component fields.

Other results obtained for the TE field from relations (5.19)–(5.21) and from Appendix A can be easily extended to the TM part. It may be mentioned that the TM field is distinguished from the TE field in that it generates the density propagation of the longitudinal field given by

$$\rho = E_z \frac{d\omega_0^2}{dz} \cdot \frac{1}{4\pi(\omega^2 - \omega_0^2)},$$

where ρ is the perturbed charge density. This relation is obtained by taking the divergence of (3.2) and utilizing the vector property

$$\operatorname{div}(N\mathbf{E}) = N \operatorname{div} \mathbf{E} + (\mathbf{E} \cdot \nabla N).$$

The TE field is free from such conversions. If we ignore the divergence, then E_x, E_z, and H_y vanish.

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APPENDIX A

Putting the values of E_y^i and E_y^r from (4.4) in (5.1) and (5.2), we get

$$\frac{dA}{dz} = -\epsilon ip\left[A + B \exp\left(2i\int^z K_1\, dz\right)\right], \quad \text{(A1)}$$

$$\frac{dB}{dz} = \epsilon ip\left[B + A \exp\left(-2i\int^z K_1\, dz\right)\right], \quad \text{(A2)}$$

where p of (5.7) is replaced by ϵp, ϵ being introduced as a parameter to facilitate expansion. The actual solution would be obtained for $\epsilon = 1$, and $\epsilon = 0$ would give $A = A_0$ and $B = B_0$ where A_0 and B_0 are constants, being actually the arbitrary constants of integration for the WKB solution. If K_1 is real, the right-hand side of (A1) and (A2) are rapidly varying functions of z. The above equations give a simple relation between A and B, namely

$$\frac{dB}{dz} = -\frac{dA}{dz} \exp\left(-2i\int^z K_1\, dz\right), \quad \text{(A3)}$$

and also the following second-order differential equation for A:

$$\epsilon p^2 \frac{d^2A}{dz^2} + \left(i\frac{dp}{dz} - 2K_1 p\right)\frac{dA}{dz} - 2iK_1\epsilon p^2 A = 0, \quad \text{(A4)}$$

and an analogous equation for B. Their solutions are mutually related to each other by (A3) or by (A1) and (A2). For convenience and clarity we seek the power-series solution in the form

$$A = A_0 + \epsilon A_1 + \epsilon^2 A_2 + \cdots, \quad \text{(A5)}$$

$$B = B_0 + \epsilon B_1 + \epsilon^2 B_2 + \cdots. \quad \text{(A6)}$$

The series solution would be the most general one, provided it is convergent, since it would contain arbitrary constants A_0 and B_0 of integration. Putting (A5) and (A6) in (A1) and (A2), and equating powers of ϵ^{m+1} from both sides, we get

$$\frac{dA_{m+1}}{dz} = -ip\left[A_m + B_m \exp\left(2i\int^z K_1\, dz\right)\right], \quad \text{(A7)}$$

$$\frac{dB_{m+1}}{dz} = ip\left[B_m + A_m \exp\left(-2i\int^z K_1\, dz\right)\right]. \quad \text{(A8)}$$

In these relations, a higher-order A or B is linearly related to both A and B of one order less multiplied by p. The constants A_0 and B_0 correspond to the uncorrelated primary incident and reflected waves respectively, one or both of which, if introduced into the plasma, will scatter secondary waves of all higher orders. Since the equations are linear in A and B, the solutions are superposable. We can, therefore, start by first putting $B_0 = 0$, i.e., assuming that only the primary incident wave is acting on the plasma, and solve for higher-order secondary scattered waves. Similarly, we can also solve for the secondary waves starting with the primary reflected wave only, i.e., with $A_0 = 0$. Then, finally, adding the two results, we get the complete solution. Let us denote by A_m^i and B_m^i the mth-order secondary quantities related to

the incident and reflected waves respectively scattered by the primary reflected wave. If we assume that the plasma is slowly varying only in the region $z' \leq z \leq z''$, then we can assign the following boundary conditions:

$$A_m^i = 0, \quad z < z',$$
$$B_m^i = 0, \quad z > z''. \tag{A9}$$

This means that, in the uniform region $z < z'$, there is no secondary incident wave, and, in the uniform region $z > z''$, there is no secondary reflected wave. In (A9), m is any positive integer and further

$$A_0^i \neq 0, \quad B_0^r \neq 0,$$
$$A_0^r = 0, \quad B_0^i = 0.$$

If the unbounded medium is throughout slowly varying then $z' = -\infty$ and $z'' = \infty$.

We have calculated A_1^i, A_1^r, B_1^i, B_1^r, and B_1^i. They have the values

$$A_1^i = -A_0 i \int_{z'}^{z} p\, dz,$$

$$A_1^r = -B_0 i \int_{z}^{z} p \exp\left(2i \int_0^z K_1\, dz\right),$$

$$B_1^i = A_0 i \int_{z'}^{z} p \exp\left(-2i \int_0^z K_1\, dz\right) dz,$$

$$B_1^r = B_0 i \int_0^z p\, dz,$$

$$\frac{A_2^i}{A_0} = -\int_{z'}^{z} p(z_1) \int_{z'}^{z} p(z_2)\, dz_1\, dz_2$$
$$+ \int_{z'}^{z} p(z_1) \exp\left(2i \int_0^{z'} K_1\, dz\right)$$
$$\times \int_{z'}^{z_1} p(z_2) \exp\left(-2i \int_0^z K_1\, dz\right) dz_1\, dz_2,$$

where

$$A_0 \equiv A_0^i \quad \text{and} \quad B_0 \equiv B_0^i.$$

By repeated application of these formulas we can derive explicit expressions for A_m^i, B_m^i, etc., in the form of m-fold integrals. An mth-order quantity would be expressed in terms of one of the two primary quantities A_0 and B_0 and m-fold integrals, whose variables of integration may be denoted by z_1, $z_2, \cdots, z_m$. As is evident from the evaluation of the second-order quantity A_2^i above, the limits of integration involve all these variables except z_m-, the last of the sequence. Each of these m-fold integrals represents the field contributions of a scattered wave that originated as a result of m-successive transmissions and reflections at levels which are the limits of integration.

[1] D. A. Tidman, Phys. Rev. **117**, 366 (1960).
[2] A. A. Vlasov, *Teoria Mnogikh Chastits* (Gos. Tekh. Izd., Moscow, 1950).
[3] K. H. Dunphy, D. Kahn, and D. Mintzer, Phys. Fluids **10**, 162, (1967).
[4] A. H. Kritz and D. Mintzer, Phys. Rev. **117**, 382 (1960).
[5] B. Chakraborty, Vestn. Mosk. Univ., Ser. III, Fiz. Astron. 30 (1966).
[6] A. Dolinsky and R. Goldman, Phys. Fluids **10**, 1250 (1967).
[7] A. M. Fedorchenko, Sov. Phys. Tech. Phys. **11**, 992 (1967).
[8] J. R. Wait, *Electromagnetic Waves in Stratified Media* (Pergamon, New York, 1962).
[9] K. G. Budden, *Radio Waves in the Ionosphere* (Cambridge U.P., New York, 1961).
[10] T. H. Stix, *The Theory of Plasma Waves* (McGraw-Hill, New York, 1962).
[11] L. M. Brekhovskikh, *Waves in Layered Media* (Academic, New York, 1960).
[12] V. L. Ginzburg, *Propagation of Electromagnetic Waves in Plasmas* (Gordon and Breach, New York, 1961).
[13] W. P. Allis, S. J. Buchsbaum, and A. Bers, *Waves in Anisotropic Plasmas* (M.I.T. Press, Cambridge, Mass., 1963).
[14] K.-M. Chen, Radio Sci. **69D**, 235 (1965).
[15] H. L. Berk, C. W. Horton, M. N. Rosenbluth, and R. N. Sudan, Phys. Fluids **10**, 2003 (1967).
[16] J. F. Denisse and J. L. Delroix, *Plasma Waves* (Interscience, New York, 1963).
[17] H. Bremmer, Physica **15**, 593 (1949).
[18] H. Bremmer, *Handbuch der Physik*, Vol. 16, 423 (1958).
[19] H. Bremmer, *Terrestial Radio Waves* (Elsevier, New York, 1949).
[20] See Ref. 8, Chap. V, and Ref. 9, Chap. 9.
[21] J. Heading, *An Introduction to Phase-Integral Methods* (Methuen, London, 1962).
[22] (a) N. Froman and P. O. Froman, *JWKB Approximation Contribution to the Theory* (North-Holland, Amsterdam, 1965). (b) F. W. Sluijter, J. Math. Anal. Appl. **27**, 282 (1969).
[23] See Eq. (17) of Ref. 17.
[24] See Eqs. (6) of Ref. 17.

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Multipole Moments. II. Curved Space

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Multipole moments are defined for static, asymptotically flat, source-free solutions of Einstein's equations. The definition is completely coordinate independent. We take one of the 3-surfaces V, orthogonal to the timelike Killing vector, and add to it a single point Λ at infinity. The resulting space inherits a conformal structure from V. The multipole moments of the solution emerge as a collection of totally symmetric, trace-free tensors P, P_a, P_{ab}, $\cdots$ at Λ. These tensors are obtained as certain combinations of the derivatives of the norm of the timelike Killing vector. (For static space-times, this norm plays the role of a "Newtonian gravitational potential.") The formalism is shown to yield the usual multipole moments for a solution of Laplace's equation in flat space, the dependence of these moments on the choice of origin being reflected in the conformal behavior of the P's. As an example, the moments of the Weyl solutions are discussed.

1. INTRODUCTION

The purpose of this paper is to define the multipole moments of static, asymptotically flat solutions of Einstein's equations.

Perhaps the most important application of our definition arises from the fact that the multipole moments of a space-time can serve as a guide to its physical interpretation. It has been a recurring problem in general relativity to interpret the exact solutions—to somehow extract physical content from a metric written in some coordinate system. The multipole moments obtained here (in a manifestly coordinate-independent way) furnish a new tool for attacking this problem. For example, having once associated with a given solution of Einstein's equations a set of multipole moments, we may proceed to construct the Newtonian gravitational field having the same moments. It would be hard to imagine a more satisfactory situation than this: We have a precise Newtonian analog of each static solution.

Consider the Weyl solutions[1,2] (the class of static, axially symmetric, source-free solutions of Einstein's equations). Certainly one of the Weyl solutions must be spherically symmetric (the Schwarzschild solution) —but which one? To construct a Weyl solution, one begins with some function α satisfying Laplace's equation in Euclidean 3-space. The Schwarzschild solution, however, corresponds to a rather complicated α (not a monopole). Using multipole moments, on the other hand, one picks out the Schwarzschild solution simply by asking for that Weyl solution whose only nonvanishing moment is the monopole. The Weyl solution corresponding to a monopole α turns out to have quadrupole as well as higher moments. The point is that, although the function α serves as a convenient label for the various Weyl solutions, α by itself has very little physical significance. The classification of Weyl solutions by their multipole moments is both coordinate independent and physically meaningful.

It is not immediately obvious that it should be possible, in curved space, to find quantities which can be interpreted as multipole moments. We might expect the curvature to have a tendency to mix together the different multipoles. As we approach infinity, the curvature, and with it this mixing effect, becomes less and less. The question is, how quickly must the curvature fall off at infinity in order that individual, pure multipoles can be identified there? It turns out, fortunately, that all static solutions which one would want to call asymptotically flat are "sufficiently asymptotically flat" to have well-defined multipole moments.

One normally thinks of multipole moments of a field in connection with the multipole expansion of that field. But such an expansion is appropriate only when the field in question satisfies a linear equation, while Einstein's equations are not at all linear. Is it not unreasonable, therefore, to discuss solutions of Einstein's equations in terms of multipole moments? In Newtonian gravitation, of course, the multipole moments have a number of equivalent interpretations, e.g., as coefficients in a multipole expansion, as moments of the source distribution, or as objects associated with the conformal group.[3] It appears to be quite difficult to generalize the first two interpretations to curved space. For example, a fundamental theorem concerning expansions—that to essentially any given set of moments there corresponds a solution of the equations—is not obvious in general relativity (although it is probably true). We shall approach multipole moments from the point of view of the conformal group. The multipole moments in Newtonian gravitation were discussed from this standpoint in Ref. 3. The moments were interpreted as multilinear mappings on the space of conformal

Killing vectors. In curved space there will, in general, be no conformal Killing vectors. However, we will still be able to recover multipole moments at infinity as objects acting on "asymptotic conformal Killing vectors."

Consider a source-free solution of Einstein's equations which is static, that is, which has a hypersurface-orthogonal, timelike Killing vector t^a. Let V denote a 3-surface orthogonal to t^a, h_{ab} the (positive-definite) induced metric on V, and D_a the covariant derivative on V (with respect to h_{ab}). Set $\psi = (-t^a t_a)^{\frac{1}{2}} - 1$. Then the Einstein equations on the 4-dimensional space–time reduce to the equations[4]

$$D^a D_a \psi = 0,$$
$$\mathcal{R}_{ab} = (1 + \psi)^{-1} D_a D_b \psi \qquad (1)$$

on V, where $\mathcal{R}_{ab}$ is the Ricci tensor of V.[5] Conversely, a 3-manifold V with positive-definite metric h_{ab} and scalar field ψ (> -1), subject to (1), defines a static solution of Einstein's equations.

It is well known that ψ plays the role of a "Newtonian gravitational potential." For example, a timelike geodesic in the 4-dimensional space–time, when projected into V, defines a curve whose acceleration is essentially the gradient of ψ. We shall take the "multipole moments" of a static solution in general relativity to mean the moments of the corresponding ψ. Thus, we have only to define the moments of a solution of Laplace's equation in a certain curved, positive-definite, 3-space.

Before defining multipole moments, we must introduce a suitable notion of asymptotic flatness. This is done in Sec. 2. The space V, h_{ab} is said to be asymptotically flat if it is possible to add to V a single point Λ "at infinity" such that the resulting space $\tilde{V}$ inherits appropriate conformal structure from V. Asymptotic properties of V and of fields on V may now be treated as local properties at Λ. The conformal behavior of a field and its equation thus plays a significant role in the asymptotic description of the field. The utility of this approach to asymptotic properties rests on the assertion that all conformally invariant constructions in $\tilde{V}$ are meaningful in terms of V. To prove this fact, we must show that $\tilde{V}$, $\tilde{h}_{ab}$ is unique, given V, h_{ab}. This uniqueness is established in the Appendix.

The multipole moments are defined in Sec. 3. "Asymptotic conformal Killing vectors" are introduced as certain combinations of tensors at Λ. Then the multipole moments, as multilinear mappings on such objects, can also be represented as tensors. We obtain in this way a collection P, P_a, P_{ab}, $\cdots$ of totally symmetric, trace-free tensors at Λ. Alternatively, these tensors can be obtained directly by assigning ψ conformal weight $-\frac{1}{2}$ and taking certain combinations of the derivatives of $\tilde{\psi}$ at Λ. The behavior of the usual multipole moments in flat space under change in the choice of origin is reflected in the present formalism in the conformal behavior of the P's.

The multipole moments of the Weyl solutions are discussed in Sec. 4. We first show that the Weyl metrics are asymptotically flat in the sense of Sec. 2. We then set up the general equations for the multipole moments of these solutions, and evaluate the first few moments explicitly.

A number of further ideas and conjectures concerning multipole moments in general relativity are introduced in Sec. 5.

2. ASYMPTOTIC FLATNESS

In this section we shall give a definition of asymptotic flatness for a 3-dimensional manifold V with positive-definite metric h_{ab}. One could approach such a definition by introducing certain coordinate systems which are to be "asymptotically Euclidean" in some appropriate sense. For example, one might say that V, h_{ab} is asymptotically flat if there exist coordinates x, y, and z with respect to which (i) the components of h_{ab} approach the unit matrix to order r^{-1} ($r^2 = x^2 + y^2 + z^2$) and (ii) the (coordinate) derivatives of these components approach zero to order r^{-2}.

Unfortunately, definitions along these lines are subject to a number of serious disadvantages. In formulating a statement concerning asymptotic behavior, one would like to be sure that he is describing a property of the space itself or of certain fields on that space and not of his particular system of coordinates. Thus, a definition of asymptotic flatness in terms of coordinates is of very little use without a complete analysis of the freedom available in the choice of permissible coordinates. Any conclusion which is drawn in one coordinate system must then be checked to ensure that the same conclusion follows in every permissible set of asymptotically Euclidean coordinates. The important feature of a given set of coordinates is their asymptotic behavior, not their precise values in V. The coordinates themselves thus contain a great deal of extra information which is irrelevant to their primary purpose: to fix the asymptotic structure of the space. To introduce a large, essentially unphysical, "gauge group" in this way makes the coordinate formalism more complicated and less natural than one would like. Furthermore, in order to formulate asymptotic statements about

fields, it is normally necessary to take limits (as $r \to \infty$) of the components of the fields and their derivatives. While such a procedure is certainly permissible from a mathematical viewpoint, it is rather awkward to be forced always to speak in terms of limits.

Fortunately, there is an alternative approach to asymptotic structure—an approach which completely avoids the shortcomings associated with coordinates. The idea is to attach an additional "point at infinity" Λ to the manifold V. Asymptotic properties of any field on V are then described in terms of the local behavior of the field at Λ. This is the approach which was used, for example, by Penrose[6] in his treatment of asymptotically flat space-times. We shall proceed in a similar way for the case of a 3-dimensional manifold with positive-definite metric.

In order to get an idea of what is involved in the introduction of a point at infinity, we begin with the example of flat 3-space. Choose coordinates x, y, and z with respect to which the metric takes the form $ds^2 = dx^2 + dy^2 + dz^2$. We now introduce new coordinates

$$\bar{x} = \frac{x}{x^2 + y^2 + z^2}, \quad \bar{y} = \frac{y}{x^2 + y^2 + z^2},$$
$$\bar{z} = \frac{z}{x^2 + y^2 + z^2}. \tag{2}$$

[The barred coordinates (2) are valid everywhere on V except at the origin.] Our metric may be written in the form

$$ds^2 = (\bar{x}^2 + \bar{y}^2 + \bar{z}^2)^{-2}(d\bar{x}^2 + d\bar{y}^2 + d\bar{z}^2). \tag{3}$$

We now require that $\bar{x}$, $\bar{y}$, and $\bar{z}$ be "good coordinates" at infinity. That is, we attach to V a single point Λ, with coordinate values $\bar{x} = \bar{y} = \bar{z} = 0$, and define the topology and differentiable structure there by insisting that $\bar{x}$, $\bar{y}$, and $\bar{z}$ define a coordinate neighborhood of Λ. The resulting manifold—consisting of V plus this point Λ at infinity—will be denoted by $\tilde{V}$. In this example, $\tilde{V}$ is topologically a 3-dimensional sphere. The metric (3) on V does not carry over smoothly to a metric on $\tilde{V}$; i.e., h_{ab} becomes singular at Λ. This is not true, however, of the conformal metric. That is,

$$\tilde{h}_{ab} = \Omega^2 h_{ab} \tag{4}$$

is smooth at Λ, where we have set[7]

$$\Omega = (\bar{x}^2 + \bar{y}^2 + \bar{z}^2) = (x^2 + y^2 + z^2)^{-1}.$$

Note that, in order that $\tilde{h}_{ab}$ be regular and nonzero at Λ, we had to choose the conformal factor in (4) to go to zero like r^{-2} at infinity. This asymptotic behavior may be characterized in the following way: we require that Ω and its derivative vanish at Λ, and that the second derivative[8] of Ω be a multiple of $\tilde{h}_{ab}$ at Λ.

We now formulate a general definition of asymptotic flatness for the curved case. Let V be a 3-dimensional manifold with positive-definite metric h_{ab}. We first require that there be a manifold $\tilde{V}$ consisting of V plus one additional point Λ. We next require that there be a metric $\tilde{h}_{ab}$ which is defined, smooth, and positive-definite everywhere on $\tilde{V}$. On V (considered as a subset of $\tilde{V}$), we further require that $\tilde{h}_{ab} = \Omega^2 h_{ab}$, where Ω is a conformal factor which is defined and C^2 everywhere on $\tilde{V}$.[9] Our discussion of flat space now suggests the additional conditions to be imposed in Ω. Firstly, asymptotic flatness of V should mean that "infinity is far away," i.e., that Ω is zero at Λ. Secondly, we should like to ensure that Ω goes to zero "like r^{-2}." We therefore require that $\tilde{D}_a\Omega = 0$ and that $\tilde{D}_a\tilde{D}_b\Omega$ be a multiple of $\tilde{h}_{ab}$ at Λ.[9]

To summarize, V, h_{ab} is said to be *asymptotically flat* if there is a manifold $\tilde{V}$ with C^∞, positive-definite metric $\tilde{h}_{ab}$ such that:

(1) $\tilde{V}$ consists of V plus one additional point Λ.

(2) On V, $\tilde{h}_{ab} = \Omega^2 h_{ab}$, where Ω is a C^2 scalar field defined on $\tilde{V}$.

(3) At Λ, $\Omega = 0$, $\tilde{D}_a\Omega = 0$, and $\tilde{D}_a\tilde{D}_b\Omega$ is a multiple of $\tilde{h}^9_{ab}$.

The question now arises as to whether our definition of asymptotic flatness is a reasonable one. Can we be sure that the class of spaces admitted by the definition consists precisely of those one would intuitively think of as being asymptotically flat? Firstly, we shall see shortly that the conditions listed above are just those needed to define multipole moments. While this argument is far from conclusive, one would certainly not expect to be able to define multipole moments in a space which is not asymptotically flat in some sense. Stronger evidence comes from the Weyl solutions. We shall show in Sec. 4 that all Weyl solutions whose "source" lies in a compact region (spatially) are asymptotically flat by our definition. Here, then, is a very large class of exact solutions which satisfy the definition. Finally, from experience with solutions of elliptic equations, it is perhaps reasonable to suppose that a static solution of Einstein's equations will either be asymptotically flat as above or else will not even faintly resemble an asymptotically flat space.[10]

As a second aspect of this question of suitability of the definition, one might ask whether $\tilde{V}$ is unique (as a conformal space), given V. This is a very important question, for we should like to be sure that,

when speaking in terms of $\tilde{V}$, we are truly describing the space–time itself and not some aspect of freedom in the construction of $\tilde{V}$.[11] The differentiable structure of $\tilde{V}$, for example, serves to determine which sets of coordinates are "good" in a neighborhood of Λ and, therefore, which coordinates on V are to be considered as "asymptotically Euclidean."[12] The differentiable structure of $\tilde{V}$ at Λ thus represents an extremely important aspect of the asymptotic structure of V. But what if this differentiable structure were not unique? The asymptotic structure of V would not then have been properly incorporated into $\tilde{V}$. In fact, such problems will not arise, for, whenever $\tilde{V}$ exists, it is unique: A proof is given in the Appendix. This appendix also contains a construction (although a rather impractical one) for obtaining $\tilde{V}$ from V.

3. MULTIPOLE MOMENTS AS TENSORS AT Λ

As discussed in Sec. 1, a static, source-free solution of Einstein's equations can be represented as a 3-dimensional manifold V with a positive-definite metric h_{ab} and a scalar field ψ (> -1), subject to the Eqs. (1). We may interpret the first Eq. (1) as representing Laplace's equation for the "Newtonian" gravitational potential. Suppose now that V, h_{ab} is asymptotically flat in the sense of Sec. 2. We might then expect that the multipole moments of our static space–time—if they can be defined at all—would appear in the asymptotic behavior of ψ, i.e., in the behavior of ψ in a neighborhood of Λ. The multipole moments will be introduced in this section: they will emerge as a collection of totally symmetric, trace-free tensors at Λ.

The tensors P, P_a, P_{ab}, $\cdots$ are defined by Eq. (20). It is not immediately clear, however, why these tensors should be taken as representing multipole moments in general relativity. We shall first show, therefore, how (20) arises naturally in the one case—flat space—in which we already know what multipole moments mean.

Let $D^a D_a \psi = 0$ in flat 3-space.[13] The multipole moments of ψ were interpreted in Ref. 3 as certain multilinear mappings on the conformal Killing vectors,[14] these mappings defined as follows. For each s ($= 0, 1, \cdots$), set

$$R_s = (4\pi)^{-1} \int_K (D_m D_{a_1} \cdots D_{a_s} \psi) \xi^{a_1} \cdots \xi^{a_s} \, dS^m, \quad (5)$$

where ξ^a is a conformal Killing vector and K is a 2-dimensional surface (topologically, a 2-sphere) which surrounds the sources. Note that, since the integrand in (5) is divergence-free, R_s is independent of the choice of K. The quantity R_s completely determines the 2^s moment of ψ.

The idea is to interpret the integral (5) as a tensor at Λ. This is done by rewriting the integrand in terms of quantities appropriate to $\tilde{V}$. The metric on $\tilde{V}$ is $\tilde{h}_{ab} = \Omega^2 h_{ab}$. We choose for the conformal factor that introduced in Sec. 2, i.e., we set $\Omega = r^{-2}$, where r is the distance from an origin O. It then follows that[15]

$$\tilde{D}_a \tilde{D}_b \Omega = 2\tilde{h}_{ab}. \quad (6)$$

[In particular, (6) implies that $\tilde{V}$, $\tilde{h}_{ab}$ is also flat.] The integral (5) may now be written in the form

$$R_s = (4\pi)^{-1}(s+1)! \sum_{r=0}^{s+1} \frac{2^{-r}(2s+1)\cdots(2s-2r+3)}{r!\,(s-r+1)!} \times \int_K \mathcal{C}[(\tilde{D}_{a_1}\Omega)\cdots(\tilde{D}_{a_r}\Omega)(\tilde{D}_{a_{r+1}}\cdots\tilde{D}_{a_{s+1}}\tilde{\psi})] \times \xi^{a_1}\cdots\xi^{a_s}\, dS^{a_{s+1}}, \quad (7)$$

where we have defined $\tilde{\psi} = \Omega^{-\frac{1}{2}}\psi$, and where $\mathcal{C}$ denotes the operation "symmetrize over all free indices and take the trace-free part." It is not difficult to evaluate (7) explicitly for the special case in which $\tilde{D}_a \xi^b = 0$, i.e., when ξ^a is a translation on $\tilde{V}$.[16] The result is

$$R_s = \sigma_s (\tilde{D}_{a_1}\cdots\tilde{D}_{a_s}\tilde{\psi})\xi^{a_1}\cdots\xi^{a_s}\big|_\Lambda, \quad (8)$$

where σ_s is a certain (rather complicated) function of the integer s.

To summarize, if ξ^a is a conformal Killing vector on V which reduces to a translation on $\tilde{V}$, then, provided Ω satisfies (6), the integral (5) reduces to (8).

Why do we single out the translations on $\tilde{V}$? The answer lies in the relation between the data[17] at the origin O and the data at Λ for a fixed conformal Killing vector ξ^a on V. The passage from O to Λ (with the accompanying conformal transformation) effectively reverses the roles of ξ^a and k_a. That is to say, a translation on $\tilde{V}$, i.e., with data at Λ of the form $(\xi^a, 0, 0, 0)$, is a conformal Killing vector on V whose data at the origin is $(0, 0, 0, k_a)$. But the 2^s moment about the origin is defined[3] by the property that, for the conformal Killing vector ξ^a whose data at O is $(0, 0, 0, k_a)$,

$$R_s = (12)^s Q^{a_1\cdots a_s} k_{a_1}\cdots k_{a_s}. \quad (9)$$

We conclude that the multipole moments of ψ are completely described by the collection

$$P_{a_1\cdots a_s} = \tilde{D}_{a_1}\cdots\tilde{D}_{a_s}\tilde{\psi}, \quad s = 0, 1, \cdots, \quad (10)$$

of totally symmetric tensors at Λ.[18] Furthermore, it follows, from the flatness of $\tilde{h}_{ab}$ and from the invariance of Laplace's equation under our conformal transformation, that $P_{a_1\cdots a_s}$ is trace-free.

One can, of course, obtain the expressions (10) directly. In terms of a Cartesian coordinate system x^a, $a = 1, 2, 3$, a quadrupole field about the origin, for example, takes the form

$$\psi = r^{-5} Q_{ab} x^a x^b, \tag{11}$$

where Q_{ab} is a symmetric, trace-free, 3×3 matrix and $r^2 = h_{ab} x^a x^b$. An appropriate set of coordinates in a neighborhood of Λ is $\bar{x}^a = r^{-2} x^a$ [c.f. Eq. (2)]. Then, setting $\Omega = r^{-2}$, we have $\tilde{\psi} = \Omega^{-\frac{1}{2}} \psi = Q_{ab} \bar{x}^a \bar{x}^b$, and so

$$P_{ab} = \tilde{D}_a \tilde{D}_b \tilde{\psi} = 2 Q_{ab}. \tag{12}$$

That is to say, P_{ab} represents the quadrupole moment about the origin.

In the discussion above, we were concerned with the moments about a particular origin O. This choice of origin was reflected in $\tilde{V}$ by our particular conformal factor Ω. We now consider what happens to the moments when the origin is permitted to change. Let O' by a new origin, and let the corresponding conformal factor be

$$\Omega' = \Omega \omega. \tag{13}$$

It is convenient to consider first the case in which $\omega - 1$ is infinitesimal: arbitrary conformal transformations can then be built up by successive application of infinitesimal ones. This restriction amounts to letting O' differ only infinitesimally from O. With the conformal factor Ω', Eq. (10) becomes

$$P'_{a_1 \cdots a_s} = P_{a_1 \cdots a_s} - \tfrac{1}{2} s(2s-1) \mathcal{T}[P_{a_1 \cdots a_{s-1}} \tilde{D}_{a_s} \omega], \tag{14}$$

where we have used the fact [which follows from (6)] that $\omega = 1$ at Λ. That is to say, under an infinitesimal conformal transformation, the 2^s moment is altered by an amount depending only on the 2^{s-1} moment. This, of course, corresponds precisely to the behavior of the usual multipole moments in their dependence on the origin. The values of the quadrupole moment about two nearby origins, for example, differ by an amount depending only on the dipole moment. (See Ref. 3.)

To summarize, the multipole moments of a solution of Laplace's equation in flat 3-space are characterized by a collection (10) of totally symmetric, trace-free tensors at Λ. The dependence of the usual moments on the choice of origin is reflected, in the present formalism, by the conformal behavior (14) of the P's.

We proceed to generalize these considerations to curved space. Assume we are given a solution ψ of[19]

$$D^a D_a \psi - \tfrac{1}{8} \mathcal{R} \psi = 0, \tag{15}$$

such that ψ vanishes at infinity. [Note, in particular, that (1) implies (15).] In flat space, we could think of the multipole moments of ψ as multilinear mappings on conformal Killing vectors. In a general curved space, on the other hand, we would not expect there to exist any conformal Killing vectors at all. We might hope, however, that the multipole moments could be interpreted as mappings on "asymptotic" conformal Killing vectors of some sort. How would one define an asymptotic conformal Killing vector? One possible definition would be as a set of data[17] at Λ, that is, as a 4-tuple $(\xi^a, F_{ab}, \varphi, k_a)$ consisting of a vector, a skew tensor, a scalar, and a vector at Λ. (In flat space, there is a one-to-point correspondence between such 4-tuples at a point and conformal Killing vectors on the space.[3]) But the multilinear mappings on sets of data at Λ can always be represented as tensors at Λ: in flat space, these tensors are precisely the $P_{a_1 \cdots a_s}$ of (10). Thus, even in curved space, we might expect to be able to define multipole moments by some formula analogous to (10).

In flat space, we were able to severely restrict our choice of conformal factor by requiring that $\tilde{h}_{ab}$ be flat in a neighborhood of Λ, i.e., by imposing (6). While we shall continue to impose this condition *at* Λ (in order to normalize Ω), it will no longer be possible to have (6) hold in a neighborhood of Λ. Thus, we cannot simply take (10) as the multipole moments in curved space, for these tensors will, in general, be neither totally symmetric nor trace-free. Furthermore, even the totally symmetric and trace-free part of (10) will not do, for these will not have the behavior (14) under conformal transformations. It is crucial for their interpretation that the moments of different rank be properly related to each other under infinitesimal conformal transformations.

Let us suppose for the moment that we have solved our problem up to and including order r. That is, assume we have obtained a collection $P, P_a, P_{ab}, \cdots, P_{a_1 \cdots a_r}$ of tensors which are totally symmetric, trace-free, and which satisfy

$$P'_{a_1 \cdots a_s} = \omega^{-\frac{1}{2}} P_{a_1 \cdots a_s} - \tfrac{1}{2} s(2s-1) \omega^{-\frac{3}{2}} \mathcal{T}[P_{a_1 \cdots a_{s-1}} \tilde{D}_{a_s} \omega] \tag{16}$$

under the infinitesimal conformal transformation (13). [Note that (16) reduces to (14) at Λ.] Our preliminary candidate for $P_{a_1 \cdots a_{r+1}}$ is

$$T_{a_1 \cdots a_{r+1}} = \mathcal{T} \tilde{D}_{a_1} P_{a_2 \cdots a_{r+1}}. \tag{17}$$

But $T_{a_1 \cdots a_{r+1}}$ does not have the correct behavior (16) under the conformal transformation (13). Instead,

we have

$$T'_{a_1\cdots a_{r+1}} = \omega^{-\frac{1}{2}}T_{a_1\cdots a_{r+1}} - \tfrac{1}{2}(4r+1)\omega^{-\frac{3}{2}}\mathcal{C}[P_{a_1\cdots a_r}\tilde{D}_{a_{r+1}}\omega] - \tfrac{1}{2}r(2r-1)\omega^{-\frac{3}{2}}\mathcal{C}[(\tilde{D}_{a_1}P_{a_2\cdots a_r})\tilde{D}_{a_{r+1}}\omega] - \tfrac{1}{2}r(2r-1)\omega^{-\frac{3}{2}}\mathcal{C}[P_{a_1\cdots a_{r-1}}\tilde{D}_{a_r}\tilde{D}_{a_{r+1}}\omega]. \quad (18)$$

The idea is to introduce into (17) additional terms involving the Ricci tensor in order to cancel out terms involving the second derivatives of ω in (18). We have for the Ricci tensor, under (13),

$$\tilde{\mathcal{R}}'_{ab} = \tilde{\mathcal{R}}_{ab} - \omega^{-1}\tilde{D}_a\tilde{D}_b\omega - \omega^{-1}\tilde{h}_{ab}(\tilde{D}^m\tilde{D}_m\omega) \quad (19)$$

to first order, From (18) and (19), we see that $P_{a_1\cdots a_{r+1}}$ will satisfy (16) provided

$$P_{a_1\cdots a_{s+1}} = \mathcal{C}[\tilde{D}_{a_1}P_{a_2\cdots a_{s+1}} - \tfrac{1}{2}s(2s-1)\tilde{\mathcal{R}}_{a_1a_2}P_{a_3\cdots a_{s+1}}] \quad (20)$$

for *both* $s = r$ and $s = r-1$. Note that we should not have been able to achieve this result were the coefficients in (18) changed. It is precisely the coefficients which appear there which allow us to collect terms of the type (20) to obtain (16).

We now define our multipole tensors by induction. Set $P = \tilde{\psi}$ $(= \Omega^{-\frac{1}{2}}\psi)$, and define $P_{a_1\cdots a_{s+1}}$ from $P_{a_1\cdots a_s}$ by (20). The resulting sequence of tensors, evaluated at Λ, defines the multipole moments of the solution ψ of (15).[20] Under infinitesimal conformal transformations, these tensors satisfy (14).

Finally, we remark that the operation of "going to the center of mass" has an analog in the present formulation. If the monopole P is nonzero, we may define

$$\mathfrak{I}_{a_1\cdots a_s} = P_{a_1\cdots a_s} + \mathcal{C}\sum_{r=0}^{s-1}\frac{s!}{r!\,(s-r)}(2s-1)(2s-3)\cdots \times (2r+1)(-P)^{r-s}P_{a_1\cdots a_r}P_{a_{r+1}}\cdots P_{a_s}. \quad (21)$$

It follows immediately from (16) that the $\mathfrak{I}_{a_1\cdots a_s}$ are conformally invariant tensors at Λ. [We have, effectively, used the dipole moment to cancel out the first derivative of ω in (16). Compare, Ref. 3.] In particular, $\mathfrak{I}_a = 0$, i.e., the dipole moment about the center of mass vanishes.

4. MULTIPOLE MOMENTS OF THE WEYL SOLUTIONS

In this section we shall apply the techniques developed in Secs. 2 and 3 to the class of asymptotically flat, static, axially symmetric solutions of Einstein's equations. These solutions may be described as follows.[1,2] Let α be any axially symmetric solution of Laplace's equation in Euclidean 3-space such that α vanishes at infinity.[21] That is, in cylindrical coordinates z, r, θ, we have

$$\partial_r\partial_r\alpha + r^{-1}\partial_r\alpha + \partial_z\partial_z\alpha = 0, \qquad \partial_\theta\alpha = 0. \quad (22)$$

The next step is to solve

$$\partial_r\beta = r[(\partial_r\alpha)^2 - (\partial_z\alpha)^2], \quad \partial_z\beta = 2r(\partial_r\alpha)(\partial_z\alpha), \quad \partial_\theta\beta = 0 \quad (23)$$

for β, subject to $\beta \to 0$ at infinity. [The integrability conditions for (23) are (22).] Then the spatial metric for a Weyl solution is

$$ds^2 = e^{2(\beta-\alpha)}(dr^2 + dz^2) + r^2e^{-2\alpha}\,d\theta^2 \quad (24)$$

with potential $\psi = e^\alpha - 1$. Note that each Weyl solution is completely and uniquely determined by some solution (α) of Laplace's equation in flat space. The problem of describing the multipole moments reduces, therefore, to the following: Given the multipole moments of α (in flat space), determine those of the corresponding Weyl solution. It is to be expected that the two sets of moments will not be identical.

We shall first show that the Weyl solutions described above are all asymptotically flat in the sense of Sec. 2. We then set up the equations giving the multipole moments of a Weyl solution in terms of those of its α. Finally, we evaluate the first few moments explicitly.

We must first re-express the Weyl solutions in terms of a set of coordinates which are applicable in a neighborhood of Λ. Set

$$\rho^2 = r^2 + z^2, \quad \bar{r} = \rho^{-2}r, \quad \bar{\rho}^2 = \rho^{-2}, \quad \bar{z} = \rho^{-2}z. \quad (25)$$

Then, defining $\tilde{\alpha} = \rho^{-1}\alpha$, we see that (22) becomes

$$\partial_{\bar{r}}\partial_{\bar{r}}\tilde{\alpha} + \bar{r}^{-1}\partial_{\bar{r}}\tilde{\alpha} + \partial_{\bar{z}}\partial_{\bar{z}}\tilde{\alpha} = 0. \quad (26)$$

The multipole moments of α are, as described in Sec. 3, the derivatives of $\tilde{\alpha}$ at Λ. (These tensors, which will be written $P^{(\alpha)}$, $P^{(\alpha)}_a, \cdots$, are automatically totally symmetric and trace free.) Expressed in terms of the coordinates (25), Eq. (23) for β takes the form

$$\partial_{\bar{r}}\beta = -\bar{r}[(\tilde{\alpha} + \bar{r}\partial_{\bar{r}}\tilde{\alpha} + \bar{z}\partial_{\bar{z}}\tilde{\alpha})^2 - (\bar{r}\partial_{\bar{z}}\tilde{\alpha} - \bar{z}\partial_{\bar{r}}\tilde{\alpha})^2], \quad \partial_{\bar{z}}\beta = -2\bar{r}[(\tilde{\alpha} + \bar{r}\partial_{\bar{r}}\tilde{\alpha} + \bar{z}\partial_{\bar{z}}\tilde{\alpha})(\bar{r}\partial_{\bar{z}}\tilde{\alpha} - \bar{z}\partial_{\bar{r}}\tilde{\alpha})]. \quad (27)$$

Finally, choosing for the conformal factor $\Omega = \rho^{-2}e^{\alpha-\beta}$, we see that the metric in a neighborhood of Λ is

$$d\bar{s}^2 = d\bar{r}^2 + d\bar{z}^2 + \bar{r}^2e^{-2\beta}\,d\theta^2, \quad (28)$$

and

$$\tilde{\psi} = 2\bar{\rho}^{-1}e^{\frac{1}{2}\beta}\sinh(\tfrac{1}{2}\tilde{\alpha}\bar{\rho}). \quad (29)$$

The situation may now be summarized as follows. Choose any solution $\tilde{\alpha}$ of (26) which vanishes at Λ ($\tilde{r} = \tilde{z} = 0$). This $\tilde{\alpha}$ is completely determined by its derivatives, $P^{(\alpha)}$, $P^{(\alpha)}_a$, $\cdots$, at Λ. Solve (27) for β, subject to $\beta = 0$ at Λ. Then we get the multipole moments of the Weyl solution from Eq. (20), using the $\tilde{\psi}$ of (29) and the metric of (28). We thus obtain expressions for the $P_{a_1 \cdots a_s}$ in terms of the $P^{(\alpha)}_{a_1 \cdots a_s}$.

It is now clear that the Weyl solutions are asymptotically flat. The differentiable structure of $\tilde{V}$ in a neighborhood of Λ is defined by the coordinates $\tilde{r}$, $\tilde{z}$, and θ. Since $\tilde{\alpha}$ satisfies Laplace's equation, $\tilde{\alpha}$ is C^∞ in a neighborhood of Λ. The smoothness of the metric $\tilde{h}_{ab}$ and of $\tilde{\psi}$ then follow (this despite the factor $\tilde{\rho}^{-1}$ in the latter). Note, however, that the conformal factor Ω is in general only C^2.

Using the prescription above, we may calculate any multipole moment of any Weyl solution.[22] For example, the first three moments of the general solution are

$$\begin{aligned} P &= P^{(\alpha)}, \\ P_a &= P^{(\alpha)}_a, \\ P_{ab} &= P^{(\alpha)}_{ab} + \tfrac{1}{8}(P^{(\alpha)})^3(\zeta_a\zeta_b - \tfrac{1}{3}\tilde{h}_{ab}), \end{aligned} \tag{30}$$

where ζ_a denotes the unit vector, at Λ, directed along the symmetry axis. We see that the monopole and dipole moments of the Weyl solutions are the same as those of α: The first correction terms appear in the quadrupole moment. This situation continues into the higher moments: The multipole moment $P_{a_1 \cdots a_s}$ depends only on the $P^{(\alpha)}$ of lower rank.

For which Weyl solution do all the moments higher than the monopole vanish? We see already from (30) that we cannot simply choose a monopole α, for the corresponding Weyl solution has a nonvanishing quadrupole moment. In fact, the α which results in the Schwarzschild solution is well known: We must choose for α the potential of a uniform rod whose length is related in a certain way to its mass density. With this choice, all the multipole moments—with the exception of the monopole—must vanish. (It appears, unfortunately, that it would have been difficult to discover this particular α through multipole moments.)

5. CONCLUSIONS

In this section we discuss a number of open questions and possible further developments concerning multipole moments in general relativity.

To what extent are the static space-times characterized by their multipole moments? In Newtonian gravitation, for example, the exterior field is uniquely determined by its moments. We might expect a similar situation in general relativity. More precisely, we may formulate

Conjecture 1: Two static solutions of Einstein's equations having identical multipole moments coincide, at least in some neighborhood of Λ.

We might also ask whether or not there are any special restrictions on the multipole moments in general relativity. Of course, the moments are not completely arbitrary, for, even in Newtonian gravitation, the 2^s moment cannot grow too fast with s without destroying the convergence of the multipole expansion.[23] However, this very weak condition is the only one required in Newtonian gravitation. We might expect, therefore,

Conjecture 2: Given any set of multipole moments, subject to the appropriate convergence condition, there exists a static solution of Einstein's equations having precisely those moments.[24]

One possible source of evidence on these conjectures is the Weyl solutions discussed in Sec. 4. Unfortunately, although we gave in that section the prescription for obtaining any multipole moment of any Weyl solution, we were unable to display an explicit formula for the general moment. Such a formula (which could, perhaps, be guessed after working out the first five or six moments explicitly) would be of great value. It could be expected not only to provide new insight into the Weyl solutions, but also to increase our confidence in (or else disprove) the conjectures above.

Can our definition of moments in the static case be extended to more general situations, for example, to stationary space-times? We would expect in this case to obtain two sets of moments: one to represent the "mass distribution" (analogous to the moments in the static case) and another to represent the "angular-momentum distribution." One would thus look for two solutions of (15)—but on what manifold? We require some 3-dimensional manifold to replace the surface (V) orthogonal to the timelike Killing vector in the static case. Fortunately, there is such an object: the 3-manifold of all trajectories of the Killing vector.[25] The equations of a stationary solution then take the form

$$\begin{aligned} \mathcal{R}_{ab} &= 2(1+\psi)^{-4}[(D_a\omega)(D_b\omega) - h_{ab}(D^m\omega)(D_m\omega)] \\ &\qquad + (1+\psi)^{-1}D_aD_b\psi, \\ D^mD_m\psi &= -2(1+\psi)^{-3}(D^m\omega)(D_m\omega), \\ D^mD_m\omega &= 3(1+\psi)^{-1}(D^m\omega)(D_m\psi), \end{aligned} \tag{31}$$

where ω represents the twist of the timelike Killing vector. One would now like to describe the moments of ψ and ω separately. Unfortunately, neither of these fields satisfy the conformally invariant Laplace equation (15). There may, nontheless, be some hope of obtaining multipole moments in the stationary case. The only point at which we used (15) in the static case was to ensure that, when ψ is assigned conformal weight $-\frac{1}{2}$, $\tilde{\psi}$ will be smooth at Λ. Perhaps there is some way to establish the necessary smoothness, in the stationary case, from (31). [*Note added in proof:* For the case of the Kerr metric, although $\tilde{h}_{ab}$ is smooth at Λ, neither $\tilde{\psi}$ nor $\tilde{\omega}$ $(= \Omega^{-\frac{1}{2}}\omega)$ is smooth there.]

One might be still more ambitious and attempt to define the multipole moments in space-times having no Killing vectors. The moments could perhaps be defined in terms of the asymptotic behavior of a set of initial data (on a spacelike 3-surface) for the solution.[26] We would certainly demand that the moments be independent of the choice of surface—in particular, that they be constant under the time-evolution of the system. (Multipole radiation would be registered on each successive 3-surface—i.e., it could not escape between different surfaces—and so would not be expected to produce changes in the moments.) On the other hand, if one wanted to define multipoles which would change with time, the appropriate definition might involve the asymptotic field at null infinity. A definition of this type has been discussed by Janis and Newman.[24] It would be interesting, in particular, to know whether their definition coincides with ours in the static case.

In Newtonian gravitation, there is a relation between the multipole moments of the field and the matter distribution which is responsible for the field: there are formulas for the moments as integrals over the matter. Do analogous formulas exist also in general relativity? (These might involve, for example, the mass integrals discussed by Dixon.[27]) This question appears to be very difficult. The moments are described at infinity—as far from the matter as possible. It is hard to see how this information could be faithfully brought in from infinity over the curved space in order to compare it locally with the matter distribution.

APPENDIX: THE UNIQUENESS OF $\tilde{V}$

Let V, h_{ab} be an asymptotically flat 3-space. Is the corresponding "conformally completed space" $\tilde{V}$, $\tilde{h}_{ab}$ unique? It is crucial for our treatment of asymptotic flatness that the answer be yes. Otherwise, the description of asymptotic structure in terms of $\tilde{V}$, $\tilde{h}_{ab}$ might well represent merely a description of our particular choice of $\tilde{V}$ rather than some aspect of the space V itself. We shall show that, if $\tilde{V}$, $\tilde{h}_{ab}$ and $\tilde{\tilde{V}}$, $\tilde{\tilde{h}}_{ab}$ both satisfy the conditions of Sec. 2, then there is a smooth mapping (with smooth inverse) from $\tilde{V}$ to $\tilde{\tilde{V}}$ which (i) reduces to the identity on V, and (ii) maps $\tilde{h}_{ab}$ to $\tilde{\tilde{h}}_{ab}$, up to a (strictly positive) conformal factor. The idea of the proof is to construct $\tilde{V}$, $\tilde{h}_{ab}$ explicitly from V, h_{ab}.

The construction of $\tilde{V}$ as a point set is easy: $\tilde{V} = V \cup \Lambda$, where Λ is an abstract point. Furthermore, there is no difficulty in assigning a topology to $\tilde{V}$: The topology on V is the usual manifold topology, while a neighborhood of Λ is to consist of Λ along with an open subset of V whose boundary is compact.[28]

It is a more difficult problem to define the differentiable structure of $\tilde{V}$. Just as topological structure on a manifold can be specified by the selection of the functions to be called "continuous" from among all functions on the point set, so the differentiable structure can be specified by the selection of the functions to be called "smooth" from among all continuous functions.[29] We must find these smooth functions. The first step in this program is to identify a suitable candidate for Ω. A conformal factor can be obtained as follows. We have seen in Sec. 3 that, if

$$(D^m D_m - \tfrac{1}{8}\mathcal{R})\varphi = 0, \tag{A1}$$

then $\tilde{\varphi} = \Omega^{-\frac{1}{2}}\varphi$ satisfies

$$(\tilde{D}^m \tilde{D}_m - \tfrac{1}{8}\tilde{\mathcal{R}})\tilde{\varphi} = 0. \tag{A2}$$

Let us suppose for the moment that we had found a suitable Ω. Let φ be any solution of (A1) which vanishes at Λ and which has a nonzero monopole moment. Then $\tilde{\varphi}$ satisfies (A2) and is therefore smooth on V. Furthermore, $\tilde{\varphi}$ does not vanish at Λ. That is to say, Ω and φ^2 differ by a factor which is smooth and nonzero in a neighborhood of Λ. We now have an intrinsic way of selecting a conformal factor: Set $\Omega = \varphi^2$ in a neighborhood of Λ, where φ is a solution of (A1) which vanishes at Λ and has nonzero monopole.[30]

Using our Ω, we are able to write down a large class of functions which are smooth at Λ: If ψ satisfies (A1) and vanishes at Λ, then $\tilde{\psi} = \Omega^{-\frac{1}{2}}\psi$ satisfies (A2) and is finite at Λ and, therefore, regular at Λ. Observe, furthermore, that any smooth function on $\tilde{V}$ has the properties: (i) It is smooth on V, and (ii) it can be written, in some neighborhood of Λ, as a C^∞ function of functions in the above class. We have thus identified the collection of all smooth functions on $\tilde{V}$, and so have defined the differentiable structure of $\tilde{V}$.

Finally, since the tensor field $\tilde{h}_{ab}$ is smooth on V, it can be extended to $\tilde{V}$ (i.e., defined at Λ so that the result is smooth everywhere on $\tilde{V}$) in at most one way.

Having constructed from V, h_{ab} the point set $\tilde{V}$, along with its topology, differentiable structure, and conformal metric, we conclude that $\tilde{V}$, $\tilde{h}_{ab}$ are unique whenever they exist.

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[1] H. Weyl, Ann. Physik **54**, 117 (1917).

[2] J. L. Synge, *Relativity: The General Theory* (North-Holland, Amsterdam, 1964), p. 312.

[3] R. Geroch, J. Math. Phys. **11**, 1955 (1970).

[4] See, for example, J. Ehlers and W. Kundt, in *Gravitation*, Ed. L. Witten, (Wiley, New York, 1962), p. 49.

[5] Our convention for the Ricci tensor is $\mathcal{R}_{ab} = \mathcal{R}^{m}{}_{amb}$, where $\mathcal{R}_{abcd}$ is defined by the condition that, for any vector field k_a, $D_{[a}D_{b]}k_c = \frac{1}{2}\mathcal{R}_{abcd}k^d$.

[6] R. Penrose, Proc. Roy. Soc. (London) **A284**, 159 (1965). In this case, "infinity" was a 3-surface rather than a point.

[7] This particular conformal factor becomes infinite at the origin. Such behavior has been permitted at this stage only to simplify the discussion—it is not at all necessary. For example, we could have set $\Omega = (x^2 + y^2 + z^2 + 1)^{-1}$ in. (4), in which case $\tilde{h}_{ab}$ would have been regular everywhere on $\tilde{V}$.

[8] Note that, when the gradient of Ω vanishes at Λ, the tensor $\tilde{D}_a\tilde{D}_b\Omega$ at Λ is independent of the choice of derivative operator $\tilde{D}_a$.

[9] While we shall require that $\tilde{h}_{ab}$ be C^∞ on V, it turns out that we must permit Ω to be only C^2 at Λ. As we shall see in the case of the Weyl solutions, the discontinuity at Λ in the third derivative of Ω essentially determines the mass of the system.

[10] For example, a solution of Laplace's equation in flat space is either very well-behaved at infinity or else divergent there.

[11] A similar point arises in the 4-dimensional case. See R. Geroch, J. Math. Phys. **9**, 450 (1968).

[12] The advantage of going to $\tilde{V}$ is, in this language, that the freedom to change from one set of asymptotically Euclidean coordinates to another is thereby put on the same footing as the freedom to change coordinates at any other point of $\tilde{V}$. We are thus able to bring the standard (coordinate-free) techniques of differential geometry to bear on asymptotic problems.

[13] That is to say, we preserve the first Eq. (1), but break the coupling between the curvature and ψ represented by the second equation.

[14] A vector field ξ^a is said to be a *conformal Killing vector* if $D_{(a}\xi_{b)} = \frac{1}{3}h_{ab}(D_m\xi^m)$.

[15] $\tilde{D}_a$ denotes the derivative operator on $\tilde{V}$ with respect to $\tilde{h}_{ab}$.

[16] Note that, although conformal Killing vectors remain conformal Killing vectors under conformal transformations, translations do not in general remain translations.

[17] The *data* for the conformal Killing vector ξ^a at a point p is defined as the values, at p, of the four tensors $(\xi^a, F_{ab}, \varphi, k_a) = (\xi^a, D_{[a}\xi_{b]}, \frac{1}{3}D_m\xi^m, \frac{1}{3}D_aD_m\xi^m)$. This information uniquely determines ξ^a everywhere. See Ref. 3.

[18] Alternatively, the multipole moments may be represented as a collection Q, Q^a, $Q^{ab}, \cdots$ of conformal Killing tensors on V (Ref. 3). The expressions (10) then represent the data, at Λ, for these fields.

[19] Equation (15) is conformally invariant, provided ψ is assigned conformal weight $-\frac{1}{2}$.

[20] Note that the only place in the argument we have used the fact that ψ satisfies (15) is to ensure that $\tilde{\psi}$ will be infinitely differentiable on $\tilde{V}$.

[21] We must, of course, permit α to have singularities in V.

[22] Of course, because of the axial symmetry, each moment $P_{a_1}\cdots a_{a_s}$ must be a multiple of $\mathcal{C}\zeta_{a_1}\cdots\zeta_{a_s}$, where ζ_a is a unit vector at Λ directed along the symmetry axis.

[23] The appropriate condition on the multipole moments is essentially the same as that for the convergence of a power series. See, for example, C. Goffman and G. Pedrick, *Functional Analysis* (Prentice-Hall, Princeton, N.J., 1965), p. 223.

[24] Compare, A. Janis and E. T. Newman, J. Math. Phys. **34**, 317 (1964).

[25] J. Ehlers, Ph.D. thesis, University of Hamburg, 1957; R. Geroch, *New Solutions of Einstein's Equations* (to be published).

[26] This program has actually been carried out in one case: that of the monopole moment. (It turns out to be essentially the discontinuity, at Λ, in the third derivative of Ω.) See, for example, D. Brill, in *Les théories relativistes de la gravitation* (Centre National de la Recherche Scientifique. Paris, 1962), p. 147.

[27] G. Dixon, Nuovo Cimento **34**, 317 (1964). See also B. Tulczyjew and W. Tulczyjew, in *Recent Developments in General Relativity* (Pergamon, New York, 1962), p. 465.

[28] If V has a "hole in the middle" which represents a singularity, then the open sets with compact boundary must first be divided into two classes, those which represent neighborhoods of Λ and those which represent neighborhoods of the singularity. See R. Geroch, *The Many-Point Compactification, Proceedings of the American Mathematical Society* (submitted for publication).

[29] See, for example, K. Nomizu, *Lie Groups and Differential Geometry* (Herald Printing, Tokyo, 1956), p. 1.

[30] It is not difficult to give an intrinsic criterion for whether a solution of (A1) has a nonvanishing monopole moment. For example, the monopole is nonzero provided ψ does not change sign in some neighborhood of Λ.

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Theory of Electrodynamics in Media in Noninertial Frames and Applications*

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The theory of local electrodynamics of media in given noninertial frames, within the Maxwell–Einstein theory, is constructed in terms of local observable EM fields and physical media parameters of its comoving frame. Localization of tensors to observables for and their relations among observers in different frames are introduced; local and global constitutive tensors and local Maxwell equations are obtained and interpreted. Also, a Lagrangian formulation for both lossless and lossy media is constructed, and boundary conditions, local conservation laws, and energy tensors are obtained. The applications concern linear accelerational and rotational media in flat space–time for which local Maxwell equations in comoving frames are obtained. Then an EM wave propagating in the direction of acceleration is studied in the accelerating frame. The first-order propagation shows a frequency shift and amplitude change which have very simple physical significances of instantaneous Doppler shift and photon density in media and which agree with familiar results in the vacuum limit. A particle model for this wave shows that the "mass-dressed" photon is dragged by the medium and does not follow a geodesic path. In the case of a rotating medium, a plane wave scattered by a rotating sphere is solved by an integral iteration method in the laboratory frame. The scattered field which is associated only with the rotation of the medium is separated from the Mie scattering. Its first-order amplitudes are found for incidences perpendicular and parallel to the rotation axis. Particular symmetry and shapes of scattering amplitude in the results agree with intuition and resemble radiation patterns of appropriately induced traveling electric and magnetic dipole sheaths.

1. INTRODUCTION

The theory and application of the electrodynamics of media in inertial and noninertial motions have been the subject of the recent interest of many authors,[1–8] but a complete theory has not been formulated. The purpose of this work is to construct directly a local electrodynamics, within the Maxwell–Einstein classical field theory,[9–12] in terms of the observable EM fields and the rest-frame physical constitutive properties of a medium in a noninertial frame. This noninertialness may be produced either by noninertial motion in flat space–time or by the presence of tidal gravitation. Then application to simple problems in flat space–time is examined.

For a simple medium moving with uniform velocity, Lee and Papas[1,4] recently found the time-harmonic Green's function and showed that dipole radiation in it has a forward-tilted far-zone Poynting vector. The time-dependent Green's functions have been obtained by other workers.[2,3] More studies[5,13] deal with different theoretical approaches and applications. The theory used is Maxwell's theory together with special relativity.

For media in noninertial frames, less work has been done.[5–9] Since macroscopic "photons" do not follow null paths nor geodesics in this case, in order to get any information concerning EM phenomena, we must start from Maxwell's equations. Two problems then arise which were not encountered in the previous study of inertial motions. The first concerns the EM fields, which are physically observable to observers in a noninertial frame and how it enters into the postulated covariant equations which govern the EM field space–time evolution. The second concerns a covariant formalism of the constitutive relations of the macroscopic media, which can only be determined locally in the medium comoving frame and which should be built into the field equations.

In the first case, Einstein's tetrad physics and the covariance principle in GRT are used to obtain a relation

$$ {}_{[1]}e^{\alpha}{}_{(\lambda)}\Lambda^{(\lambda)}{}_{(\bar{\delta})}\,{}_{[2]}e^{(\bar{\delta})}{}_{\beta}\frac{\partial x^{\beta}}{\partial x^{\gamma}} = \delta^{\alpha}{}_{\gamma}, \tag{1.1} $$

which reduces the tensor transform $\partial x^{\beta}/\partial x^{\gamma}$ to the instantaneous Lorentz transform $\Lambda^{(\lambda)}{}_{(\bar{\delta})}$, for those observables whose observers are in different frames $\{x^{\mu}\}$ and $\{x^{\bar{\mu}}\}$, by the localization transforms ${}_{[1]}e_{(\alpha)}{}^{\beta}$ and ${}_{[2]}e_{(\bar{\alpha})}{}^{\bar{\beta}}$. Equation (1.1) explicitly states the form in which physical observables, whose measurements locally in GRT are identical with those of SRT, combine with the noninertialness of the frame and/or space–time to put the laws of physics in a covariant form. This relation and the localization transform are

useful, especially when one is interested in local physics, e.g., electrodynamics in media. The general local Maxwell equations are obtained later; these equations also show the extent of the approximation in using the usual 3-vector Maxwell equations for a neighborhood of noninertial space–time.

In the second case, based on a covariance assumption for EM equations in media, a constitutive tensor expressed by the 4-velocity $\hat{v}$ and the rest-frame local properties $\epsilon^{(i)}{}_{(j)}$, $K^{(i)}{}_{(j)}$ of a linear medium is constructed for the first time:

$$C^{\mu\nu\alpha\beta} = \tfrac{1}{2}K_{\gamma\delta}({}^*v)^{\mu\nu\gamma}({}^*v)^{\alpha\beta\delta} + \tfrac{1}{2}[v^\alpha(\epsilon^{\nu\beta}v^\mu - \epsilon^{\mu\beta}v^\nu) - v^\beta(\epsilon^{\nu\alpha}v^\mu - \epsilon^{\mu\alpha}v^\nu)], \quad (1.2)$$

such that $G^{\mu\nu} = C^{\mu\nu\alpha\beta}F_{\alpha\beta}$. Previous confusion[5–7] in not distinguishing physical observables from their tensors, which also led to a misinterpretation of the $C^{\mu\nu\alpha\beta}$ as physical properties of media, are all cleared up. With this covariant formalism to build the constitutive parameters of media into EM theory, we also find the Lagrangian formulations for the lossless and lossy media, local boundary conditions, local conservation laws, and energy–momentum tensor.

In the latter part of this work (Secs. 5 and 6), applications to motions of media in flat space–time, such as uniform linear (hyperbolic) acceleration and steady rotation, are considered. For both cases, exact local Maxwell equations in comoving frames are found. In the rotational case, the error in a previous work[8] is corrected. Special problems are then solved in detail.

In a uniform linearly accelerated simple medium, the EM wave propagating along the direction of acceleration is studied by comoving observers. The first-order solution gives two terms that correspond to traveling against and traveling with the apparent gravitation in that frame. A frequency shift and amplitude decrease (or increase) result for this first-order propagation and have the simple meanings of equivalent gravitational red (or blue) shift and instantaneous "photon" density. The coordinate phase velocity is time dependent. If we identify the instantaneous frequency and phase velocity of the wave as energy and velocity of the corresponding "mass-dressed" photon,[14] then the photon has a time-dependent mass and does not follow a geodesic. Physically, this means photons are dragged by the noninertial motion of the medium.

In the rotational case, a plane wave scattered by a rotating simple sphere is studied by using integral iteration method in the laboratory frame. The scattered field purely due to the rotation of the medium is separated from the Mie scattering.[15] This is the only scattering, provided that the rotating medium is the same as its surrounding medium. The first-order amplitude of this rotational scattered field is evaluated and plotted for incidences perpendicular and parallel to the axis of rotation. Particular symmetry and the shapes of scattering amplitude result; they agree with intuition and resemble the radiation patterns of appropriately induced traveling electric and magnetic dipole sheaths.

In the following section, Eq. (1.1) for frame comoving observers introduces localization. In Sec. 3, we give the constitutive tensor. In Sec. 4, we derive the general local Maxwell equations, least-action formalism, and boundary conditions, and we investigate local conservation laws and the energy–momentum tensor. In Sec. 5, there is the application to linear accelerated media, whereas in Sec. 6, there is the application to steady rotating media. Appendices contain remarks and some derivations; also, geometrized units $c = 1$, $k = 1$, and $G = 1$ are used for convenience.[16]

2. LOCAL PHYSICAL TENSOR OF FRAME COMOVING OBSERVERS AND THEIR TRANSFORMS

A. Reviews and Coordinate-Basis Vectors

Consider a 4-dimensional differentiable manifold S_4 labeled with the permissible coordinate frame $\{x^\mu\}$ which represents a space–time continuum. An affine-connected geometry is constructed in the usual way.[17] We define the parallel transport of vectors by a set of affine numbers $\Gamma^\mu{}_{\alpha\beta}$, and then define the geodesic as a path generated by the parallel transport dx^μ. We define the geometrical scalar distance $ds^2 = g_{\mu\nu}\,dx^\mu\,dx^\nu$ between neighboring points by a symmetric metric tensor $g_{\mu\nu}$ and define the path of extreme length by $\delta\int ds = 0$. Finally, we identify the path of extreme length with the geodesic.[18] The geometry thus constructed is identified with the space–time of physics by the postulate that free-falling neutral particles follow a geodesic.

Now, at a space–time point P, the coordinate contravariant and covariant basis vectors $\{\hat{\mathbf{e}}_\mu\}$ and $\{\hat{\mathbf{e}}^\mu\}$ of $\{x^\mu\}$ are defined by[19]

$$d\hat{\mathbf{x}} \equiv dx^\mu\hat{\mathbf{e}}_\mu \equiv dx_\mu\hat{\mathbf{e}}^\mu, \quad \mu = 0, 1, 2, 3, \quad (2.1)$$

where the dx^μ are infinitesimal coordinate increments of x^μ at P and $dx_\mu \equiv g_{\mu\nu}\,dx^\nu$. Then the scalar length

$dx^2 \equiv d\hat{\mathbf{x}}^\nu \cdot d\hat{\mathbf{x}}$ implies that

$$\hat{\mathbf{e}}_\mu \cdot \hat{\mathbf{e}}_\nu = g_{\mu\nu}, \quad \hat{\mathbf{e}}^\mu \cdot \hat{\mathbf{e}}_\nu = \delta^\mu{}_\nu, \quad \hat{\mathbf{e}}^\mu \cdot \hat{\mathbf{e}}^\nu = g^{\mu\nu}. \quad (2.2)$$

Thus, $\hat{\mathbf{e}}_\mu$ is a vector with length $|g_{\mu\mu}|^{\frac{1}{2}}$, pointing in the tangent direction of x^μ for $\{x^\mu\}$ at P, and $\hat{\mathbf{e}}^\mu$ is a vector with length $|g^{\mu\mu}|^{\frac{1}{2}}$, which is perpendicular to the constant x^μ hypersurface. From (2.1), we have that

$$\hat{\mathbf{e}}_\mu = \frac{\partial x^{\bar{\alpha}}}{\partial x^\mu}\hat{\mathbf{e}}_{\bar{\alpha}} \quad \text{and} \quad \hat{\mathbf{e}}^\mu = \frac{\partial x^\mu}{\partial x^{\bar{\alpha}}}\hat{\mathbf{e}}^{\bar{\alpha}} \quad (2.3)$$

relate the basis vectors for different $\{x^\mu\}$ and $\{x^{\bar{\mu}}\}$ at the same point P.

Similarly to (2.1), any vector field $\hat{\mathbf{V}}$ at P can now be expressed as

$$\hat{\mathbf{V}} \equiv V^\mu \hat{\mathbf{e}}_\mu \equiv V_\mu \hat{\mathbf{e}}^\mu. \quad (2.4)$$

Then (2.2) implies that

$$V^\mu = \hat{\mathbf{V}} \cdot \hat{\mathbf{e}}^\mu, \quad V_\mu = \hat{\mathbf{V}} \cdot \hat{\mathbf{e}}_\mu, \quad (2.5)$$

and (2.3) implies that

$$V^\mu = \frac{\partial x^\mu}{\partial x^{\bar{\alpha}}} V^{\bar{\alpha}}, \quad V_\mu = \frac{\partial x^{\bar{\alpha}}}{\partial x^\mu} V_{\bar{\alpha}}. \quad (2.6)$$

Thus, contravariant and covariant vectors are actually components of a vector on the respective coordinate basis. The above equations apply to tensors of higher rank, just with more indices written, e.g.,

$$\hat{\mathbf{T}} = T^{\mu\nu\alpha}\hat{\mathbf{e}}_\mu\hat{\mathbf{e}}_\nu\hat{\mathbf{e}}_\alpha, \quad T^{\mu\nu\alpha} = \hat{\mathbf{e}}^\alpha\hat{\mathbf{e}}^\nu\hat{\mathbf{e}}^\mu \cdots \hat{\mathbf{T}}, \quad \text{etc.} \quad (2.7)$$

B. Localization of Tensors to Observables for Frame Comoving Observers

Consider temporarily a flat space-time described by an inertial Minkowskian $\{X^{\bar{\mu}}\}$ and a noninertial $\{x^\mu\}$. Consider one observer $\{O\}$ in $\{x^\mu\}$ with world lines $\{\Gamma\} \equiv \{x^i = \text{fixed}, x^0 \text{ varies}\}$ passing an inertial $\bar{O}$ of $\{X^{\bar{\mu}}\}$ momentarily at P. From the equivalence principle, a vector $d\hat{\mathbf{x}}$ observed by $\bar{O}$ as $dX^{\bar{\mu}}$ will be observed by O as

$$dx^{(\mu)} \equiv dX^{\mu'} = \Lambda^{\mu'}{}_{\bar{\alpha}}\frac{\partial X^{\bar{\alpha}}}{\partial x^\lambda}dx^\lambda \equiv \Lambda^{(\mu)}{}_{\bar{\alpha}}\frac{\partial X^{\bar{\alpha}}}{\partial x^\lambda}dx^\lambda, \quad (2.8)$$

where $dX^{\mu'}$ is the value of $d\hat{\mathbf{x}}$ observed by O' who is comoving with O at P on his Minkowskian basis $\{\hat{\mathbf{e}}_{\mu'}\}$[19] which is related to the $\{\hat{\mathbf{e}}_{\bar{\mu}}\}$ of $\bar{O}$ by a Lorentz transform $\Lambda^{\mu'}{}_{\bar{\alpha}}$. Identifying locally the $\{\hat{\mathbf{e}}_{\mu'}\}$ as the physical tetrad basis vectors $\{\hat{\mathbf{e}}_{(\mu)}\}$ of O such that $d\hat{\mathbf{x}} = dx^{(\mu)}\hat{\mathbf{e}}_{(\mu)}$ gives

$$\hat{\mathbf{e}}_{(\mu)} \cdot \hat{\mathbf{e}}_{(\nu)} = \eta_{\mu\nu}, \quad e^{(\mu)} \cdot \hat{\mathbf{e}}_{(\nu)} = \delta^\mu{}_\nu, \quad e^{(\mu)} \cdot \hat{\mathbf{e}}^{(\nu)} = \eta^{\mu\nu}. \quad (2.9)$$

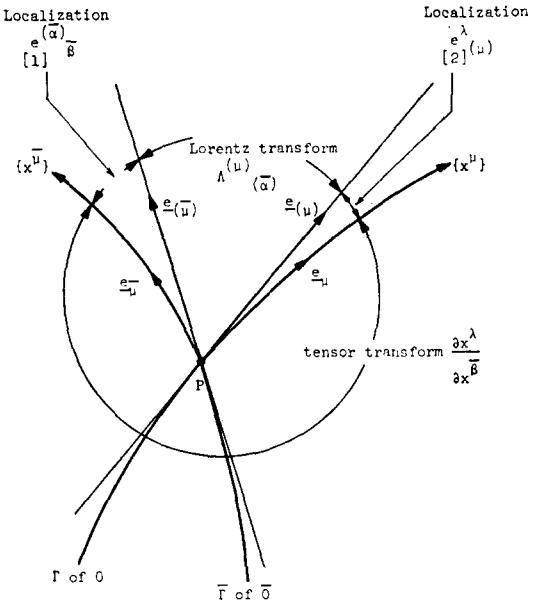


FIG. 1. A sketch of (2.13). Γ and $\bar{\Gamma}$ are world lines of O and $\bar{O}$ which comove in $\{x^\mu\}$ and $\{x^{\bar{\mu}}\}$, respectively.

Now we can rewrite (2.8) and define localization $e^{(\mu)}_\lambda$ by

$$dx^{(\mu)} = e^{(\mu)}{}_\lambda\, dx^\lambda, \quad e^{(\mu)}{}_\lambda \equiv \Lambda^{(\mu)}{}_{\bar{\alpha}}\frac{\partial X^{\bar{\alpha}}}{\partial x^\lambda} \quad (2.10)$$

and, with (2.1) and (2.2), we have

$$e^{(\mu)}{}_\lambda = \hat{\mathbf{e}}^{(\mu)} \cdot \hat{\mathbf{e}}_\lambda, \quad e^{(\mu)\lambda} = \hat{\mathbf{e}}^{(\mu)} \cdot \hat{\mathbf{e}}^\lambda, \quad e_{(\mu)\lambda} = \hat{\mathbf{e}}_{(\mu)} \cdot \hat{\mathbf{e}}_\lambda,$$
$$e_{(\mu)}{}^\lambda = \hat{\mathbf{e}}_{(\mu)} \cdot \hat{\mathbf{e}}^\lambda. \quad (2.11)$$

Thus, we see that to physically observe a vector or tensor quantity by $\{O\}$ in $\{x^\mu\}$ is to observe its local components as (2.10) on a local Minkowskian basis $\{\hat{\mathbf{e}}_{(\mu)}\}$ of $\{O\}$. But this local result also applies to $\bar{O}$ in $\{X^{\bar{\mu}}\}$; thus, we do not require that $\{X^{\bar{\mu}}\}$ be an inertial frame, i.e., the space-time need not be flat. Thus, in general, (2.10) becomes

$$dx^{(\mu)} = {}_{[2]}e^{(\mu)}{}_\lambda\, dx^\lambda, \quad dx^{(\bar{\mu})} = {}_{[2]}e^{(\bar{\mu})}{}_{\bar{\lambda}}\, dx^{\bar{\lambda}}, \quad (2.12a)$$
$$dx^\lambda = {}_{[2]}e^\lambda{}_{(\mu)}\, dx^{(\mu)}, \quad dx^{\bar{\lambda}} = {}_{[2]}e^{\bar{\lambda}}{}_{(\bar{\mu})}\, dx^{(\bar{\mu})}, \quad (2.12b)$$

and

$$\delta^\gamma{}_\lambda = {}_{[1]}e^\gamma{}_{(\mu)}\Lambda^{(\mu)}{}_{(\bar{\alpha})}\,{}_{[2]}e^{(\bar{\alpha})}{}_\beta\frac{\partial x^\beta}{\partial x^\lambda} \quad (2.13)$$

for arbitrary $\{x^\mu\}$ and $\{x^{\bar{\mu}}\}$ frames for the comoving observers $\{O\}$ and $\{\bar{O}\}$ with physical tetrad bases $\{{}_{[1]}\hat{\mathbf{e}}_{(\mu)}\}$ and $\{{}_{[2]}\hat{\mathbf{e}}_{(\bar{\mu})}\}$, respectively. Equations (2.12) and (2.13) explicitly state that measurements in general relativity are locally identical as in special relativity and localize tensor transforms among different frames to be instantaneous local Lorentz transforms for physically observable values of that tensor. These relations are graphically represented by Fig. 1. They

are especially useful when local physics is emphasized, e.g., electrodynamics in media, because with them we can avoid tensors and talk only about local observables which are the quantities of eventual physical interest.

For observations by the $\{O\}$ on any $\hat{\mathbf{V}}$ or higher-rank tensors, relations similar to (2.12) apply, as in (2.5) and (2.7) with $\hat{\mathbf{e}}_\mu$ replaced by $\hat{\mathbf{e}}_{(\mu)}$.

C. Coordinate Transport of Comoving Basis

To find the physical tetrad basis $\{\hat{\mathbf{e}}_{(\mu)}\}$ and the appropriate way that they are carried along by $\{O\}$ comoving in $\{x^\mu\}$ with velocity $\hat{\mathbf{u}}$, we first set

$$\hat{\mathbf{e}}_{(0)} = (g_{00})^{-\frac{1}{2}}\hat{\mathbf{e}}_0 \equiv \hat{\mathbf{u}}, \tag{2.14}$$

since the observer's proper-time lapse during dx^0 is $d\tau = (g_{00})^{\frac{1}{2}}\,dx^0$, i.e., the local proper-time direction for $\{O\}$ is the coordinate-time direction there, only rescaled by a factor of $(g_{00})^{-\frac{1}{2}}$. Since the local spatial basis vectors $\{\hat{\mathbf{e}}_{(i)}\}$ must be orthogonal to $\hat{\mathbf{e}}_{(0)}$ and are orthonormalized among themselves for convenience, they are only defined within a spatial rotation; thus, within (2.9),[20]

$$\{\hat{\mathbf{e}}_{(i)}\} = \text{O.N.}\,\{\hat{\mathbf{d}}_i \equiv \hat{\mathbf{e}}_i - (g_{0i}/g_{00})\hat{\mathbf{e}}_0\}, \tag{2.15}$$

where the $\hat{\mathbf{d}}_i$ are just the time-orthogonalized coordinate triads.

Now (2.14) specified $\hat{\mathbf{e}}_{(0)}$, but (2.15) left free the ways in which $\{0\}$ can carry $\{\hat{\mathbf{e}}_{(i)}\}$ along $\{\Gamma\}$. But, in order to have simple formalism for local physics, the medium-fixed observers should also keep their $\{\hat{\mathbf{e}}_{(i)}\}$, as a whole, not rotating with respect to the medium. Thus, the simple Fermi transport of $\{\hat{\mathbf{e}}_{(i)}\}$, which preserves the $\{\hat{\mathbf{e}}_{(\mu)}\}$ but fixes the $\{\hat{\mathbf{e}}_{(i)}\}$ directions with respect to distant stars, is not convenient. A study of the local geometry reveals that, for an $\{x^\mu\}$ with

$$(\hat{\mathbf{d}}_i \cdot \hat{\mathbf{d}}_j)^2/(\hat{\mathbf{d}}_i \cdot \hat{\mathbf{d}}_i)(\hat{\mathbf{d}}_j \cdot \hat{\mathbf{d}}_j) \text{ time independent}, \tag{2.16}$$

neighboring frame-comoving observers will not see each other's rotation if $\{\hat{\mathbf{e}}_{(i)}\}$ is carried along $\{\Gamma\}$ of $\{O\}$ by

$$\{\hat{\mathbf{e}}_{(i)}\} = \text{O.N.}\{\hat{\mathbf{n}}_i\}, \text{ with time-independent coefficients and Eq. (2.11)}, \tag{2.17}$$

where the $\{\hat{\mathbf{n}}_i\}$ are just the Frenet–Serret normals to $\{\Gamma\}$[21]:

$$\begin{aligned} D\hat{\mathbf{u}}/Ds &\equiv a_1\hat{\mathbf{n}}_1, \\ D\hat{\mathbf{n}}_1/Ds &\equiv a_1\hat{\mathbf{u}} + a_2\hat{\mathbf{n}}_2, \\ D\hat{\mathbf{n}}_2/Ds &\equiv -a_2\hat{\mathbf{n}}_1 + a_3\hat{\mathbf{n}}_3, \quad \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_i \equiv -1, \end{aligned} \tag{2.18}$$

along Γ. Thus, the observers attached to the frame which is comoving with the medium should coordinate transport $\{\hat{\mathbf{e}}_{(i)}\}$ according to (2.17), so as to have a locally nonrotating spatial triad with respect to each other. By (2.13), the coefficients in (2.17) can be chosen to make $\{\hat{\mathbf{e}}_{(\mu)}\}$ the instantaneous Lorentz transform of the $\{\hat{\mathbf{e}}_{(\bar{\mu})}\}$ of some frame $\{x^{\bar{\mu}}\}$ which has a particularly simple geometry although it may not comove with the medium.

If (2.16) does not hold in $\{x^\mu\}$, then this frame $\{x^\mu\}$ is not "locally rigid," e.g., $u^{\bar{i}}/u^{\bar{0}}$ is position dependent for an $\{x^\mu\}$ moving in an inertial $\{X^{\bar{\mu}}\}$. Then it is impossible to have any orthogonal $\{\hat{\mathbf{e}}_{(i)}\}$ for $\{O\}$ in $\{x^\mu\}$ which also hold unrotated with respect to their neighbors in $\{x^\mu\}$. In this case, we still coordinate transport $\{\hat{\mathbf{e}}_{(i)}\}$ according to (2.17) to keep it orthonormal and the least locally rotated.

3. ELECTROMAGNETIC CONSTITUTIVE TENSORS OF MEDIA

From the covariance postulate of macroscopic Maxwell equations in media, we found[22] that the constitutive tensor for a linear medium with 4-velocity $\hat{\mathbf{v}}$ was

$$\begin{aligned} G^{\mu\nu} &= C^{\mu\nu\alpha\beta}F_{\alpha\beta}, \\ C^{\mu\nu\alpha\beta} &= \tfrac{1}{2}K_{\gamma\delta}(^*v)^{\mu\nu\gamma}(^*v)^{\alpha\beta\delta} + \tfrac{1}{2}[v^\alpha(\epsilon^{\nu\beta}v^\mu - \epsilon^{\mu\beta}v^\nu) \\ &\quad - v^\beta(\epsilon^{\nu\alpha}v^\mu - \epsilon^{\mu\alpha}v^\nu)], \end{aligned} \tag{3.1}$$

whose physical meaning is revealed by its local form

$$G^{(\mu)(\nu)} = C^{(\mu)(\nu)(\alpha)(\beta)}F_{(\alpha)(\beta)}. \tag{3.2}$$

Here, the local components of $\hat{\mathbf{K}}$ and $\hat{\boldsymbol{\epsilon}}$ on a coordinate-transported physical tetrad $\{\hat{\mathbf{e}}_{(\mu)}\}$ in the *frame comoving with the medium* have the values

$$\begin{aligned} &\epsilon^{(i)}{}_{(0)} \equiv 0, \quad \epsilon^{(0)}{}_{(i)} \equiv 0, \quad K^{(i)}{}_{(0)} \equiv 0, \quad K^{(0)}{}_{(i)} \equiv 0, \\ &\epsilon^{(0)}{}_{(0)} = \tfrac{1}{3}\sum_{i=1}^{3}\epsilon^{(i)}{}_{(i)}, \quad K^{(0)}{}_{(0)} \equiv \tfrac{1}{3}\sum_{i=1}^{3}K^{(i)}{}_{(i)}. \end{aligned} \tag{3.3}$$

$\epsilon^{(i)}{}_{(j)}$ and $K^{(i)}{}_{(j)}$ with respect to $\{O\}$ in that frame have the physical meaning

$$D^{(i)} = \epsilon^{(i)}{}_{(j)}E^{(j)}, \quad H^{(i)} = K^{(i)}{}_{(j)}B^{(j)}. \tag{3.4}$$

With (3.1)–(3.4), the intrinsic physical properties of the linear medium enter covariantly into the EM formalism. For a vacuum, C reduces to $C^{\mu\nu}{}_{\alpha\beta} = \frac{1}{2}\delta^{\mu\nu}{}_{\alpha\beta}$, so that $G^{\mu\nu} = F^{\mu\nu}$ in any frame and $\mathbf{D} = \mathbf{E}$ and $\mathbf{B} = \mathbf{H}$ for any observer.

4. GENERAL LOCAL ELECTRODYNAMICS IN MEDIA

A. Local Maxwell Equations and Wave Equations

In a general $\{x^\mu\}$, the Einstein–Maxwell theory postulates the field equations in vacuum $F^{\mu\nu}{}_{;\nu} = -J^\mu$

and $(^*F)^{\mu\nu}{}_{;\nu} = 0$.[23] Now, postulating the similar covariant form for macroscopic Maxwell equations in media gives

$$G^{\mu\nu}{}_{;\nu} = -J^{\mu}, \tag{4.1a}$$

$$(^*F)^{\mu\nu}{}_{;\nu} = 0 \leftrightarrow \exists\, A_{\mu} \ni F_{\mu\nu} = A_{\nu,\mu} - A_{\mu,\nu}, \tag{4.1b}$$

and the constitutive tensor relations (3.1). Here the ";" denotes the covariant derivative and the "*" denotes the dual; these are defined by

$$\begin{aligned} V^{\mu}{}_{;\lambda} &\equiv V^{\mu}{}_{,\lambda} + \Gamma^{\mu}{}_{\lambda\alpha}V^{\alpha}, \\ T^{\mu\nu}{}_{;\lambda} &\equiv T^{\mu\nu}{}_{,\lambda} + \Gamma^{\mu}{}_{\lambda\alpha}T^{\alpha\nu} + \Gamma^{\nu}{}_{\lambda\alpha}T^{\mu\alpha}, \quad \text{etc.}, \\ (^*F)^{\mu\nu} &\equiv \tfrac{1}{2}(-g)^{-\frac{1}{2}}\eta^{\mu\nu\alpha\beta}F_{\alpha\beta}. \end{aligned} \tag{4.2}$$

The Christoffel symbols are

$$\begin{aligned} \Gamma^{\mu}{}_{\lambda\alpha} &\equiv g^{\mu\beta}\Gamma_{\beta|\lambda\alpha}, \\ \Gamma_{\beta|\lambda\alpha} &\equiv \tfrac{1}{2}(g_{\beta\lambda,\alpha} + g_{\beta\alpha,\lambda} - g_{\lambda\alpha,\beta}), \end{aligned} \tag{4.3}$$

Finally, $(\ )_{,\lambda} \equiv \partial/\partial x^{\lambda}$, $g \equiv \det(g_{\mu\nu})$, and $\eta^{\mu\nu\alpha\beta} = 1$, -1, or 0 if $\pi(\mu\nu\alpha\beta) =$ even $\pi(0123)$, odd $\pi(0123)$, or otherwise, respectively.

But now the EM field $F^{(\mu)(\nu)}$, $G^{(\mu)(\nu)}$, and current $J^{(\mu)}$, which are physically observable to the observers $\{O\}$ in $\{x^{\mu}\}$, are the local components of $\hat{\mathsf{F}}$, $\hat{\mathsf{G}}$, and $\hat{\mathsf{J}}$ on the $\{\hat{\mathbf{e}}_{(\mu)}\}$ of $\{O\}$:

$$\begin{aligned} F^{(0)(i)} &= -E^{(i)}, \quad (^*F)^{(0)(i)} = -B^{(i)}, \\ G^{(0)(i)} &= -D^{(i)}, \quad (^*F)^{(0)(i)} = -H^{(i)}, \\ J^{(\mu)} &= (\rho, J^{(1)}, J^{(2)}, J^{(3)}). \end{aligned} \tag{4.4}$$

The tensors as mathematical symbols, in whose forms these physical quantities combine the curvatures of both the coordinate frame and space-time in order to enter the postulated simple covariant equations, have no direct physical significance. We wish to avoid unnecessary divergence, which may occur to the tensor quantities. Furthermore, we wish to have the local physics of eventual interest under direct consideration such that we have a physical feeling about the quantities being handled and such that we are able to simplify equations with intuitive symmetry arguments when such physical symmetry happens locally. Accordingly, we prefer dealing with local equations. To get such equations for $\{O\}$, first from (2.14) and (2.15), the observer's $\{\hat{\mathbf{e}}_{(\mu)}\}$ satisfies

$$e_{(0)}{}^{\mu} = (g_{00})^{-\frac{1}{2}}\delta_0{}^{\mu}, \quad e_{(0)\mu} = (g_{00})^{-\frac{1}{2}}g_{0\mu}, \quad e_{(i)0} = 0. \tag{4.5}$$

Then, substituting quantities of (4.4) into Eqs. (4.1) by use of the localization (2.12) on the above $\{\hat{\mathbf{e}}_{(\mu)}\}$, we obtain the local Maxwell equations in a medium for observers $\{O\}$ in $\{x^{\mu}\}$ as

$$[(-g)^{\frac{1}{2}}e_{(i)}{}^{j}D^{(i)}(g_{00})^{-\frac{1}{2}}]_{,j} + [(-g)^{\frac{1}{2}}\eta^{0ijk}e_{(i)}{}^{0}e_{(j)}{}^{l}H_{(k)}]_{,l} = (-g)^{\frac{1}{2}}(\rho(g_{00})^{-\frac{1}{2}} + J^{(i)}e_{(i)}{}^{0}), \tag{4.6a}$$

$$[(-g)^{\frac{1}{2}}\eta^{0ikl}e_{(i)}{}^{j}e_{(k)}{}^{\nu}H_{(l)}]_{,\nu} = [(-g)^{\frac{1}{2}}e_{(i)}{}^{j}D^{(i)}(g_{00})^{-\frac{1}{2}}]_{,0} + (-g)^{\frac{1}{2}}J^{(i)}e_{(i)}{}^{j}, \tag{4.6b}$$

$$[(-g)^{\frac{1}{2}}e^{j}{}_{(i)}B^{(i)}(g_{00})^{-\frac{1}{2}}]_{,j} - [(-g)^{\frac{1}{2}}\eta^{0ijk}e_{(i)}{}^{0}e_{(j)}{}^{l}E_{(k)}]_{,l} = 0, \tag{4.6c}$$

$$[(-g)^{\frac{1}{2}}\eta^{0ikl}e_{(i)}{}^{j}e_{(k)}{}^{\nu}E_{(l)}]_{,\nu} = -[(-g)^{\frac{1}{2}}e_{(i)}{}^{j}B^{(i)}(g_{00})^{-\frac{1}{2}}]_{,0}, \tag{4.6d}$$

and the local constitutive relations (3.2), which simply reduce to (3.4) if $\{x^{\mu}\}$ is the frame which is comoving with the medium.

Physically, in (4.6a), the mix of local current density $\mathbf{J}$ into charge density ρ and the presence of the curl-like term of $\mathbf{H}$ compensate for the fact that the coordinate divergence of $\mathbf{D}$ is not taken purely spatially; similar remarks apply to (4.6b)–(4.6d). In fact, if we express the coordinate differential operators by local differential operators through $d\hat{\mathbf{x}} = dx^{\mu}\hat{\mathbf{e}}_{\mu} = dx^{(\alpha)}\hat{\mathbf{e}}_{(\alpha)}$, then (4.6a) and (4.6b) become, respectively,

$$\begin{aligned} &(-g)^{\frac{1}{2}}(g_{00})^{-\frac{1}{2}}\left[\frac{\partial D^{(i)}}{\partial x^{(i)}} - \rho\right] \\ &\quad + (-g)^{\frac{1}{2}}e^{0}{}_{(j)}\left[\eta^{0jik}\frac{\partial H_{(k)}}{\partial x^{(i)}} - \frac{\partial D^{(j)}}{\partial x^{0}} - J^{(j)}\right] \\ &\quad + [(-g)^{\frac{1}{2}}e^{j}{}_{(i)}(g_{00})^{-\frac{1}{2}}]_{,j}D^{(i)} \\ &\quad + [(-g)^{\frac{1}{2}}\eta^{0jik}e^{0}{}_{(j)}e^{l}{}_{(i)}]_{,l}H_{(k)} = 0 \end{aligned} \tag{4.7a}$$

and

$$\begin{aligned} &e^{j}{}_{(i)}(-g)^{\frac{1}{2}}\left[\eta^{0ijk}\frac{\partial H_{(k)}}{\partial x^{(j)}} - J^{(i)} - \frac{\partial D^{(i)}}{\partial x^{0}}\right] \\ &\quad - [(-g)^{\frac{1}{2}}e^{j}{}_{(i)}(g_{00})^{-\frac{1}{2}}]_{,0}D^{(i)} \\ &\quad + [(-g)^{\frac{1}{2}}\eta^{0ikl}e^{j}{}_{(i)}e^{\nu}{}_{(k)}]_{,\nu}H_{(l)} = 0, \end{aligned} \tag{4.7b}$$

from which the vanishing of the large square brackets will give the flat space-time EM equations

$$\frac{\partial D^{(i)}}{\partial x^{(i)}} = \rho \quad \text{and} \quad \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t},$$

approximately, in a small enough neighborhood if the change of $g_{\mu\nu}$ in there is neglected. Similar remarks apply for (4.6c) and (4.6d). Although coordinate conditions can be imposed on $\{x^{\mu}\}$ to simplify (4.6), such a frame is, in general, not medium comoving; then the mixed constitutive relations make it difficult to decouple the equations, and the motion of such frames relative to the medium obscure the local physics.

When the $\{x^\mu\}$ has synchronous metric, i.e., $g_{0i} \equiv 0$, all $e_{(0)}{}^i$, $e_{(0)i}$, $e^{(0)}{}_i$, and $e^{(0)i}$ vanish; we can rescale time so that $g_{00} \equiv 1$ and define the operators $\nabla \times$ and $\nabla \cdot$ in 3-space according to (4.6) such that

$$\nabla \cdot \mathbf{D} = \rho, \quad \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial}{\partial t}\mathbf{D} + \alpha \cdot \mathbf{D},$$
$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} - \alpha \cdot \mathbf{B}, \tag{4.8}$$

where $\alpha^{(j)}{}_{(i)} \equiv e^{(j)}{}_k[(-g)^{\frac{1}{2}}e^k{}_{(i)}]_{,0}$. If, in addition, the $g_{\mu\nu}$ are not functions of time, (4.8) will just reduce to the ordinary 3-vector equations in curvilinear coordinates.

In a linear medium expressed by $C^{\mu\nu\alpha\beta}$ as (3.1), the general wave equations in it are

$$(C^{\mu\nu\alpha\beta}A_{\alpha;\beta})_{;\nu} = \tfrac{1}{2}J^\mu, \tag{4.9}$$

in which a divergence gauge freedom exists for $\hat{\mathbf{A}}$. For the special case of local-isotropic medium in which $\epsilon^{(\mu)}{}_{(\nu)} = \epsilon\delta^\mu{}_\nu$, $K^{(\mu)}{}_{(\nu)} = K\delta^\mu{}_\nu$,[24] and a frame in which $Dv^\mu/Dx^\lambda \equiv 0$, Eq. (4.9) then becomes

$$[-\mu^{-1}A^{\mu;\nu} + (\mu^{-1} - \epsilon)v_\beta v^\nu A^{\mu;\beta}]_{;\nu} + [\mu^{-1}R^{\lambda\mu} + (\mu^{-1} - \epsilon)R^{\beta\lambda\mu\nu}v_\beta v_\nu]A_\lambda = -[J^\mu + (\mu^{-1} - \epsilon)v^\mu v_\beta J^\beta], \tag{4.10a}$$

where an invariant gauge condition of the form

$$\mu^{-1}A^\nu{}_{;\nu} - (\mu^{-1} - \epsilon)v_\beta v^\nu A^\beta{}_{;\nu} = 0 \tag{4.10b}$$

has been used and $R^{\mu\nu\alpha\beta}$ and $R^{\mu\nu}$ are the Riemann and Ricci curvature tensors, respectively.[25] Equations (4.10) and (4.11) in the inertial Minkowskian limit reduce to the familiar results in a linear medium.[26]

B. Lagrangian Formulation

For a lossless linear medium with $C^{\mu\nu\alpha\beta} = C^{\alpha\beta\mu\nu}$, the Maxwell equation (4.1a) can be obtained from

$$\delta\int L(-g)^{\frac{1}{2}}d^4x = 0, \tag{4.11a}$$

$$L = -\tfrac{1}{4}G^{\mu\nu}F_{\mu\nu} - J^\mu A_\mu \equiv L_{\text{EM}} + L_{\text{int}} \tag{4.11b}$$

by varying A_μ which is defined by (4.1b). But in a lossy medium the $\epsilon^{(i)}{}_{(j)}$ and the $K^{(i)}{}_{(j)}$ in the medium-comoving frame are not symmetrical; thus $C^{\mu\nu\alpha\beta}$ in any frame is not symmetric[27] in $(\mu\nu) \rightleftarrows (\alpha\beta)$ and can be decomposed into a symmetric and an antisymmetric part,

$$C^{\mu\nu\alpha\beta} \equiv \tfrac{1}{2}(C^{\mu\nu\alpha\beta} + C^{\alpha\beta\mu\nu}) + \tfrac{1}{2}(C^{\mu\nu\alpha\beta} - C^{\alpha\beta\mu\nu}) \equiv {}_sC^{\mu\nu\alpha\beta} + {}_aC^{\mu\nu\alpha\beta} \tag{4.12}$$

such that ${}_aC^{\mu\nu\alpha\beta} = -{}_aC^{\alpha\beta\mu\nu}$ and ${}_sC^{\mu\nu\alpha\beta} = C^{\alpha\beta\mu\nu}$. In this lossy medium, the above $L_{\text{EM}} = -\frac{1}{4}G^{\mu\nu}F_{\mu\nu}$ only picks up that part of $G^{\mu\nu}$ corresponding to the symmetric part of $\epsilon^{(\mu)}{}_{(\nu)}$ and $K^{(\mu)}{}_{(\nu)}$; i.e., ${}_sG^{\mu\nu} = {}_sC^{\mu\nu\alpha\beta}F_{\alpha\beta}$; thus (4.1a) cannot be obtained simply from (4.11a).

However, a local consideration of the losses on a closed path of field states in the **B**–**H** and **E**–**D** spaces for a linear lossy medium reveals[27] that all the losses in unit 4-volume for a $\delta\mathbf{B}$ and $\delta\mathbf{E}$ change of field strength are due to the "antisymmetric" part ${}_aG^{\mu\nu} \equiv {}_aC^{\mu\nu\alpha\beta}F_{\alpha\beta}$ as

$$\delta W_{\text{loss}} = {}_a\mathbf{H} \cdot \delta\mathbf{B} - {}_a\mathbf{D} \cdot \delta\mathbf{E} = \tfrac{1}{2}{}_aG^{(\mu)(\nu)}\delta F_{(\mu)(\nu)} = \tfrac{1}{2}{}_aG^{\mu\nu}\delta F_{\mu\nu}. \tag{4.13}$$

Then an action principle in a lossy medium can be stated for the difference of the field Lagrangian and the energy loss as

$$\delta I \equiv \delta\int d^4x(-g)^{\frac{1}{2}}(L - W_{\text{loss}}) = 0 \tag{4.14}$$

by varying A_μ, where L is given by (4.11b) and W_{loss} enters in the sense of (4.13). Performing the variation, we see that (4.14) gives

$$0 = \int(-g)^{\frac{1}{2}}d^4x\left[\frac{\partial L}{\partial A_\mu} - \frac{1}{(-g)^{\frac{1}{2}}}\left((-g)^{\frac{1}{2}}\frac{\partial L}{\partial A_{\mu,\nu}}\right)_{,\nu} - \frac{1}{(-g)^{\frac{1}{2}}}((-g)^{\frac{1}{2}}{}_aG^{\mu\nu})_{,\nu}\right]\delta A_\mu,$$

from which immediately follows

$$-J^\mu - (-g)^{-\frac{1}{2}}[(-g)^{\frac{1}{2}}{}_aG^{\mu\nu} + (-g)^{\frac{1}{2}}{}_sG^{\mu\nu}]_{,\nu} = 0. \tag{4.15}$$

We see the ${}_aG^{\mu\nu}$ in the lossy part and the ${}_sG_{\mu\nu}$ in the L_{EM} combine back to give the total $G^{\mu\nu}$ as required in (4.1a). In the above, $A_\mu \equiv 0$ at spatial infinity and Gauss' theorem has been used.

C. Boundary Conditions, Local Conservative Quantities, and Energy Tensor

The boundary conditions at the interface of two different media are obtained by integrating Maxwell equations over appropriate infinitesimal 3-hypersurfaces and by making use of Gauss' theorem:

$$\tfrac{1}{2}\oint_{V_2} S^{\alpha\mu\nu}\,d\Sigma^*{}_{\mu\nu} = \int_{V_3} S^{\alpha\mu\nu}{}_{,\nu}\,d\Sigma^*{}_\mu. \tag{4.16}$$

In a time-orthogonal frame $\{x^\mu\}$, the immediate results can be expressed by local physical quantities

for observers $\{O\}$ in that frame as the usual forms[27]

$$\mathbf{n}\cdot({}_{II}\mathbf{D}-{}_{I}\mathbf{D})=\sigma,\qquad \mathbf{n}\cdot({}_{II}\mathbf{B}-{}_{I}\mathbf{B})=0,$$
$$\mathbf{n}\times({}_{II}\mathbf{E}-{}_{I}\mathbf{E})=0,\quad \mathbf{n}\times({}_{II}\mathbf{H}-{}_{I}\mathbf{H})=\mathbf{k},\quad (4.17)$$

where $\mathbf{n}$ is unit normal of the intersurface pointing from medium II to medium I and σ and $\mathbf{k}$ are the *physical* surface charge and current densities on that surface to $\{O\}$. But (4.17) as a local result then holds for any observer. Thus, the boundary conditions of the observable EM field for observers in any frame are given by (4.17), which is anticipated, since the geometry $g_{\mu\nu}$ is continuous without abrupt changes and thus contributes nothing to local limiting processes.

Now the conservation of physical charge for $\{O\}$ is just implied by (4.1a), i.e.,

$$\frac{\partial}{\partial t}\left[(-g)^{\frac{1}{2}}\left(\frac{\rho}{(g_{00})^{\frac{1}{2}}}+g^{0j}e_{j(i)}J^{(i)}\right)\right]=-(e^{i}_{(j)}J^{(j)})_{,i},\quad (4.18)$$

or as an integral over an $x^0=$ const spacelike 3-hypersurface S:

total conserved charge

$$=\int_S(-g)^{\frac{1}{2}}d^3x\left(\frac{\rho}{(g_{00})^{\frac{1}{2}}}+g^{0j}e_{(i)j}J^{(i)}\right)$$
$$=\int_S[-\det(g_{ij})]^{\frac{1}{2}}d^3x\rho,\quad \text{if } \{x^\mu\} \text{ is synchronous.}\quad (4.18')$$

So, in general, the total conserved charge is not the physically observable charge alone but, in addition, the current $\mathbf{J}$.

Concerning the energy tensor, such a quantity with field-equation-implied physical meaning and generating conservative law by its divergence cannot be found for macroscopic EM fields in media because it includes the averaged interaction with the medium and forms a nonclosed system.[28]

However, a tensor which partially fulfills these purposes with limited physical meaning can be found as the generalization of the vacuum case. First, in the frame comoving with the medium, extrapolating the meaning of $\frac{1}{2}(\mathbf{E}\cdot\mathbf{D}+\mathbf{B}\cdot\mathbf{H})$ in the static case to be local energy density $T^{(0)(0)}$ and interpreting the rewritten special-relativity local field energy balance

$$\frac{\partial}{\partial T}T^{(0)(0)}$$
$$=-\mathbf{E}\cdot\mathbf{J}-\nabla\cdot(\mathbf{E}\times\mathbf{H})+\frac{1}{2}\left(B^{(i)}B^{(j)}\frac{\partial}{\partial T}K_{(i)(j)}-E^{(i)}E^{(j)}\frac{\partial}{\partial T}\epsilon_{(i)(j)}\right)\quad (4.19)$$

lead us to identify mechanically $\mathbf{E}\times\mathbf{H}$ as field momentum density $T^{(0)(i)}$ and the last term as power stored in the medium to keep field strength constant during a change of media properties. Now the force acted on a medium by EM field can be found from an infinitesimal displacement of it by

$$\delta\int d^3X\tfrac{1}{2}(\mathbf{H}\cdot\mathbf{B}+\mathbf{E}\cdot\mathbf{D})=-\int d^3X\mathbf{f}\cdot\delta\mathbf{x}$$
$$\Rightarrow\mathbf{f}=\rho\mathbf{E}+\mathbf{J}\times\mathbf{B}+\frac{1}{2}\left(B^{(i)}B^{(j)}\nabla K_{(i)(j)}-E^{(i)}E^{(j)}\nabla\epsilon_{(i)(j)}\right)+\frac{\partial}{\partial T}(\mathbf{D}\times\mathbf{B}).\quad (4.20)$$

The above defined $T^{(0)(0)}$ and $T^{(0)(i)}$ can then be used to construct a local tensor $T^{(\mu)(\nu)}$, of which they are $(0)(\mu)$ components,

$$T^{(\mu)(\nu)}\equiv -F^{(\mu)(\lambda)}G^{(\nu)}{}_{(\lambda)}+\tfrac{1}{4}\eta^{(\mu)(\nu)}F^{(\alpha)(\beta)}G_{(\alpha)(\beta)}.\quad (4.21)$$

Also, this $T^{(i)(j)}{}_{,(j)}$ gives exactly the $\mathbf{f}$ obtained in (4.20) such that $T^{(i)(j)}$ has the meaning of stress; moreover, this $T^{(\mu)(\nu)}$ reduces to the familiar form in the vacuum limit. Thus, we can just define it to be the local energy tensor of the EM field in media whose only physical meaning is $T^{(0)(0)}$ as energy density, $T^{(0)(i)}$ as momentum density, and $T^{(i)(j)}$ as stress of local EM field. Its nonsymmetry just results from the nonclosedness of the field and is completely irrelevant. In general relativity, a delocalization (2.12b) immediately gives

$$T^{\mu\nu}=-F^{\mu\lambda}G^{\nu}{}_{\lambda}+\tfrac{1}{4}g^{\mu\nu}F_{\alpha\beta}F^{\alpha\beta}\quad (4.22)$$

as the energy tensor. Computing the divergence $T^{\mu\nu}{}_{;\nu}$, we see that the energy momentum conservation takes the form

$$T^{\mu\nu}{}_{;\nu}=-F^{\mu\nu}J_\nu+\tfrac{1}{4}g^{\mu\nu}{}_{\mathrm{s}}C^{\alpha\beta\gamma\delta}{}_{;\nu}F_{\alpha\beta}F_{\gamma\delta}+\tfrac{1}{2}g^{\mu\nu}{}_{\mathrm{a}}C^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta;\nu}\quad (4.23)$$

or

$$(T^{\mu\nu}+t^{\mu\nu}_{\text{charges}})_{;\nu}+{}_{\mathrm{s}}F^{\mu}+{}_{\mathrm{a}}F^{\mu}=0,\quad (4.23')$$

which means that, in addition to a Lorentz force acted on the explicit charges, the EM field supplies an averaged conservative power force to alter the stored energy during a change of media properties and a power force to provide the medium losses. In other words, what is conserved is the total energy–momentum $T^{\mu\nu}+t^{\mu\nu}_{\text{charges}}$ of the EM field and the explicit charges, plus the energy–momentum stored in and dissipated to the medium, such as (4.24).

D. Discussions

For media in inertial frames, the assumption of covariance of $\mathbf{D}$ and $\mathbf{H}$ equations and their $G^{\mu\nu}$ tensor,

and thus the whole formalism actually does not assume any new law of macroscopic EM physics, even if observed in an accelerated frame. The formalism is just a convenient way to present the well-accepted rest-frame physics of (3.4) and the usual Maxwell equations to other frames by using $G^{\mu\nu}$ as an intermediate concept. But, for a medium in a noninertial frame, (4.1) is an additional assumption on the behavior of the averaged medium-EM interactions even in the medium comoving frame. One reason for us to make this assumption is that the theory so formulated surely holds for noninertial observers moving with respect to a medium at an inertial frame; the principle of relativity then suggests its applicability the other way around and, thus, in general frames.

Also, the physical constitutive properties must be discussed locally only. Mistaken results, such as **D** depends constitutively on **B** even for vacuum,[29] will occur if one does not treat the constitutive physics and constitutive tensor properly, as in Sec. 3.

5. APPLICATION TO LINEAR ACCELERATED MEDIUM

A. Formulation

Let $\{X^{\bar\mu}\} \equiv \{X^{\bar 0}, X^{\bar 1}, X^{\bar 2}, X^{\bar 3}\} \equiv \{T, X, Y, Z\}$ be a laboratory inertial Minkowskian frame. If a medium is uniformly linear accelerated, its comoving frame[30] can be described by an $\{x^\mu\}$ that

$$T = a^{-1}\sinh at, \qquad Y = y,$$
$$X = a^{-1}(\cosh at - 1) + x, \quad Z = z, \tag{5.1}$$

as in Fig. 2 where origins have been adjusted so that at $t = 0 = T$ their relative velocity is zero. $\{x^\mu\}$ is medium coaccelerating in the sense that each point of fixed (x^i) has X-uniform acceleration

$$V = \tanh at, \tag{5.2}$$

with respect to $\{X^{\bar\mu}\}$, and has metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & -\sinh at & 0 & 0 \\ -\sinh at & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{5.3}$$

This $\{x^\mu\}$ is just a convenient frame describing the medium motion and is neither synchronous nor static. However, t is the proper time of medium comoving observers $\{O\}$.

Now observable values of a tensor to $\{O\}$ are its physical components on a conveniently coordinate-transported local tetrad basis $\{\hat{\mathbf{e}}_{(\mu)}\}$ which, because of (2.13) and as explained at the end of Sec. 2, can be chosen as the instantaneous Lorentz transform of the $\hat{\mathbf{e}}_{(\bar\mu)}$ of $\{X^{\bar\mu}\}$:

$$\hat{\mathbf{e}}_{(0)} = \hat{\mathbf{e}}_0, \quad \hat{\mathbf{e}}_{(2)} = \hat{\mathbf{e}}_2,$$
$$\hat{\mathbf{e}}_{(1)} = \frac{1}{\cosh at}(\hat{\mathbf{e}}_1 + \sinh at\, \hat{\mathbf{e}}_0), \quad \hat{\mathbf{e}}_{(3)} = \hat{\mathbf{e}}_3, \tag{5.4}$$

where the $\{\hat{\mathbf{e}}_\mu\}$ are the coordinate bases of $\{x^\mu\}$ and the instantaneous Lorentz transform from $\{\hat{\mathbf{e}}_{(\mu)}\}$ to $\{\hat{\mathbf{e}}_{(\bar\mu)}\}$ is

$$\Lambda^{\bar\alpha}{}_{(\lambda)} = \begin{pmatrix} \cosh at & \sinh at & & 0 \\ \sinh at & \cosh at & & \\ & & 1 & \\ 0 & & & 1 \end{pmatrix}. \tag{5.5}$$

Then, by (2.12) and (2.13),[31]

$$J^\mu = \frac{\partial x^\mu}{\partial X^{\bar\alpha}}\Lambda^{\bar\alpha}{}_{(\lambda)}J^{(\lambda)} \quad \text{or} \quad J^\mu = e^\mu{}_{(\lambda)}J^{(\lambda)} \Rightarrow J^\mu = \left(\rho + \tanh at J^{(x)}, \frac{J^{(x)}}{\cosh at}, J^{(y)}, J^{(z)}\right), \tag{5.6a}$$

$$F^{\mu\nu} = \frac{\partial x^\mu}{\partial X^{\bar\alpha}}\frac{\partial x^\nu}{\partial X^{\bar\beta}}\Lambda^{\bar\alpha}{}_{(\lambda)}\Lambda^{\bar\beta}{}_{(\tau)}F^{(\lambda)(\tau)} \quad \text{or} \quad F^{\mu\nu} = e^\mu{}_{(\alpha)}e^\nu{}_{(\beta)}F^{(\alpha)(\beta)}$$
$$\Rightarrow F^{\mu\nu} = \begin{pmatrix} 0 & \dfrac{-E^{(x)}}{\cosh at} & -(E^{(y)} + \tanh at B^{(z)}) & -E^{(z)} + \tanh at B^{(y)} \\ & 0 & \dfrac{-B^{(z)}}{\cosh at} & \dfrac{B^{(y)}}{\cosh at} \\ - & & 0 & -B^{(x)} \\ & & & 0 \end{pmatrix}, \tag{5.6b}$$

and, similarly,

$$G^{\mu\nu} = [\mathbf{E} \to \mathbf{D}, \mathbf{B} \to \mathbf{H} \text{ in (5.6b)}] \tag{5.6c}$$

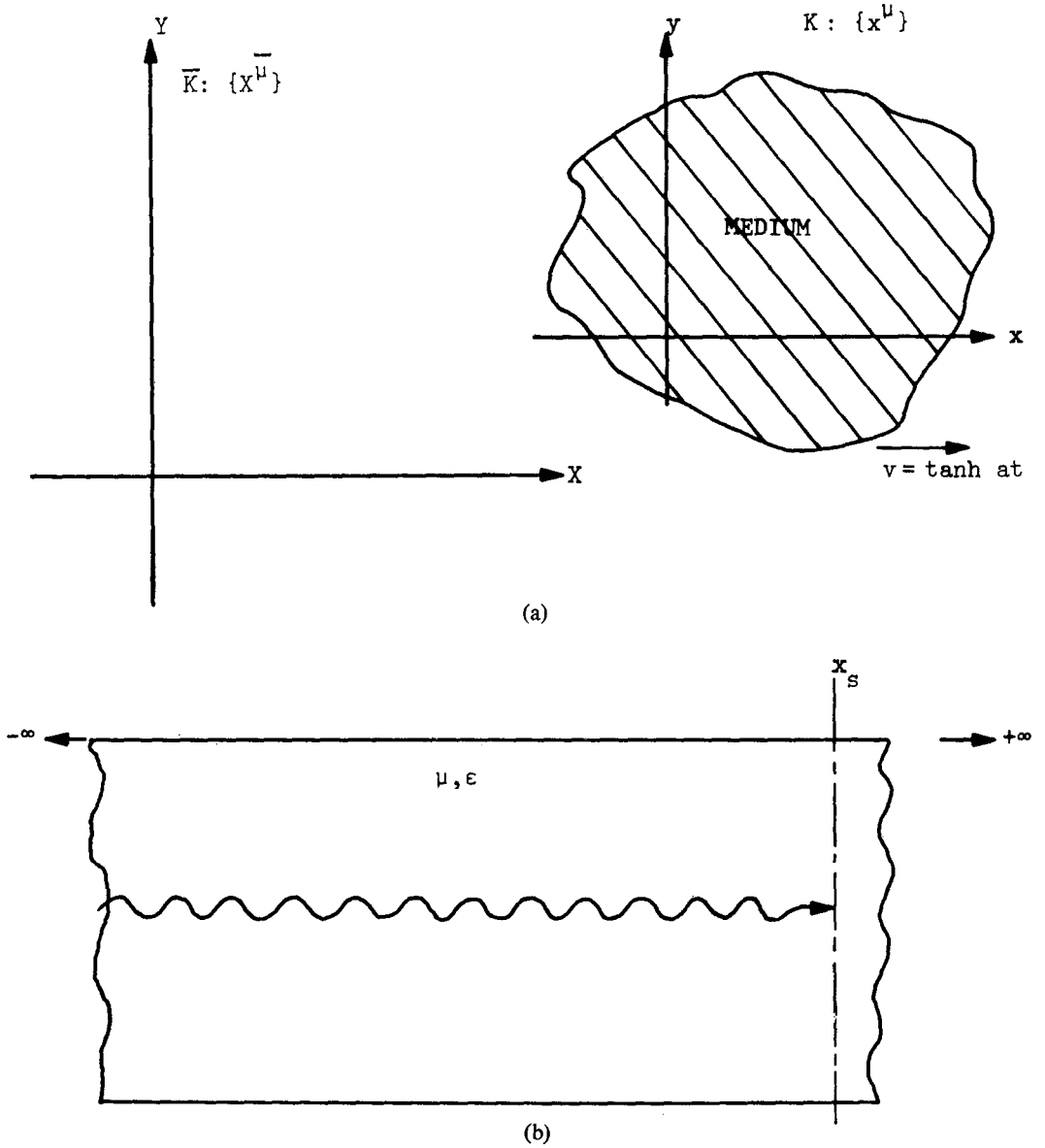


FIG. 2. (a) Linear accelerated medium. (b) EM wave propagation in an accelerated simple medium; at $t = 0$ it begins to accelerate, whence the propagation obeys a new law.

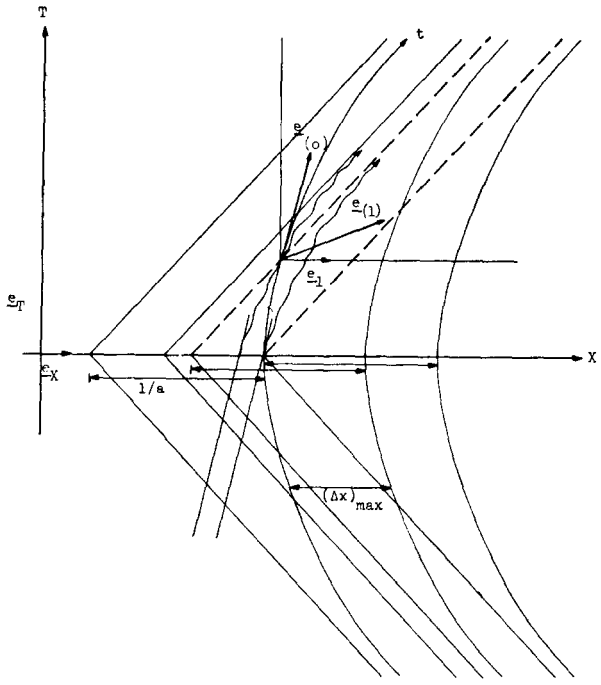


FIG. 3. Space–time diagram of observer in accelerated medium and wave propagation in it (wavy lines).

express that local observables of $\{O\}$ combine with geometry of $\{x^\mu\}$ into tensors. The physical meaning is as in Sec. 2B and is now caused by the local non-time-orthogonality and nonnormalization of $\hat{\mathbf{e}}_x$ and can be seen in Fig. 3.

Now in $\{x^\mu\}$, with (5.6) and the only nonzero Christoffel symbols $\Gamma^0_{00} = a \tanh at$, $\Gamma^1_{00} = a \operatorname{sech} at$, and $\Gamma_{1/00} = -a \cosh at$, the local Maxwell equations (4.6a) and (4.6b) in this accelerated frame are

$$\nabla \cdot \mathbf{D} + \mathbf{V} \cdot (\nabla \times \mathbf{H}) = \rho + \mathbf{V} \cdot \mathbf{J}, \quad (5.7a)$$

$$\nabla \times \mathbf{H} + \mathbf{a} \times \mathbf{H} + \mathbf{V} \times \frac{\partial}{\partial t}\mathbf{H} = \mathbf{J} + \frac{\partial}{\partial t}\mathbf{D} - \mathbf{V} \times (\mathbf{a} \times \mathbf{D}), \quad (5.7b)$$

where the conventions[32] are

$$\nabla \equiv \left(\frac{1}{\cosh at}\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right);$$

$\partial/\partial t$ does not act on $\hat{\mathbf{e}}_{(i)}$, and 3-vectors are componented on $\hat{\mathbf{e}}_{(i)}$ so that $\mathbf{D} \equiv (D^{(1)}, D^{(2)}, D^{(3)})$, etc., and $\mathbf{V} \equiv \tanh at\, \mathbf{e}_{(x)}$, $\mathbf{a} \equiv a\mathbf{e}_{(x)}$.

Similarly, (4.6c) and (4.6d) become

$$\nabla \cdot \mathbf{B} = \mathbf{V} \cdot \nabla \times \mathbf{E}, \quad (5.8a)$$

$$\nabla \times \mathbf{E} + \mathbf{a} \times \mathbf{E} + \mathbf{V} \times \frac{\partial}{\partial t}\mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B} + \mathbf{V} \times (\mathbf{a} \times \mathbf{B}). \quad (5.8b)$$

Also, (5.7) implies the local continuity equation

$$-\nabla \cdot \mathbf{J} - \mathbf{a} \cdot \mathbf{J} = \frac{\partial}{\partial t}\rho + \mathbf{V} \cdot \frac{\partial}{\partial t}\mathbf{J} + \rho \mathbf{a} \cdot \mathbf{V}. \quad (5.9)$$

Now, in addition to (5.7) and (5.8), since this $\{x^\mu\}$ is medium comoving, the constitutive relations are just

$$D^{(i)} = \epsilon^{(i)}{}_{(j)} E^{(j)}, \quad H^{(i)} = K^{(i)}{}_{(j)} B^{(j)}, \quad (5.10)$$

where $\epsilon^{(i)}{}_{(j)}$ and $K^{(i)}{}_{(j)}$ are the comoving local medium parameters which, if changes due to accelerated strain are neglected, are simply equal to their values when this medium is in an inertial frame.

For a tensor description of (5.10), first the $\epsilon^{\mu\nu}$ and the $K^{\mu\nu}$ in $\{x^\mu\}$ are just

$$\epsilon^{\mu\nu} = e^\mu{}_{(\alpha)} e^\nu{}_{(\beta)} \epsilon^{(\alpha)(\beta)} = \begin{pmatrix} \epsilon^{(0)(1)} + \epsilon^{(1)(1)} \tanh^2 at & \operatorname{sech} at \tanh at\, \epsilon^{(1)(1)} & \tanh at\, \epsilon^{(1)(2)} & \tanh at\, \epsilon^{(1)(3)} \\ \operatorname{sech} at \tanh at\, \epsilon^{(1)(1)} & \operatorname{sech}^2 at\, \epsilon^{(1)(1)} & \operatorname{sech} at\, \epsilon^{(1)(2)} & \operatorname{sech} at\, \epsilon^{(1)(3)} \\ \tanh at\, \epsilon^{(2)(1)} & \operatorname{sech} at\, \epsilon^{(2)(1)} & \epsilon^{(2)(2)} & \epsilon^{(2)(3)} \\ \tanh at\, \epsilon^{(3)(1)} & \operatorname{sech} at\, \epsilon^{(3)(1)} & \epsilon^{(3)(2)} & \epsilon^{(3)(3)} \end{pmatrix}, \quad (5.11a)$$

$$K^{\mu\nu} = [\text{replacing } \epsilon^{(\alpha)(\beta)} \to K^{(\alpha)(\beta)} \text{ in (5.11a)}]. \quad (5.11b)$$

Then $C^{\mu\nu\alpha\beta}$ in this $\{x^\mu\}$ is constructed on the above $\epsilon^{\mu\nu}$ and $K^{\mu\nu}$ and 4-velocity of the medium $\hat{\mathbf{V}}$ according to (3.1); thus, the $C^{\bar{\mu}\bar{\nu}\bar{\alpha}\bar{\beta}}$ in any $\{x^{\bar{\mu}}\}$ is obtained by a tensor transform. In particular, evaluating

$$G^{(\bar{\mu})(\bar{\nu})} = e^{(\bar{\mu})}{}_{\bar{\alpha}} e^{(\bar{\nu})}{}_{\bar{\beta}} C^{\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}} F_{\bar{\gamma}\bar{\delta}}$$

in the laboratory directly gives[33]

$$(D^{\bar{i}}) = \begin{Bmatrix} \epsilon^{(1)}{}_{(1)} & \cosh at\, \epsilon^{(1)}{}_{(2)} & \cosh at\, \epsilon^{(1)}{}_{(3)} \\ \cosh at\, \epsilon^{(2)}{}_{(1)} & (\cosh^2 at\, \epsilon^{(2)}{}_{(2)} - \sinh^2 at\, K^{(3)}{}_{(3)}) & (\cosh^2 at\, \epsilon^{(2)}{}_{(3)} + \sinh^2 at\, K^{(3)}{}_{(2)}) \\ \cosh at\, \epsilon^{(3)}{}_{(1)} & (\cosh^2 at\, \epsilon^{(3)}{}_{(2)} + \sinh^2 at\, K^{(2)}{}_{(3)}) & (\cosh^2 at\, \epsilon^{(3)}{}_{(3)} - \sinh^2 at\, K^{(2)}{}_{(2)}) \end{Bmatrix}$$

$$\times (E^{\bar{i}}) + \sinh at \begin{Bmatrix} 0 & \epsilon^{(1)}{}_{(3)} & -\epsilon^{(1)}{}_{(2)} \\ K^{(3)}{}_{(1)} & & \\ -K^{(2)}{}_{(1)} & \cosh at \begin{pmatrix} K^{(3)}{}_{(2)} + \epsilon^{(2)}{}_{(3)}, & K^{(3)}{}_{(3)} - \epsilon^{(2)}{}_{(2)} \\ -K^{(2)}{}_{(2)} + \epsilon^{(3)}{}_{(3)}, & -K^{(2)}{}_{(3)} - \epsilon^{(3)}{}_{(2)} \end{pmatrix} \end{Bmatrix} (B^{\bar{j}}), \quad (5.12a)$$

$$H^{(\bar{i})} = [\text{replacing } \epsilon^{(i)}{}_{(j)} \to K^{(i)}{}_{(j)},\ K^{(i)}{}_{(j)} \to \epsilon^{(i)}{}_{(j)},\ E^{(\bar{i})} \to B^{(\bar{i})},\ B^{(\bar{i})} \to -E^{(\bar{i})} \text{ in (5.12a)}] \quad (5.12b)$$

as the constitutive relations for the accelerating medium in the laboratory frame.

The boundary conditions (4.17) directly apply to observable EM fields in the accelerated frame. If there are no local surface charge and current, then the quantities

$$\mathbf{n}\cdot\mathbf{D},\quad \mathbf{n}\cdot\mathbf{B},\quad \mathbf{n}\times\mathbf{E},\quad \mathbf{n}\times\mathbf{H} \quad (5.13)$$

are continuous across the boundary of different media. In particular, if the boundary is perpendicular to the x direction ($\mathbf{n} \parallel \mathbf{e}_{(x)}$), then $D^{(x)}$, $B^{(x)}$, $E^{(y)}$, $E^{(z)}$, $H^{(y)}$, and $H^{(z)}$ are continuous; if the boundary has its normal in the y direction ($\mathbf{n} \parallel \mathbf{e}_{(y)}$), then $D^{(y)}$, $B^{(y)}$, $E^{(x)}$, $E^{(z)}$, $H^{(x)}$, and $H^{(z)}$ are continuous.

B. Wave Propagation along Acceleration in a Simple Medium

For a simple accelerated medium in $\{x^\mu\}$, Eq. (5.10) reduces to $\mathbf{D} = \epsilon\mathbf{E}$, $\mathbf{H} = \mu^{-1}\mathbf{B}$. Then, in a sourceless region, (5.7) becomes

$$\nabla\cdot\mathbf{E} + (\mu\epsilon)^{-1}\mathbf{V}\cdot(\nabla\times\mathbf{B}) = 0, \quad (5.14a)$$

$$\nabla\times\mathbf{B} + \mathbf{a}\times\mathbf{B} + \mathbf{V}\times\frac{\partial}{\partial t}\mathbf{B} = \mu\epsilon\left(\frac{\partial}{\partial t}\mathbf{E} - \mathbf{V}\times(\mathbf{a}\times\mathbf{E})\right). \quad (5.14b)$$

Consider now a planelike wave propagating along the x direction; the medium homogeneity leads to the assumption that nothing is y and z dependent. Then (5.8a) and (5.14a) give

$$\frac{\partial}{\partial x}B^{(x)} = 0, \quad \frac{\partial}{\partial x}E^{(x)} = 0, \quad (5.15)$$

so that $E^{(x)}$ and $B^{(x)}$ are spatial constants. But no source can produce a time varying field which is spatially uniform; thus they are space–time constants, and we can put them equal to 0. Then the other Maxwell equations of this transverse TEM wave are

$$\boldsymbol{\Phi}\times\mathbf{E} = -\psi\mathbf{B},$$
$$\boldsymbol{\Phi}\times\mathbf{B} = +\mu\epsilon\psi\mathbf{E}, \quad (5.16)$$

where, for abbreviation, the operators are defined as

$$\boldsymbol{\Phi} \equiv \Phi\mathbf{e}_{(x)} \equiv \mathbf{e}_{(x)}\left(\operatorname{sech} at\frac{\partial}{\partial x} + a + \tanh at\frac{\partial}{\partial t}\right)$$
$$\psi \equiv \left(\frac{\partial}{\partial t} + a\tanh at\right) \quad (5.17)$$

$$[\Phi, \psi] = a\operatorname{sech}^2 at\left(\sinh at\frac{\partial}{\partial x} - \cosh at\frac{\partial}{\partial t}\frac{1}{\cosh at}\right). \quad (5.18)$$

We see that $\boldsymbol{\Phi}$ and ψ are the natural corresponding operators of ∇ and $\partial/\partial T$ in an inertial frame. We thus solve the problem with approximation to these operators. From (5.16),

$$(\Phi^2 - \mu\epsilon\psi^2)\mathbf{E} = [\Phi, \psi]\mathbf{e}_{(x)}\times\mathbf{B},$$
$$(\Phi^2 - \mu\epsilon\psi^2)\mathbf{B} = -\mu\epsilon[\Phi, \psi]\mathbf{e}_{(x)}\times\mathbf{E}, \quad (5.19)$$

from which $(\Phi + \mu^{\frac{1}{2}}\psi)$ will give the $+x$ traveling wave and $(\Phi - \mu^{\frac{1}{2}}\psi)$ will give the $-x$ traveling wave. We solve (5.19) in the following way: First we neglect the mixed effect $[\Phi, \psi]$ corresponding to interaction of opposite traveling waves on the right side which is of order (a) and approaches to zero for large (at) as $\operatorname{sech}^2 at$; obtaining this E, B as the first approximation, we then put it back into the right side of (5.19) and proceed to solve for the next approximation, and so on. Now assume that, when the medium is at rest with respect to the laboratory at $t = 0$, a plane wave is propagating in the $+x$ direction, i.e., $E, B \sim e^{i(kx-\omega t)}$ at $t \sim 0$. Now we rewrite (5.19) as

$$[\Phi - (\mu\epsilon)^{\frac{1}{2}}\psi][\Phi + (\mu\epsilon)^{\frac{1}{2}}\psi]\mathbf{E} = [\Phi, \psi][-(\mu\epsilon)^{\frac{1}{2}}\mathbf{E} + \mathbf{e}_{(x)}\times\mathbf{B}], \quad (5.20a)$$

$$[\Phi - (\mu\epsilon)^{\frac{1}{2}}\psi][\Phi + (\mu\epsilon)^{\frac{1}{2}}\psi]\mathbf{B} = -(\mu\epsilon)^{\frac{1}{2}}[\Phi, \psi][\mathbf{B} + (\mu\epsilon)^{\frac{1}{2}}\mathbf{e}_{(x)}\times\mathbf{E}]. \quad (5.20b)$$

Then we neglect $[\Phi, \psi]$, solve $E^{(y)}$ and $E^{(z)}$ by substituting the Fourier transform of **E** into (5.20a) and breaking it into two first order d.e.'s. Thus,

$$(\Phi - \mu^{\frac{1}{2}}\psi)\mathbf{F}(k, t) = 0, \tag{5.21a}$$

and

$$(\Phi + \mu^{\frac{1}{2}}\psi)\mathbf{E}(k, t) = \mathbf{F}(\mathbf{k}, t), \tag{5.21b}$$

where $\partial/\partial x$ is replaced by ik in Φ. Then their solutions are

$$\mathbf{F}(\mathbf{k}, t) = \alpha \exp\left(-\int_0^t \frac{a[\cosh at - (\mu\epsilon)^{\frac{1}{2}} \sinh at] + ik}{\sinh at - (\mu\epsilon)^{\frac{1}{2}} \cosh at}\, dt\right), \tag{5.22a}$$

$$\mathbf{E}(\mathbf{k}, t) = \exp\left(-\int_0^t \frac{a[\cosh at + (\mu\epsilon)^{\frac{1}{2}} \sinh at] + ik}{\sinh at + (\mu\epsilon)^{\frac{1}{2}} \cosh at}\, dt\right) \times \left[\boldsymbol{\beta} + \int_0^t \frac{\mathbf{F}(k, \eta)}{(\mu\epsilon)^{\frac{1}{2}} + \tanh a\eta} \times \exp\left(\int_0^\eta d\xi \frac{ik + a[\cosh a\xi + (\mu\epsilon)^{\frac{1}{2}} \sinh a\xi]}{\sinh a\xi + (\mu\epsilon)^{\frac{1}{2}} \cosh a\xi}\right) d\eta\right]. \tag{5.22b}$$

Examining the behavior near $t \sim 0$ reveals that the **F** term of **E** in (5.22) represents a $-x$ traveling wave with increasing amplitude as $t \gtrsim 0$. Since, initially, we have only $+x$ traveling wave and the boundary conditions (5.14) eliminate reflected waves for propagation along the direction of acceleration in a simple medium, then $\mathbf{a} = \mathbf{0}$ and we can orient the yz axis to have the solution

$$E^{(x)} = 0, \quad E^{(z)} = 0,$$

$$E^{(y)} = \int \frac{dk}{2\pi} e^{ikx}\beta(k) \times \exp\left(-\int_0^t \frac{a[\cosh at + (\mu\epsilon)^{\frac{1}{2}} \sinh at] + ik}{(\sinh at + (\mu\epsilon)^{\frac{1}{2}} \cosh at)}\, dt\right) \tag{5.23a}$$

as the first approximation; the corresponding **B** is then obtained by (5.20) with an initial $B^{(z)} = (\mu\epsilon)^{\frac{1}{2}} e^{ikx}$ and no (y, x) components:

$$B^{(x)} = 0, \quad B^{(y)} = 0, \quad B^{(z)} = (\mu\epsilon)^{\frac{1}{2}} E^{(y)}. \tag{5.23b}$$

A higher Nth-order solution is obtained by substituting (5.23) into the right side of (5.20) and solving the two first order d.e.'s as (5.21) but with source in (5.21a).

If near $t \sim 0$ the propagation has a single wavelength $2\pi/k_0$, then we have $\beta(k) = 2\pi\delta(k - k_0)$ and $E^{(y)}$ is

$$E^{(y)} = e^{ik_0 x} \exp\left(-ik_0 \int_0^t \frac{dt}{\sinh at + (\mu\epsilon)^{\frac{1}{2}} \cosh at}\right) \times \exp\left(-a \int_0^t \frac{1 + (\mu\epsilon)^{\frac{1}{2}} \tanh at}{(\mu\epsilon)^{\frac{1}{2}} + \tanh at}\, dt\right), \quad t > 0. \tag{5.24}$$

This is the first-order (neglecting $[\Phi, \psi]$) steady-state wave propagation in an accelerated simple medium with its phase and amplitude chosen with respect to an arbitrary origin of coordinate time t, namely, $t = 0$ at which time the physical wavelength to all $\{O\}$ is $2\pi/k_0$. Physically, we can interpret that, for $t < 0$, a $\omega_0 \equiv k_0/(\mu\epsilon)^{\frac{1}{2}}$ plane wave has already been propagating in the inertial simple medium; then at $t = 0$ the medium is a-accelerated and the wave begins to obey the new law (5.19), as in Fig. 2. Since no reflection exists, whether there is acceleration or not, it propagates according to (5.24) in first order; also for region $x > x_s$, in which the wave has not reached at $t = 0$, a step function $S[x - x_s - w(t)]$ is multiplied to solution (5.24). Here

$$w(t) \equiv [(\mu\epsilon)^{\frac{1}{2}} \cosh at + \sinh at]^{-1} \tag{5.25}$$

is the new coordinate phase velocity, but its proper physical value to $\{0\}$ is, by using (2.8),

$$w^{(x)} = (\mu\epsilon)^{-\frac{1}{2}}, \tag{5.26}$$

which shows to local observers in $\{x^\mu\}$ that acceleration does not affect the phase velocity. Since, if the wave is once $e^{ik_0 x}$ x-dependent, it is always so; the acceleration can begin at any time $t < 0$ and (5.24) still holds with normalization fixed with respect to that $t = 0$ arbitrarily. The instantaneous red-shifted proper frequency to $\{O\}$ is

$$\omega = \frac{k_0}{(\mu\epsilon)^{\frac{1}{2}} \cosh at + \sinh at} \xrightarrow{at \to \text{large}} \frac{2k_0}{1 + (\mu\epsilon)^{\frac{1}{2}}} e^{-at}, \tag{5.27}$$

which results as propagating in the simple medium against an equivalent gravity. The constant-phase wavefront can propagate a maximum coordinate

distance

$$\Delta(x)_{\max} = \int_0^\infty w(t)\,dt$$

$$= \begin{cases} \dfrac{2}{a}\dfrac{\tan^{-1}\{(\mu\epsilon-1)^{\frac{1}{2}}/[(\mu\epsilon)^{\frac{1}{2}}+1]\}}{(\mu\epsilon-1)^{\frac{1}{2}}} & \text{if } \mu\epsilon > 1, \\ \dfrac{2}{a}\dfrac{\tanh^{-1}\{(1-\mu\epsilon)^{\frac{1}{2}}/[1+(\mu\epsilon)^{\frac{1}{2}}]\}}{(1-\mu\epsilon)^{\frac{1}{2}}} & \text{if } \mu\epsilon < 1 \end{cases}$$

$$\xrightarrow{\mu\epsilon\to 1} \frac{1}{a}, \tag{5.28}$$

which shows in the equivalent gravitation that an EM wave can propagate arbitrarily far into a medium iff $\mu\epsilon \to 0$ which is the case of infinite phase velocity in the rest frame of the medium. See Fig. 3.

The third term in (5.24),

$$\exp\left(-a\int_0^t \frac{1+(\mu\epsilon)^{\frac{1}{2}}\tanh at}{(\mu\epsilon)^{\frac{1}{2}}+\tanh at}\,dt\right) = \frac{1}{\cosh at + (\mu\epsilon)^{-\frac{1}{2}}\sinh at}, \tag{5.29}$$

shows amplitude decreasing. This can be interpreted as the slowing down of the coordinate phase velocity which reduces the number of waves in unit time passing some $\{O\}$ or as the decrease of the "dressed photons" density with respect to the initial value by applying instantaneous Lorentz transform (5.5) to velocity (5.26).[34] Also, (5.24) reveals that polarization of this propagation is not affected by the apparent gravity.

Finally, if we want to make a particlelike photon model for this wave, then with

$$\omega = \text{proper energy of photon} = \hat{\mathbf{P}}\cdot\hat{\mathbf{u}} = P_0,$$

$$\frac{P^1}{P^0} = \frac{w^1}{w^0} = \frac{dx^1}{dx^0} = w(t),$$

where $\hat{\mathbf{w}}$ is the photon 4-velocity, we get a dressed mass

$$m = \frac{k_0(\mu\epsilon-1)^{\frac{1}{2}}}{(\mu\epsilon)^{\frac{1}{2}}[(\mu\epsilon)^{\frac{1}{2}}\cosh at + \sinh at]} \tag{5.30a}$$

and w_1 or P_1,

$$w_1 = \frac{-[\cosh at + (\mu\epsilon)^{\frac{1}{2}}\sinh at]}{(\mu\epsilon-1)^{\frac{1}{2}}},$$

$$P_1 = \frac{-k_0[\cosh at + (\mu\epsilon)^{\frac{1}{2}}\sinh at]}{(\mu\epsilon)^{\frac{1}{2}}[(\mu\epsilon)^{\frac{1}{2}}\cosh at + \sinh at]}, \tag{5.30b}$$

which shows, since $g_{\mu\nu}$ independent of x^1 implies $w_1 = \text{const}$ for a massy particle and $P_1 = \text{const}$ for a massless particle along their geodesics,[35] that this "photon in accelerated media" does not propagate along a geodesic nor is it massless and path null. This just demonstrates again that a wave in a noninertial moving medium is dragged along by it. (See Fig. 3.)

All these results are caused partly by the particular behavior of the accelerated coordinate and partly by the presence of the medium. If we instantaneously Lorentz transform (5.24) to the lab. $\{X^{\bar\mu}\}$, then

$$E^Y = \frac{(\mu\epsilon)^{\frac{1}{2}}[1+(\mu\epsilon)^{\frac{1}{2}}\tanh at]}{(\mu\epsilon)^{\frac{1}{2}}+\tanh at} \times \exp ik_0(X - a^{-1}(1+a^2T^2)^{\frac{1}{2}})e^{-ik_0A(T)}, \tag{5.31}$$

where

$$A(t) \equiv \begin{cases} \dfrac{2}{a}\dfrac{1}{(1-\mu\epsilon)^{\frac{1}{2}}}\left[\tanh^{-1}\left(\dfrac{(1-\mu\epsilon)^{\frac{1}{2}}}{1+(\mu\epsilon)^{\frac{1}{2}}}\right) - \tanh^{-1}\left(\dfrac{(1-\mu\epsilon)^{\frac{1}{2}}}{1+(\mu\epsilon)^{\frac{1}{2}}}e^{-at}\right)\right] & \text{if } \mu\epsilon < 1, \\ \dfrac{2}{a}\dfrac{1}{(\mu\epsilon-1)^{\frac{1}{2}}}\left[\tan^{-1}\left(\dfrac{(\mu\epsilon-1)^{\frac{1}{2}}}{1+(\mu\epsilon)^{\frac{1}{2}}}\right) - \tan^{-1}\left(\dfrac{(\mu\epsilon-1)^{\frac{1}{2}}}{1+(\mu\epsilon)^{\frac{1}{2}}}e^{-at}\right)\right] & \text{if } \mu\epsilon > 1, \end{cases} \tag{5.32}$$

and $A(t)$ approaches $T/(\mu\epsilon)^{\frac{1}{2}}$ for small at such that

$$E^Y \begin{cases} \xrightarrow{\mu\epsilon\to 1} e^{ik_0(X-T)} \\ \xrightarrow{a\to 0} e^{ik_0[X-T/(\mu\epsilon)^{\frac{1}{2}}]}. \end{cases} \tag{5.33}$$

So, as it should be, (5.24) in the vacuum limit is nothing but a simple plane wave in $\{X^{\bar\mu}\}$ seen by accelerated observers $\{O\}$, and in the $a \to 0$ limit is just a plane wave in ordinary simple media. The instantaneous phase velocity in $\{X^{\bar\mu}\}$ from (5.31) is

$$\left.\frac{dX}{dT}\right|_{\text{constant phase}} = \frac{1}{(1+a^2T^2)^{\frac{1}{2}}}\left(aT + 2[(1+a^2T^2)^{\frac{1}{2}} - aT] \times \frac{1}{[1+(\mu\epsilon)^{\frac{1}{2}}] + [(\mu\epsilon)^{\frac{1}{2}}-1][(1+a^2T^2)^{\frac{1}{2}} - aT]^2}\right) \tag{5.34}$$

which, as it approaches 1 in the vacuum limit, is dragged along by the medium accordingly increasing (or decreasing) from $(\mu\epsilon)^{-\frac{1}{2}}$ to 1 from $T=0$ to $T=\infty$, when the medium velocity approaches $+1$ as it should be that any velocity in its rest frame approaches 1 in $\bar{K}$. The instantaneous frequency $\bar{\omega}$ in $\{X^{\bar{\mu}}\}$ is just (5.34) multiplied by k_0 and changes from ω_0 $[\equiv k_0/(\mu\epsilon)^{\frac{1}{2}}]$ to $\omega_0(\mu\epsilon)^{\frac{1}{2}}$ as the medium accelerates fast. The amplitude of E^Y is dragged from the initial 1 to $(\mu\epsilon)^{\frac{1}{2}}$ as $T\to\infty$.

The above dragging effects in $\{X^{\bar{\mu}}\}$ manifest themselves for small $V=\tanh aT\sim aT$ since

$$\frac{\bar{\omega}}{\omega_0}=1+V(\mu\epsilon)^{\frac{1}{2}}-\frac{V}{(\mu\epsilon)^{\frac{1}{2}}}+O(V^2)$$

and

$$|E^Y|=1+V(\mu\epsilon)^{\frac{1}{2}}-\frac{V}{(\mu\epsilon)^{\frac{1}{2}}}+O(V^2),\quad \text{as}\quad V\to 0. \tag{5.35}$$

But, in $\{X^{\bar{\mu}}\}$, the corresponding observations of a steady EM plane wave, which x-propagates with frequency ω_0 and amplitude 1 in a simple medium having a small velocity β in the $+X$ direction relative to $\{X^{\bar{\mu}}\}$, are

$$\bar{\omega}/\omega_0=1+\beta(\mu\epsilon)^{\frac{1}{2}}+O(\beta^2),$$
$$|E^Y|=1+\beta(\mu\epsilon)^{\frac{1}{2}}+O(\beta^2). \tag{5.36}$$

Comparing (5.35) with (5.36), we see that, the "denser" $(\mu\epsilon\gg 1)$ the medium is, the more obvious the dragging manifests itself.

6. APPLICATION TO STEADY ROTATING MEDIA

A. Formulation

Consider a lab. cylindrical inertial frame $\{X^{\bar{\mu}}\}\equiv\{T,R,\Phi,Z\}$; then

$$T=t,\quad R=r,\quad \Phi=\phi+\Omega(r)t,\quad Z=z \tag{6.1}$$

carry $\{X^{\bar{\mu}}\}$ to a steady medium-corotating frame $\{x^\mu\}\equiv\{t,r,\phi,z\}$ so that a fixed point (x^i) rotates with $\Omega\equiv\Omega(r)$ about the Z axis in the lab. $\bar{K}$. Since Ω must satisfy $r\Omega<1$, it is impossible to have $\Omega=$ const rotation for large media, and the most possible "rightlike" continuous rotation $\Omega(r)$ should be

$$\Omega(r)=\Omega_0+O(\Omega_1 r),\quad \text{as}\quad \Omega_0 r\ll 1,$$
$$\Omega(r)\to r^{-1},\quad \text{as}\quad r\to\infty, \tag{6.2}$$
$$\Omega(r_1)>\Omega(r_2),\quad \text{if}\quad r_1<r_2.$$

For example, if the proper centrifugal acceleration of a rotating observer is to be proportional to r with proportionality constant Ω_0^2, then

$$\Omega(r)=\Omega_0/(1+r^2\Omega_0^2)^{\frac{1}{2}},$$

which satisfies (6.2) and can be taken as the relativistic analog to "rigid" rotation.

Now, in the $\{x^\mu\}$ of (6.1), we have metric

$$g_{\mu\nu}=\begin{pmatrix}1-r^2\Omega^2 & -r^2t\Omega\Omega' & -r^2\Omega & 0\\ -r^2t\Omega\Omega' & -(1+\Omega'^2r^2t^2) & -r^2t\Omega' & 0\\ -r^2\Omega & -r^2t\Omega' & -r^2 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}, \tag{6.3}$$

and a use of (2.13) and (2.15) gives a convenient local tetrad $\{\hat{\mathbf{e}}_{(\mu)}\}$ for the corotating observers $\{O\}$ as

$$\hat{\mathbf{e}}_{(t)}=(1-r^2\Omega^2)^{-\frac{1}{2}}\hat{\mathbf{e}}_t,$$
$$\hat{\mathbf{e}}_{(r)}=\hat{\mathbf{e}}_r-\Omega' t\hat{\mathbf{e}}_\phi,$$
$$\hat{\mathbf{e}}_{(\phi)}=\frac{(1-r^2\Omega^2)^{\frac{1}{2}}}{r}\left(\hat{\mathbf{e}}_\phi+\frac{r^2\Omega}{1-r^2\Omega^2}\hat{\mathbf{e}}_t\right), \tag{6.4}$$
$$\hat{\mathbf{e}}_{(z)}=\hat{\mathbf{e}}_z,$$

so that they are instantaneous Lorentz transforms of $\{\hat{\mathbf{e}}_{(\bar{\mu})}\}$ of $\bar{K}$. Then, similarly to (5.6), in $\{x^\mu\}$,

$$J^\mu=(l(\rho+r\Omega J^{(\phi)}),J^{(r)},(J^{(\phi)}/lr)-\Omega' tJ^{(r)},J^{(z)}), \tag{6.5a}$$

$$F^{0i}=(l(-E^{(r)}+r\Omega B^{(z)}),(-E^{(\phi)}/r)+l\Omega' t(E^{(r)}-r\Omega B^{(z)}),-l(E^{(z)}+r\Omega B^{(r)})),$$
$$F^{12}=-B^{(r)}/r,\quad F^{13}=B^{(\phi)},$$
$$F^{23}=(-B^{(r)}/lr)-\Omega' tB^{(\phi)}, \tag{6.5b}$$

$$G^{\mu\nu}=[\text{replacing }(\mathbf{E},\mathbf{B})\to(\mathbf{D},\mathbf{H})\text{ in (6.5b)}] \tag{6.5c}$$

express the tensor current and EM field in terms of their local physical values to $\{0\}$, where $l\equiv(1-r^2\Omega^2)^{-\frac{1}{2}}$. Also, since $\{O\}$ is fixed to the medium, this physical constitutive relation is simply (5.10). Now,

with (6.4), for $\{O\}$ in $\{x^\mu\}$, we obtain the local Maxwell equations

$$\begin{cases} \left(\frac{1}{lr}\frac{\partial}{\partial r}(lrD^{(r)}) + \frac{1}{lr}\frac{\partial}{\partial\phi}D^{(\phi)} + \frac{\partial}{\partial z}D^{(z)}\right) \\ \qquad + \Omega' t\frac{\partial}{\partial\phi}(r\Omega H^{(z)} - D^{(r)}) \\ \quad = \rho + r\Omega J^{(\phi)} - r\Omega\frac{\partial}{\partial z}H^{(r)} + \frac{1}{lr}\frac{\partial}{\partial r}(lr^2\Omega H^{(z)}), \\ \left(\frac{1}{lr}\frac{\partial}{\partial\phi}H^{(z)} - \frac{\partial}{\partial z}H^{(\phi)}\right) + lr\Omega\frac{\partial}{\partial t}H^{(z)} \\ \quad = J^{(r)} + l\frac{\partial}{\partial t}D^{(r)}, \qquad (6.6) \\ \left(\frac{\partial}{\partial z}H^{(r)} - \frac{\partial}{\partial r}H^{(z)}\right) + l^2r\Omega^2H^{(z)} + \Omega' t\frac{\partial}{\partial\phi}H^{(z)} \\ \quad = J^{(\phi)} + l\frac{\partial}{\partial t}D^{(\phi)} - l^2r\Omega' D^{(r)}, \\ \left(\frac{1}{r}\frac{\partial}{\partial r}(rH^{(\phi)}) - \frac{1}{lr}\frac{\partial}{\partial\phi}H^{(r)}\right) \\ \qquad - lr\Omega\frac{\partial}{\partial t}H^{(r)} - \Omega' t\frac{\partial H^{(\phi)}}{\partial\phi} \\ \quad = J^{(z)} + l\frac{\partial}{\partial t}D^{(z)}, \end{cases}$$

[replacing $\mathbf{D}\to\mathbf{B}$, $\mathbf{H}\to-\mathbf{E}$, $\mathbf{J}\to 0$ in (6.6)] (6.7)

and, from (6.6), the continuity equations

$$\left(\frac{1}{r}\frac{\partial}{\partial r}rJ^{(r)} + \frac{1}{lr}\frac{\partial}{\partial\phi}J^{(\phi)} + \frac{\partial}{\partial z}J^{(z)}\right) - \Omega' t\frac{\partial}{\partial\phi}J^{(r)} = -l\frac{\partial}{\partial t}(\rho + r\Omega J^{(\phi)}). \quad (6.8)$$

The boundary conditions for $\{O\}$ at the media discontinuity are again just (4.17). The behavior of the rotating local $\{\hat{\mathbf{e}}_{(\mu)}\}$ and coordinate $\{\hat{\mathbf{e}}_\mu\}$ in the inertial $\bar{K}$ is easily seen in Fig. 4 which explains the mixing and scaling in (6.5).

The $\hat{\mathbf{e}}$ and $\hat{\mathbf{K}}$ have components in this $\{x^\mu\}$, expressed by their local physical values $\epsilon^{(\mu)(\nu)}$ and $K^{(\mu)(\nu)}$ to $\{O\}$:

$$\epsilon^{\mu\nu} = \begin{pmatrix} l^2(\epsilon^{(0)(0)} + r^2\Omega^2\epsilon^{(2)(2)}) & lr\Omega\epsilon^{(2)(1)} & -lr\Omega\Omega' t\epsilon^{(2)(1)} + \Omega\epsilon^{(2)(2)} & lr\Omega\epsilon^{(2)(3)} \\ lr\Omega\epsilon^{(1)(2)} & \epsilon^{(1)(1)} & -\Omega' t\epsilon^{(1)(1)} + (lr)^{-1}\epsilon^{(1)(2)} & \epsilon^{(1)(3)} \\ -lr\Omega\Omega' t\epsilon^{(1)(2)} + \Omega\epsilon^{(2)(2)} & -\Omega' t\epsilon^{(1)(1)} + (lr)^{-1}\epsilon^{(2)(1)} & \Omega'^2t^2\epsilon^{(1)(1)} - \frac{\Omega' t}{lr}(\epsilon^{(1)(2)} + \epsilon^{(2)(1)}) + \frac{1}{l^2r^2}\epsilon^{(2)(2)} & -\Omega' t\epsilon^{(1)(3)} + \frac{1}{lr}\epsilon^{(2)(3)} \\ lr\Omega\epsilon^{(3)(2)} & \epsilon^{(3)(1)} & -\Omega' t\epsilon^{(3)(1)} + (lr)^{-1}\epsilon^{(3)(2)} & \epsilon^{(3)(3)} \end{pmatrix} \quad (6.9)$$

$$K^{\mu\nu} = [\text{replacing } \epsilon^{(\mu)(\nu)}\to K^{(\mu)(\nu)} \text{ in (6.9)}], \quad (6.10)$$

which then construct an observer-independent constitutive tensor $C^{\mu\nu\alpha\beta}$ according to (3.1).

Finally, consider the special case of a rotating medium, with $r\Omega \ll 1$ throughout, which rotates rigidly. Then $\Omega' = 0$ and the local equations (6.6)–(6.8) for $\{O\}$ can be written in 3-vector forms, respectively, as

$$\begin{cases} \nabla\times\mathbf{H} + l\frac{\partial}{\partial t}[(\boldsymbol{\Omega}\times\mathbf{r})\times\mathbf{H}] + l^2\boldsymbol{\Omega}\times[\boldsymbol{\Omega}\times(\mathbf{r}\times\mathbf{H})] \\ \qquad = \mathbf{J} + l\frac{\partial}{\partial t}\mathbf{D}, \qquad (6.11) \\ \nabla\cdot\mathbf{D} - l^2\mathbf{D}\cdot\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\mathbf{r}) \\ \qquad = \rho + (1+l^2)\boldsymbol{\Omega}\cdot\mathbf{H} + \boldsymbol{\Omega}\times\mathbf{r}\cdot(\mathbf{J} - \nabla\times\mathbf{H}), \end{cases}$$

$$\begin{cases} \nabla\times\mathbf{E} + l\frac{\partial}{\partial t}[(\boldsymbol{\Omega}\times\mathbf{r})\times\mathbf{E}] + l^2\boldsymbol{\Omega}\times[\boldsymbol{\Omega}\times(\mathbf{r}\times\mathbf{E})] \\ \qquad = -l\frac{\partial}{\partial t}\mathbf{B}, \qquad (6.12) \\ \nabla\cdot\mathbf{B} - l^2\mathbf{B}\cdot\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times\mathbf{r}) \\ \qquad = -(1+l^2)\boldsymbol{\Omega}\cdot\mathbf{E} + \boldsymbol{\Omega}\times\mathbf{r}\cdot\nabla\times\mathbf{E}, \\ \nabla\cdot\mathbf{J} = -l\frac{\partial}{\partial t}(\rho + \mathbf{J}\cdot\boldsymbol{\Omega}\times\mathbf{r}) \qquad (6.13) \end{cases}$$

in the above $\mathbf{r} \equiv r\mathbf{e}_{(r)}$ and $l^{-1}\partial/\partial\phi$ replaces $\partial/\partial\phi$ in ∇; also, it corrects the previous mistake[36] in trying to get the $\nabla\times$ equations.

B. Plane-Wave Scattering by a Simple Rotating Sphere

Consider a rigidly rotating simple sphere of radius a surrounded by an ϵ_0, μ_0 simple medium in the inertial laboratory frame $\bar{K}$. This sphere then scatters plane waves as shown in Fig. 5. If we neglect medium internal strain changes due to rotation, the constitutive relations are just $\mathbf{D} = \epsilon\mathbf{E}$ and $\mathbf{H} = \mu^{-1}\mathbf{B}$ to corotating $\{O\}$. But now the local Maxwell equations are most naturally expressed in the spherical corotating frame $\{x^\mu\} \equiv \{t, r, \theta, \phi\}$ related to the laboratory $K\{x^{\bar\mu}\} \equiv \{T, R, \Theta, \Phi\}$ by[37]

$$T = t, \quad R = r, \quad \Theta = \theta, \quad \Phi = \phi + \Omega t, \quad \Omega = \text{const} \quad (6.14)$$

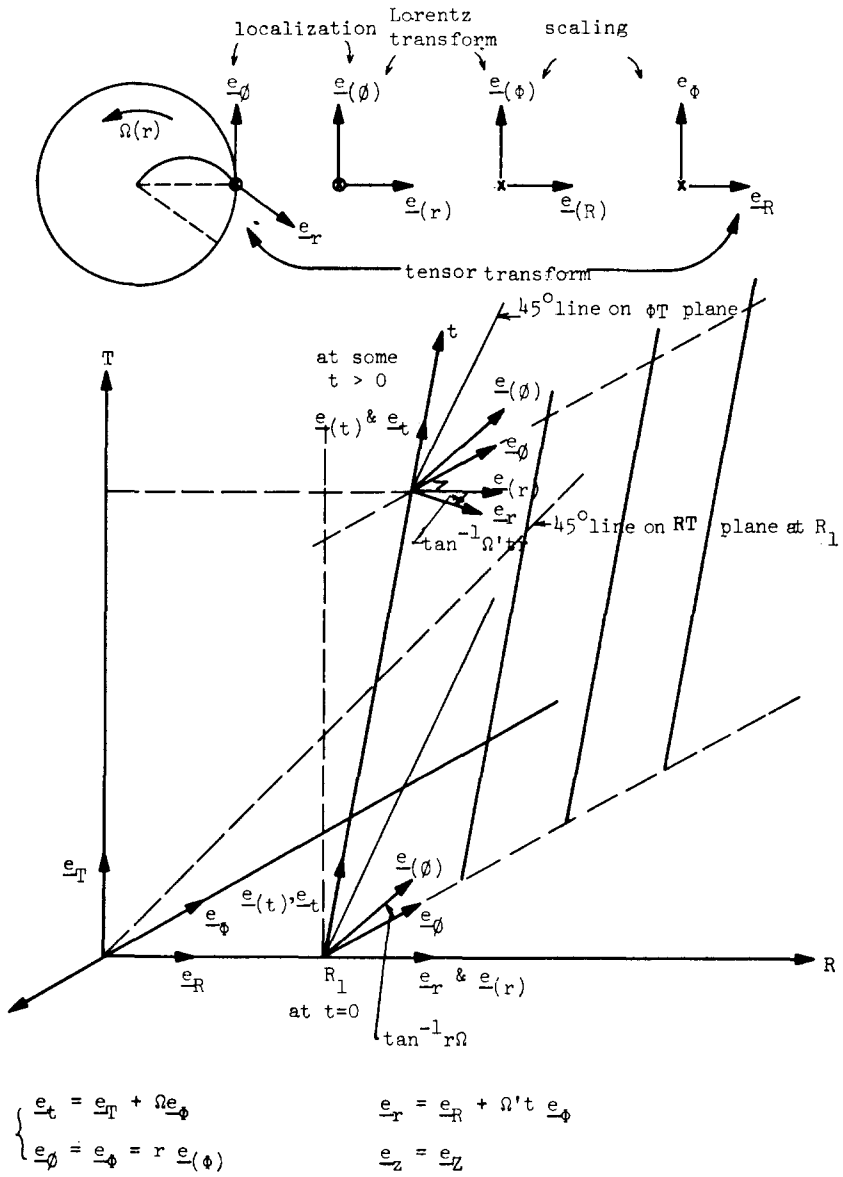


FIG. 4. Space-time diagram and physical picture showing relations among $\{\hat{\mathbf{e}}_{(\mu)}\}$, $\{\hat{\mathbf{e}}_{\mu}\}$, and $\{\hat{\mathbf{e}}^{\mu}\}$.

to fit the boundary and thus simplify the mathematics. But the spherical $\{O\}$ in this $\{x^{\mu}\}$ of (6.14) only differs from those $\{O\}$ in $\{x^{\mu}\}$ of (6.1) by their spatial triad orientations. So, for the spherical rotating observers, choosing the local basis

$$\hat{\mathbf{e}}_{(t)} = l\hat{\mathbf{e}}_t, \quad \hat{\mathbf{e}}_{(r)} = \hat{\mathbf{e}}_r, \quad \hat{\mathbf{e}}_{(\theta)} = r^{-1}\hat{\mathbf{e}}_\theta,$$
$$\hat{\mathbf{e}}_{(\phi)} = lr\Omega \sin\theta\hat{\mathbf{e}}_t + (lr\sin\theta)^{-1}\hat{\mathbf{e}}_\phi, \tag{6.15}$$

we see that the local Maxwell equations are just the 3-vector interpretation of (6.11) and (6.12) in spherical coordinate convention; here, $l \equiv (1 - r^2\Omega^2\sin^2\theta)^{-\frac{1}{2}}$.

Now, substituting $\mathbf{D} = \epsilon\mathbf{E}$ and $\mathbf{H} = \mu^{-1}\mathbf{B}$ into (6.11) gives

$$\nabla \times \mathbf{B} + l\frac{\partial}{\partial t}[(\boldsymbol{\Omega} \times \mathbf{r}) \times \mathbf{B}] + l^2\boldsymbol{\Omega} \times [\boldsymbol{\Omega} \times (\mathbf{r} \times \mathbf{B})]$$
$$= l\mu\epsilon\frac{\partial}{\partial t}\mathbf{E} + \mu\mathbf{J}, \tag{6.16}$$

$$\nabla \cdot \mathbf{E} - l^2\mathbf{E} \cdot \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \mathbf{r}) - \rho/\epsilon$$
$$= (\mu\epsilon)^{-1}(1 + l^2)\boldsymbol{\Omega} \cdot \mathbf{B} - (\mu\epsilon)^{-1}\boldsymbol{\Omega} \times \mathbf{r} \cdot \nabla \times \mathbf{B},$$

which, with (6.12) and suitable boundary conditions, gives the whole local electrodynamics in rotating frame.

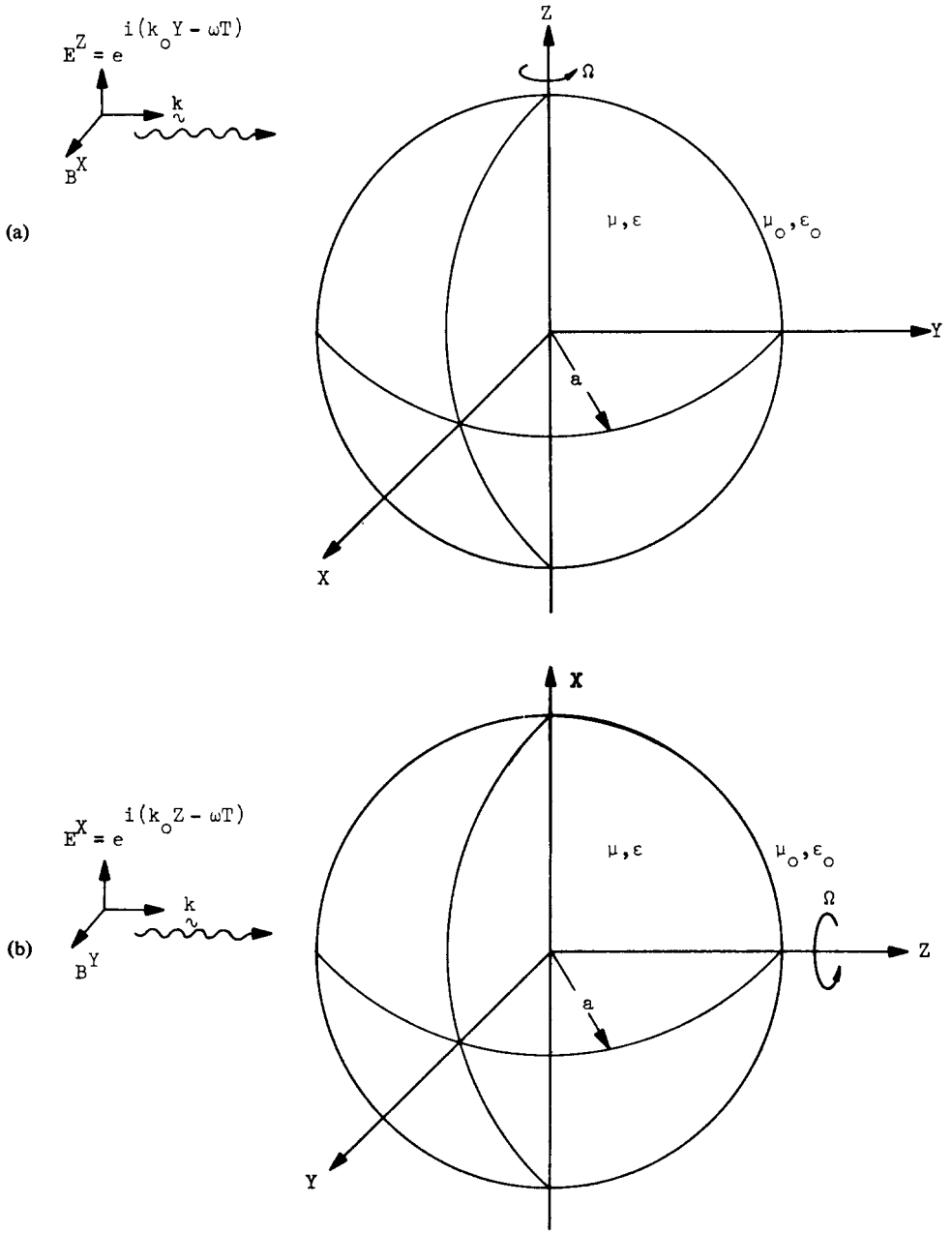


FIG. 5. (a) Perpendicular incidence of rotational scattering; (b) parallel incidence of rotational scattering.

But now, instead of solving EM scattering for rotating observers, we are interested in the scattered field in $\bar{R}$. Thus, we must find the transformed local equations (6.12) and (6.16) in $\bar{R}$ by substituting tensor transforms $\partial/\partial x^\alpha = (\partial X^\lambda/\partial x^\alpha)(\partial/\partial X^\lambda)$ from (6.14) and instantaneous Lorentz transforms. Then (6.16) gives

$$R < a \begin{cases} \bar{\nabla} \times \bar{\mathbf{B}} = -\left(\Omega \dfrac{\partial}{\partial \Phi} \bar{\mathbf{E}} - \mathbf{V} \bar{\nabla} \cdot \bar{\mathbf{E}}\right) + \left(\dfrac{\partial}{\partial T} + \Omega \dfrac{\partial}{\partial \Phi}\right)[\mu\epsilon \bar{\mathbf{E}} + (l^2 - 1)(\mu\epsilon - 1)\bar{\mathbf{E}}_\perp + l^2(\mu\epsilon - 1)\mathbf{V} \times \bar{\mathbf{B}}], \\ \epsilon \bar{\nabla} \cdot \bar{\mathbf{E}} = -\dfrac{(\mu\epsilon - 1)}{\mu} \bar{\nabla} \cdot [(l^2 - 1)\bar{\mathbf{E}}_\perp + l^2 \mathbf{V} \times \bar{\mathbf{B}}], \end{cases} \tag{6.17}$$

and (6.12) just gives the ordinary equations

$$\bar{\nabla} \times \bar{\mathbf{E}} = -\frac{\partial}{\partial T}\bar{\mathbf{B}}, \quad \bar{\nabla} \cdot \bar{\mathbf{B}} = 0, \quad \text{all } R, \tag{6.18}$$

as it should; in the above, the source term is zero in the present scattering problem and bar denotes quantities in $\bar{K}$.

Since no coefficients in (6.17) and (6.18) are time dependent, we can simplify equations by assuming $e^{-i\omega T}$ time dependence to $\bar{\mathbf{E}}$, $\bar{\mathbf{B}}$ and obtain wave equation for $\bar{\mathbf{E}}$ inside the region of rotating medium

$$\bar{\nabla} \times \bar{\nabla} \times \bar{\mathbf{E}} - k^2\bar{\mathbf{E}} = i\omega \mathbf{S} \cdot \bar{\mathbf{E}}, \quad R < a, \tag{6.19}$$

where

$$\begin{aligned} \mathbf{S} \equiv & \left[\mathbf{V}\bar{\nabla} + (\mu\epsilon - 1)\Omega\frac{\partial}{\partial\Phi}\mathsf{U}\right] \\ & + (\mu\epsilon - 1)\left(-i\omega + \Omega\frac{\partial}{\partial\Phi}\right) \\ & \times \left[(l^2 - 1)\left(\mathsf{U} - \frac{\mathbf{VV}}{V^2}\right) + \frac{l^2\Omega}{\omega i}\boldsymbol{\lambda}\right] \end{aligned} \tag{6.20}$$

and $k^2 \equiv \omega^2\mu\epsilon$, $\mathsf{U} \equiv$ unit dyadic δ_{ij}, and

$$\boldsymbol{\lambda} \equiv \begin{pmatrix} \dfrac{-\partial}{\partial\Phi} & 0 & \sin\Theta\dfrac{\partial}{\partial R} \\ 0 & \dfrac{-\partial}{\partial\Phi} & \dfrac{\partial}{\partial\Theta}(\sin\Theta) \\ 0 & 0 & 0 \end{pmatrix} \tag{6.21}$$

Compared with the wave equation in a simple medium at rest, the wave equation for outside the sphere now takes the form

$$\bar{\nabla} \times \bar{\nabla} \times \bar{\mathbf{E}} - k_0^2\bar{\mathbf{E}} = 0, \quad R > a, \quad k_0^2 = \omega^2\mu_0\epsilon_0. \tag{6.22}$$

We see that the S in (6.19) is zero either when the sphere is not rotating $\Omega = 0$ or when there is nothing but $\mu = 1 = \epsilon$ vacuum being rotated. Thus, S is purely medium rotating effect.

Now (6.19) and (6.22), with outward going radiation condition on the scattered field at $R = \infty$ and BC's

$$\begin{aligned} & \mu_0^{-1}B^{(\Phi)})_{R=a^+} = \mu^{-1}B^{(\Phi)})_{R=a^-}, \\ & \mu_0^{-1}B^{(\Theta)})_{R=a^+} \\ & \quad = l^2[B^{(\Theta)}(\mu^{-1} - \epsilon V^2) + E^{(R)}V(\epsilon - \mu^{-1})]_{R=a^-}, \\ & \epsilon_0 E^{(R)})_{R=a^+} \\ & \quad = l^2[E^{(R)}(\epsilon - V^2/\mu) - B^{(\Theta)}V(\epsilon - \mu^{-1})]_{R=a^-}, \end{aligned} \tag{6.23}$$

and $B^{(R)}$, $E^{(\Theta)}$, and $E^{(\Phi)}$ continuous across $R = a$, form BVP of scattering. But it is difficult to solve it in closed form, because the inside waves are coupled in modes and cannot be expanded as simple sums of familiar spherical partial waves with arbitrary constants. It can be solved by using an integral iteration method.

First, we combine (6.19) and (6.22) to give us

$$\bar{\nabla} \times \bar{\nabla} \times \bar{\mathbf{E}} - k_0^2\bar{\mathbf{E}} = p(R)[(k^2 - k_0^2)\mathsf{U} + i\omega\mathbf{S}(\mathbf{R})] \cdot \mathbf{E}, \tag{6.24}$$

where $P(R) \equiv 1$ or 0 for $R < a$ or $R > a$, respectively. Now, making use of the familiar Green's function of (6.24),[38]

$$\Gamma(\mathbf{R}, \mathbf{R}') = \left(\mathsf{U} + \frac{1}{k_0^2}\bar{\nabla}\bar{\nabla}\right)\frac{e^{ik|\mathbf{R}-\mathbf{R}'|}}{4\pi|\mathbf{R} - \mathbf{R}'|}, \tag{6.25}$$

we can change (6.24) into an integral equation

$$\begin{aligned} \bar{\mathbf{E}}(\mathbf{R}) = \bar{\mathbf{E}}^{\text{homo}}(\mathbf{R}) + & \int_{R'<a} d^3R'\Gamma(\mathbf{R}, \mathbf{R}') \\ & \cdot [(k^2 - k_0^2)\mathsf{U} + i\omega\mathbf{S}(\mathbf{R}')] \cdot \bar{\mathbf{E}}(\mathbf{R}'), \quad \text{all } R. \end{aligned} \tag{6.26}$$

The $\bar{\mathbf{E}}^{\text{homo}}$ is the solution without the rotating and different medium, so $\bar{\mathbf{E}}^{\text{homo}} = \bar{\mathbf{E}}^{\text{inc}}$. Thus, (6.26) is an integral equation for $R < a$, whose solution then serves as a source of current density

$$\begin{aligned} \mathbf{J}^{\text{equivalent}}(\mathbf{R}) = & (i\omega\mu_0)^{-1} \\ & \times [(k^2 - k_0^2)\mathsf{U} + i\omega\mathbf{S}(\mathbf{R})] \cdot \bar{\mathbf{E}}(\mathbf{R}), \\ & R < a. \end{aligned} \tag{6.27}$$

The iteration approximation is as follows: first we roughly approximate the integrand $\bar{\mathbf{E}}(\mathbf{R}')$ of (6.26) by incident wave and get the first-order total solution; then we put it inside the integration to get the next-order solution, and so on, assuming the iterating series converges. This gives

$$\bar{\mathbf{E}}(R) = \bar{\mathbf{E}}^{\text{inc}}(\mathbf{R}) + \bar{\mathbf{E}}^{\text{sc}}_{\text{Mie}} + \bar{\mathbf{E}}^{\text{sc}}_{\text{Mixed}} + \bar{\mathbf{E}}^{\text{sc}}_{\text{rotating medium}}, \tag{6.28}$$

where scatterings due to different effects were separated as

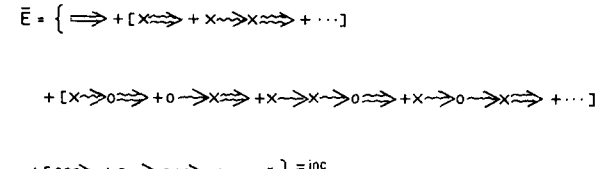
$$\begin{aligned} \bar{\mathbf{E}}^{\text{cs}}_{\text{Mie}} = (k^2 - k_0^2) & \int_{R'<a} d^3R'\Gamma(\mathbf{R}, \mathbf{R}') \\ & \cdot \bar{\mathbf{E}}^{\text{inc}}(\mathbf{R}') + (k^2 - k_0^2)^2 \\ & \times \iint_{R', R''<a} d^3R'd^3R''\Gamma(\mathbf{R}, \mathbf{R}') \\ & \cdot \Gamma(\mathbf{R}', \mathbf{R}'') \cdot \bar{\mathbf{E}}^{\text{inc}}(\mathbf{R}'') + \cdots, \end{aligned} \tag{6.29a}$$

$$\bar{\mathbf{E}}^{sc}_{mixed} = i\omega(k^2 - k_0^2) \iint_{R',R''<a} d^3\mathbf{R}'d^3\mathbf{R}''\Gamma(\mathbf{R},\mathbf{R}') \cdot [\Gamma(\mathbf{R}',\mathbf{R}'')\cdot\mathbf{S}(\mathbf{R}'') + \mathbf{S}(\mathbf{R}') \cdot \Gamma(\mathbf{R}',\mathbf{R}'')]\cdot\bar{\mathbf{E}}^{inc}(\mathbf{R}'') + \cdots, \quad (6.29b)$$

$$\bar{\mathbf{E}}^{sc}_{rotation} = i\omega\int_{R'<a} d^3R'\Gamma(\mathbf{R},\mathbf{R}')\cdot\mathbf{S}(\mathbf{R}')\cdot\bar{\mathbf{E}}^{inc}(\mathbf{R}') + (i\omega)^2 \iint_{R',R''<a} d^3R'd^3R''\Gamma(\mathbf{R},\mathbf{R}') \cdot \mathbf{S}(\mathbf{R}')\cdot\Gamma(\mathbf{R}',\mathbf{R}'')\cdot\mathbf{S}(\mathbf{R}'')\cdot\bar{\mathbf{E}}^{inc}(\mathbf{R}'') + \cdots. \quad (6.29c)$$

The $\bar{\mathbf{E}}^{sc}_{Mie}$ is the well-known Mie[39] scattering of a plane wave by a sphere expressed in different form from the Mie's spherical partial Hertz wave expansion. The $\bar{\mathbf{E}}^{sc}_{rotating}$ is the scattering caused purely by the "something rotating" which occurs even when the rotating sphere is made of the same μ_0 and ϵ_0 medium as its surroundings and when the Mie scatter vanishes. $\bar{\mathbf{E}}^{sc}_{mixed}$ is the scattered field caused by the mixed effects of both the "medium rotation" and the "medium difference," which is a second-order effect.

The physical meaning of (6.28) and (6.29) can be clearly seen graphically. We draw ⇝ for $\Gamma(\mathbf{R},\mathbf{R}')$ as a propagator for waves going from $\mathbf{R}'$ to $\mathbf{R}$, x for $(k^2 - k_0^2)\mathsf{U}$ as a Mie scatterer at $\mathbf{R}'$, o for $i\omega\mathbf{S}(\mathbf{R}')$ as a rotating-medium scatterer at $\mathbf{R}'$, and → as a propagator for direct propagation. Then (6.28) and (6.29) can be represented as



(6.30)

where only double propagator can propagate to all R and integrations are understood. Now, obviously, we can interpret the total field as the sum of these incident waves which directly go through and hit nothing, which are Mie-scattered in the sphere once and propagate out, which are rotationally scattered, propagated to other points in the sphere, Mie-scattered and then propagated out, etc.

From (6.20) and (6.24), the ratio

$$\left|\frac{E^{sc}_{Rot}}{E^{sc}_{Mie}}\right| \sim \frac{(\mu\epsilon - 1)(\mu_0\epsilon_0)^{\frac{1}{2}}a\Omega}{(\mu\epsilon - \mu_0\epsilon_0)} \quad (6.31)$$

is small if $a\Omega \ll 1$, unless $\mu\epsilon \sim \mu_0\epsilon_0$. In either case, the second-order mix-scattering can be neglected and the first-order $\bar{\mathbf{E}}^{sc}_{rot}$ will give a good description of the rotational scattering.

Now consider two kinds of incidences, as in Fig. 5: For Fig. 5(a), we have from (6.29c)

$$\bar{\mathbf{E}}^{inc} = \mathbf{e}_Z e^{i(k_0 Y - \omega T)},$$

$$\bar{\mathbf{E}}^{sc}_{Rot,1st\,order} = i\omega\int_{R'<a} d^3R'\Gamma(\mathbf{R},\mathbf{R}')\cdot\mathbf{S}(\mathbf{R}')\cdot\hat{\mathbf{e}}_Z e^{i(k_0Y' - \omega T)}. \quad (6.32)$$

Then, at far zone $R \gg R'$, $k_0R \gg 1$, we get

$$\bar{\mathbf{E}}^{sc}_{Rot,1st,Far\,zone} = \frac{e^{ik_0R}}{4\pi R} i\omega(\mu\epsilon - 1)(\mathsf{U} - \mathbf{e}_R\mathbf{e}_R)\cdot\mathbf{e}_Z\int_{R'<a} d^3R' \times \left\{-i\omega(l^2 - 1) + l^2ik_0V'\left[2\cos\Phi' + \frac{1}{i\omega}(\Omega\sin\Phi' - ik_0V'\cos^2\Phi')\right]\right\}e^{ik_0(Y' - \mathbf{e}_R\cdot\mathbf{R}')}, \quad (6.33)$$

which integrates to the first order of Ω:

$$\bar{\mathbf{E}}^{sc}_{rot.,\,far\,zone,\,1st} = i8\pi\frac{e^{i(k_0R - \omega T)}}{4\pi R}(\mu\epsilon - 1) \times \frac{\Omega a^2}{(\mu_0\epsilon_0)^{\frac{1}{2}}} f(\Theta,\Phi)\mathbf{e}_{(\Theta)} + O(\Omega^2), \quad (6.34a)$$

$$f(\Theta,\Phi) = \frac{(k_0a)^3\sin^2\Theta\cos\Phi[(3 - \delta^2)\sin\delta - 3\delta\cos\delta]}{\delta^5},$$

$$\delta \equiv k_0a\sqrt{2}(1 - \sin\Theta\sin\Phi). \quad (6.34b)$$

The antisymmetry of this first-order rotational scattering with respect to the (Y, Z) plane is a result of opposite rotational motion of the sphere as seen at the $-Y$ axis of incidence; its symmetry about the $\theta = \frac{1}{2}\pi$ plane results from the fact that the upper and lower halves of the sphere are in identical motion with respect to the incident wave [Fig. 6(a-1)]. Plots of (6.34b) show that, on the $\Theta = \frac{1}{2}\pi$ plane [Figs. 6(a-2, 3)] it has a resemblance to quadrupole radiation such that it can be simply interpreted as radiation from successive electric quadrupole sheaths at $|y| = \text{const}$ caused by induced $\mathbf{V}\times\mathbf{B}^{inc}$ electric polarization at the sphere, however, with forward bending lobes as the effect from traveling wave antennas. This is caused by the traveling of the inducing incident wave, there is no scattering at backward $\Phi = -\frac{1}{2}\pi$ and forward $\Phi = \frac{1}{2}\pi$; but the main lobes bend from side ends toward forward direction more as k_0a becomes larger. Equation

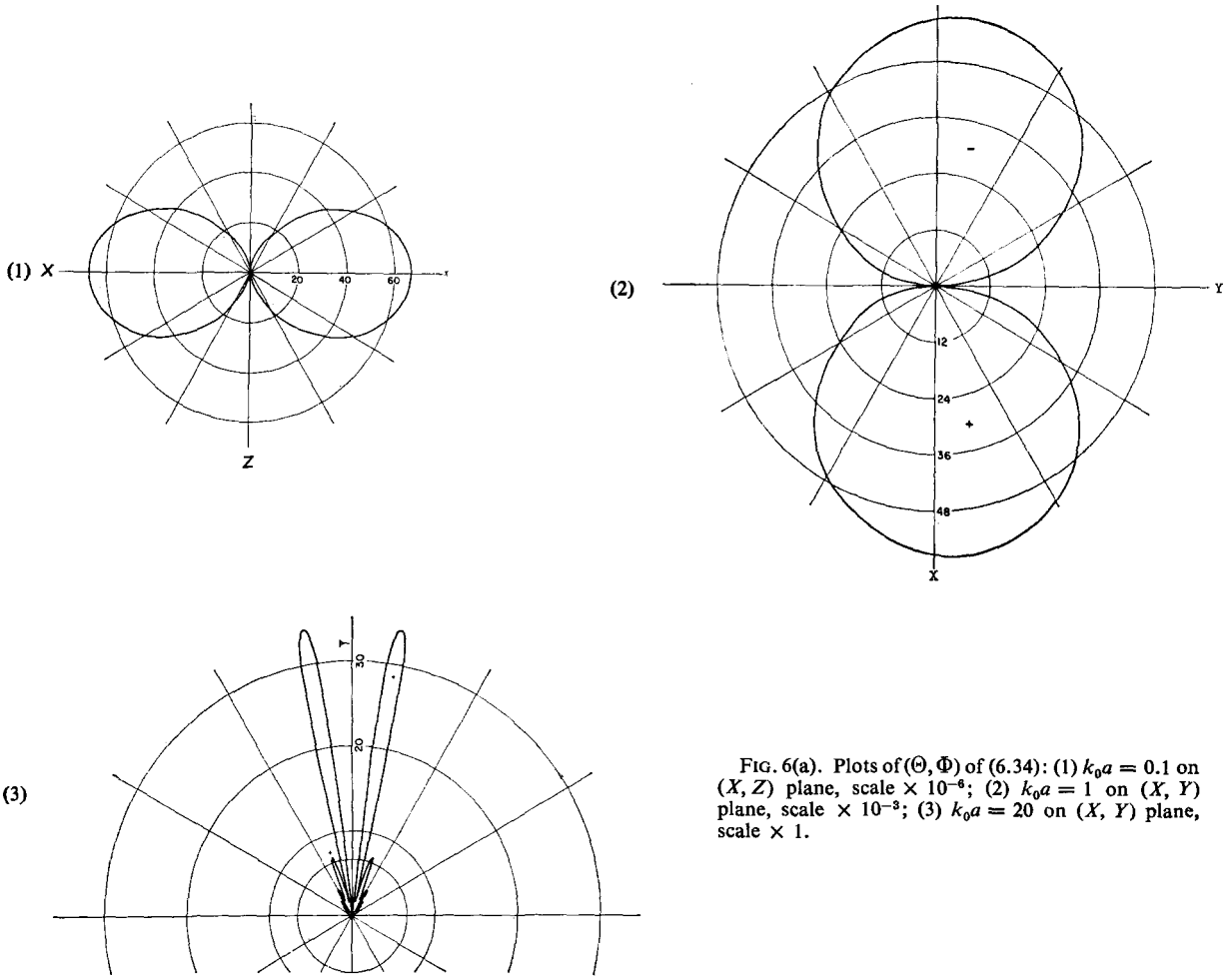


FIG. 6(a). Plots of (Θ, Φ) of (6.34): (1) $k_0a = 0.1$ on (X, Z) plane, scale $\times 10^{-6}$; (2) $k_0a = 1$ on (X, Y) plane, scale $\times 10^{-3}$; (3) $k_0a = 20$ on (X, Y) plane, scale $\times 1$.

(6.34) has only a θ component as the first-order Mie scattering, although the latter has a dipole pattern for scatter amplitude. Also, there is no Doppler frequency shift since the motion of the scatterer is tangential to its boundary and the scattered wave is in the same medium as the incident wave.

For Fig. 5b, we have

$$\mathbf{E}^{\text{inc}} = \mathbf{e}_X e^{i(k_0 Z - \omega T)};$$

then by similar integration, we obtain

$$\mathbf{E}^{\text{sc}}_{\text{rot, far zone, 1st}} = \frac{e^{i(k_0 R - \omega T)}}{4\pi R} 4\pi a^3(\mu\epsilon - 1)i\omega\Omega \cdot \mathbf{f}(\Theta, \Phi) + O(\Omega^2), \quad (6.35a)$$

$$\mathbf{f}(\Theta, \Phi) = -\mathbf{e}_{(\Theta)} \cdot \sin\Phi \left(\cos\Theta \frac{\sin\delta_1 - \delta_1 \cos\delta_1}{\delta_1^3} + (k_0a)^2 \sin^2\Theta \frac{(3 - \delta_2^2)\sin\delta_2 - 3\delta_2\cos\delta_2}{\delta_2^5} \right) - \mathbf{e}_{(\Phi)} \cos\Phi \frac{\sin\delta_1 - \delta_1\cos\delta_1}{\delta_1^3}, \quad (6.35b)$$

where $\delta_1 \equiv 2k_0a \sin\frac{1}{2}\Theta$ and $\delta_2 \equiv k_0a[2(1 - \cos\Theta)]^{\frac{1}{2}}$. The $E^{(\theta)} \sim \sin\Phi$ and $E^{(\Phi)} \sim \cos\Phi$ Φ dependences which are just opposite to those of the corresponding Mie scattering[40] change the polarization of the total scattering. Unlike the previous case, where we had the induced $\nabla \times \mathbf{M} \sim \nabla \times (\mathbf{V} \times \mathbf{E}) \sim 0$, this scattering has contributions from both the P-like and M-like induced polarization sheaths at $|Y| = \text{const}$ as $\mathbf{P} \sim VB \sin\Phi \mathbf{e}_Z$ and $\nabla \times \mathbf{M} \sim \Omega E \mathbf{e}_Y$; accordingly, one can interpret that on the $\Theta = \frac{1}{2}\pi$ plane an $E^{(\theta)} \sim \sin\Phi$ from $\mathbf{P}$ and an $E^{(\Phi)} \sim \cos\Phi$ from $\mathbf{M}$. Plots of (6.35b) show on the (X, Z) plane only an $E^{(\Phi)} \sim \text{const}$ from $\mathbf{M}$ [Fig. 6(b-1, 2)], on the (Y, Z) plane an $E^{(\theta)} \sim \sin\Theta$ from $\mathbf{P}$ and an $E^{(\theta)} \sim \cos\Theta$ from $\mathbf{M}$ [Fig. 6(b-3, 4)]; all are forward drifted or bent from the traveling wave effect as before. The forward and backward rotational scattering which is 90° rotated with respect to the E^{inc} and in the Y direction are perpendicular to the X-polarized Mie scattering and elliptically polarize the total scattered field.

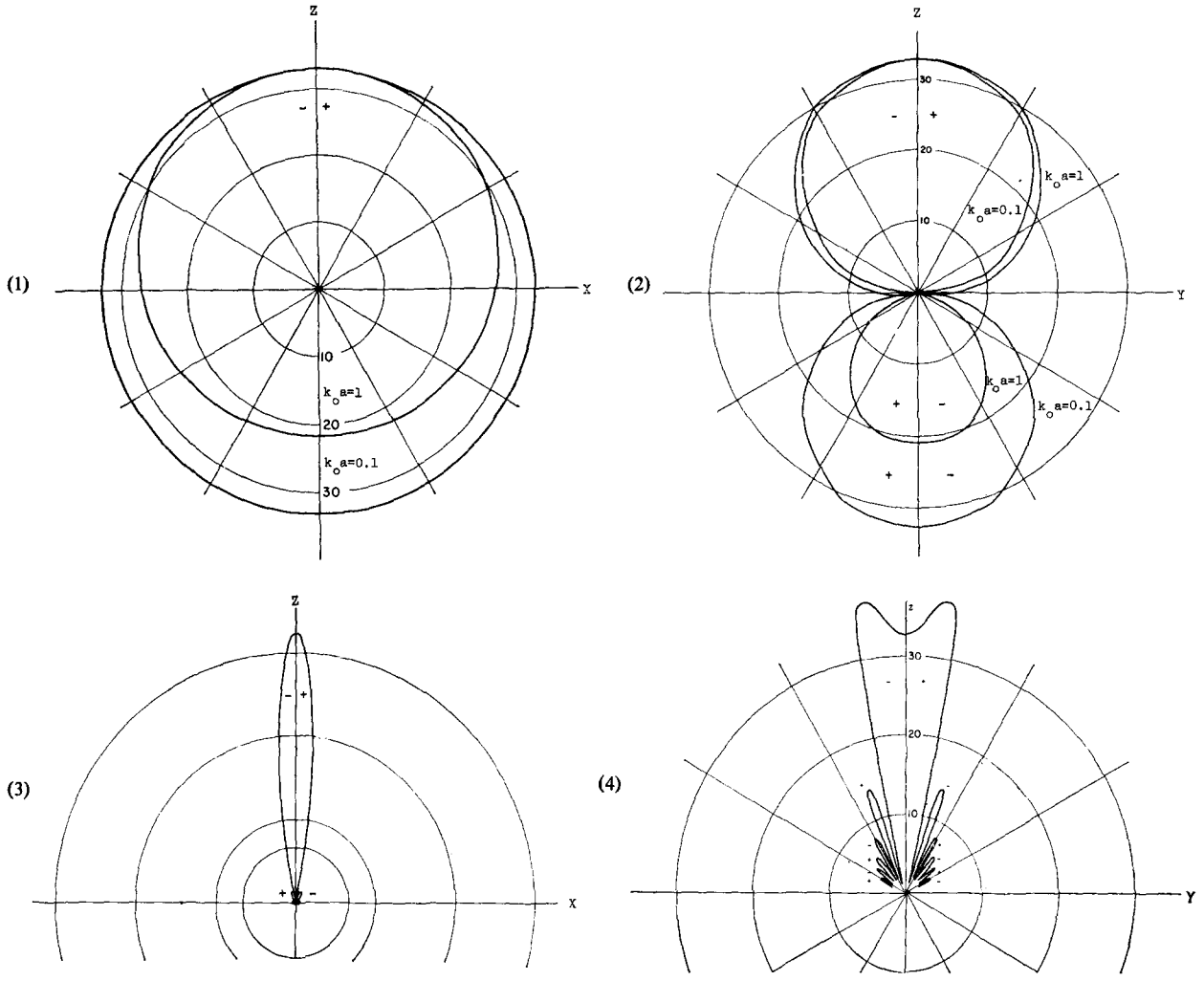


FIG. 6(b). Plots of $f(\Theta, \Phi)$ of (6.35): (1) $k_0 a = 0.1, 1, f^{(\Theta)}$ on (X, Z) plane, scale $\times 10^{-2}$; (2) $k_0 a = 0.1, 1, f^{(\Phi)}$ on (Y, Z) plane, scale $\times 10^{-2}$; (3) $k_0 a = 20, f^{(\Theta)}$ on (X, Z) plane, scale $\times 10^{-3}$; (4) $k_0 a = 20, f^{(\Phi)}$ on (Y, Z) plane, scale $\times 10^{-2}$.

C. Summary of Applications

Applying the theory of Secs. 2–4 to media in linear acceleration and rotation, we find electrodynamic equations for local observable EM fields and sources with physical constitutive relations in these comoving noninertial frames. Studying in detail wave propagation in a simple accelerated medium reveals that EM wave is dragged by the medium with its amplitude changed, frequency shifted and phase velocity dragged along reasonably; its path is neither null nor a geodesic. Scattering of a plane EM wave by a rotating sphere is solved by an integral iteration in the laboratory frame. The rotational scattering is separated from the Mie scattering, and its first-order amplitude for incidences parallel and perpendicular to the rotation axis are evaluated and plotted which agree with intuition and can be interpreted simply as radiation from properly induced traveling electric and magnetic polarization sheaths.

Also, as the simplest cases of coordinate transport (2.17), it turns out that the local physical tetrads for coaccelerating and corotating observers, chosen respectively as the instantaneous Lorentz transforms of the basis of the natural laboratory Cartesian and cylindrical coordinates, are just the unit tangents and Frenet normals of the world lines of these observers. One can easily show that, for $\{\hat{\mathbf{e}}_{(i)}\}$ of the accelerational (5.4),

$$a_x = a, \quad a_y = 0, \quad a_z = 0, \tag{6.36a}$$

and that, for $\{\hat{\mathbf{e}}_{(i)}\}$ of the cylindrical rotational (6.4),

$$a_{r_c} = \frac{-r_c\Omega^2}{1 - r_c^2\Omega^2}, \quad a_\phi = \frac{\Omega}{1 - r_c^2\Omega^2}, \quad a_z = 0, \tag{6.36b}$$

where the a_i are curvatures defined in (2.18).

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† Alfred Sloan Research Fellow, Caltech.

[1] K. S. H. Lee and C. H. Papas, J. Math. Phys. **5**, 1668 (1964); also, IEEE Trans. Antennas Propagation **13**, 799 (1965).

[2] R. T. Compton, Jr., J. Math. Phys. **7**, 2145 (1966); **9**, 1865 (1968).

[3] C. T. Tai, J. Math. Phys. **8**, 646 (1967); also, Radio Sci. **2**, 245 (1967).

[4] P. Daly, K. S. H. Lee, and C. H. Papas, IEEE Trans. Antennas Propagation **13**, 583 (1965).

[5] E. J. Post, Rev. Mod. Phys. **39**, 475 (1967).

[6] E. J. Post and A. Yildiz, Phys. Rev. Letters **15**, 177 (1965).

[7] A. Yildiz and C. Tang, Phys. Rev. **146**, 947 (1966); C. V. Heer, Phys. Rev. **134A**, 799 (1964); C. V. Heer, J. Little, and J. Bupp, Ann. Inst. Henri Poincaré **8**, 311 (1968).

[8] W. M. Irvine, Physica **30**, 1160 (1964).

[9] C. Lanczos, J. Math. Phys. **7**, 316 (1966); **8**, 829 (1967); also, Rev. Mod. Phys. **29**, 337 (1957); V. Bargmann, Rev. Mod. Phys. **29**, 161 (1957).

[10] J. L. Synge, *General Relativity* (Interscience, New York, 1960).

[11] L. Landau and E. Lifshitz, *Classical Theory of Fields* (Addison-Wesley, Reading, Mass., 1962); *Electrodynamics of Continuous Media* (Pergamon, New York, 1960).

[12] A. Einstein, *The Meaning of Relativity* (Princeton U.P., Princeton, N.J., 1955).

[13] P. Penfield and H. Haus, "Electrodynamics of Moving Media," MIT Monograph, Cambridge, Mass., 1967.

[14] See, H. T. Yura, Ph.D. thesis, Caltech, 1961; also, in media, even in an inertial frame, this identification is arbitrary and a $\pm$ sign is included in the definition of the dressed mass. Also, it is obvious that the path is not null.

[15] H. C. Van de Hulst, *Light Scattering by Small Particles* (Wiley, New York, 1957).

[16] For conversion of units to MKS, see T. C. Mo, Ph.D. thesis, Caltech, 1969.

[17] J. A. Wheeler, *Gravitation and Relativity*, H. Y. Chiu and W. F. Hoffman, Eds. (Benjamin, New York, 1964), lectures 3, 4; R. Dicke, *ibid.*, lecture 1; J. A. Anderson, *ibid.*, lecture 2; also, L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1926) and *An Introduction to Differential Geometry* (Princeton U.P., Princeton, N.J., 1940); also the notations $\mu = 0, 1, 2, 3$, $i = 1, 2, 3$, Minkowskian signature $\equiv [+---]$ and $\{x^\mu\} \equiv$ coordinate frame $\{x^\mu\}$ are used throughout. Also, the caret $\hat{}$ denotes 4-space quantities.

[18] This is possible because Etvos' experiment showed $M_{\text{grav}} = M_{\text{inertial}}$, present accuracy 10^{-11}.

[19] For $\{\hat{\mathbf{e}}_{(\mu')}\}$ notice that the local spatial orthogonality to time must be done for geometrical model to coincide with physics; spatial orthogonality within itself is just a convenient choice.

[20] O.N. $\equiv$ orthonormal combinations of.

[21] a_i are curvatures of Γ in $\hat{\mathbf{n}}_i$ direction; also, (2.18) implies $(D/DS)\hat{\mathbf{n}}_3 = -a_3\hat{\mathbf{n}}_2$, D/DS is invariant differentiation.

[22] Reference 16.

[23] Neglect the perturbation of EM field on geometry.

[24] Reference 16.

[25] K. S. Thorne, "Relativistic Stellar Structure and Dynamics," Orange Aid Preprint Series in Nuclear Astrophysics, Caltech, 1966, p. 43.

[26] C. H. Papas, *Theory of Electromagnetic Wave Propagation* (McGraw-Hill, New York, 1965), p. 239.

[27] Reference 16.

[28] C. Møller, *Theory of Relativity* (Oxford U.P., Oxford, 1952), p. 202. Also on momentum density, R. P. Feynman, Lecture Notes on Quantum Mechanics, 1966, Caltech.

[29] See Footnotes 5 and 6.

[30] W. Rindler, Phys. Rev. **119**, 2082 (1960).

[31] The minus sign in the matrix means negative values of the upper right elements.

[32] Here 3-vector notations are in usual convention: $\mathbf{e}_{(i)}$ denotes $\hat{\mathbf{e}}_{(i)}$ not being acted on by $\partial/\partial x^\mu$.

[33] With (2.13), (5.13) can also be obtained by substituting instantaneous Lorentz transform into (5.11) and solving for $\bar{H}$, $\bar{D}$.

[34] Reference 16.

[35] Reference 25, p. 114.

[36] Reference 8.

[37] $\mathbf{r}$ represents spherical $\mathbf{r}$ and the cylindrical radius will be denoted by $\mathbf{r}_c$ from here on.

[38] Reference 26, p. 32.

[39] Reference 15, Chap. 9.

[40] Reference 39.

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Topological Analysis of a Nonlinear Field Theory*

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This paper is concerned with a class of nonlinear field theories that exhibit conserved particlelike structures. An example of such a theory is quoted. Fields belonging to this theory are classical fields, single-valued under the action of the rotation group. It is explained how, when the theory is quantized, the quantum mechanical states which correspond to 1-particle systems in the unquantized theory may have properties similar to fermion states. In particular, it is shown that it is possible for wavefunctionals to exist which are double-valued under 2π rotations. This is the first known example in which a single-valued field theory can give rise to a quantized theory with half-odd spin properties.

1. INTRODUCTION

It is well known that the quantization of a classical field introduces a quantity that can be interpreted as a particle number. Since by a classical field we mean a field that is single-valued under the action of the rotation group, it follows that the particles involved must be bosons. However, a number of authors[1–7] have studied field theories which possess particlelike structures even in the classical theory. Such structures are called "kinks," and such theories are said to "admit kinks." The aim of these studies has been to examine the possibility that, when theories of this type are quantized, the states corresponding to a 1-kink classical-field configuration are, in fact, fermion states.

Finkelstein[5] has investigated these ideas from the point of view of algebraic topology and has given necessary and sufficient conditions for the existence of kinks in terms of the homotopy groups appropriate to the theory involved. One of the characteristic properties of a many-fermion state is the double-valuedness of the wavefunctional under exchange. For the type of theories considered in this paper, it has been shown[6] that double-valuedness under exchange implies the double-valuedness of the 1-kink wavefunctional under 2π rotation. If a theory is given for which kinks exist and if it is also possible to define, on the space of fields, functionals which are double-valued under 2π rotation, then we follow the terminology of Finkelstein and say that the theory "admits spin."

An example of a 1-dimensional field theory that admits kinks is found by considering the set of all mappings[8] α from the real line R^1 into the circle S^1,

$$\alpha: R^1 \to S^1.$$

S^1 can be parametrized by two real variables (ϕ_1, ϕ_2) whose squares add up to 1. To prevent the escape of interesting structures at infinity, it is necessary to impose boundary conditions. Hence, we consider only α for which

$$\alpha(x) \to (0, 1) \quad \text{as} \quad x \to \pm\infty,$$

where x is any point in R^1 and $(0, 1)$ is a fixed point in S^1. A field α may then be illustrated pictorially by a narrow strip stretching from $x = -\infty$ to $x = +\infty$ such that the angular twist of the strip about its center line specifies the value of $\alpha(x)$ for a given x. For a 1-kink field, the configuration is similar to the twist in the familiar Möbius strip (except that the Möbius strip has a twist through π, whereas the 1-kink field has a twist through 2π). Dynamics may be introduced into this theory, and it has been shown[1] how a quantum mechanical operator can be constructed which creates kinks and which anticommutes with itself.

The concept of spin has no meaning in one dimension. However, the simple 1-dimensional model has been generalized by Skyrme,[2,3] who introduces mappings φ from 3-dimensional space R^3 into the 3-sphere S^3,

$$\varphi: R^3 \to S^3. \tag{1.1}$$

S^3 can be parametrized by four real variables $(\phi_1, \phi_2, \phi_3, \phi_4)$ subject to the restriction

$$\sum_{i=1}^{4} \phi_i^2 = 1.$$

There are three independent fundamental fields which might be used to represent the three π-meson fields of nature. The number of kinks present is equal to the degree of the mapping φ, and it is hoped that this may be interpreted as the number of baryons. As before, to ensure the conservation of kinks, we impose a boundary condition

$$\varphi(\mathbf{x}) \to (0, 0, 0, 1) \quad \text{as} \quad |\mathbf{x}| \to \infty, \tag{1.2}$$

where x is any point in R^3 and (0, 0, 0, 1) is a fixed point in S^3. It is the purpose of this paper to show that this 3-dimensional theory admits spin.

2. TOPOLOGICAL CONSIDERATIONS

In this section, we review for completeness the general theory of kink fields as given by Finkelstein and Rubenstein.[6] Let θ be a mapping from n-dimensional Euclidean space R^n into some manifold Y,

$$\theta: R^n \to Y, \tag{2.1}$$

subject to the condition

$$\theta(x_1, \cdots, x_n) \to y_0 \quad \text{as any} \quad |x_i| \to \infty, \tag{2.2}$$

where $(x_1, \cdots, x_n)$ is any point of R^n and y_0 is a fixed point of Y. We let Q denote the set of all such mappings θ. Q is divided into a collection of pathwise-connected components $Q_a, Q_b, Q_c, \cdots$ called homotopy classes. Any two members of the same homotopy class can be joined by a path, but members of different homotopy classes cannot. The collection of homotopy classes form a group called the nth homotopy group of Y, denoted by $\pi_n(Y, y_0)$. We assume that the manifold Y is pathwise connected, in which case the group structure of $\pi_n(Y, y_0)$ is independent of which particular fixed point y_0 is chosen. We write simply $\pi_n(Y)$. If θ_a and θ_b are mappings belonging to distinct homotopy classes Q_a and Q_b, then it is impossible to join θ_a and θ_b by a path. Since time is a continuous parameter that may be used to label a path, this means that mappings belonging to Q_a possess a certain characteristic structure that cannot develop with the passage of time into a structure characteristic of mappings belonging to Q_b. As an illustration, let us consider the special case in which Y is the n-sphere S^n. It is well known from tables[9] that

$$\pi_n(S^n) = Z,$$

where Z is the additive group of integers. Thus, each homotopy class may be characterized by an integer which can be interpreted as the number of particles or kinks. The homotopy classes may be denoted by $\cdots, Q_{-2}, Q_{-1}, Q_0, Q_1, Q_2, \cdots$. For example, the $n = 1$ case refers to the 1-dimensional theory mentioned previously. Mappings belonging to Q_1 then have a single twist through 2π. This is clearly not deformable into a mapping without a twist. Similarly, the $n = 3$ case applies to the 3-dimensional theory. The number of kinks is equal to the degree of the mapping.

Let us now consider mappings θ as given by Eqs. (2.1) and (2.2), and focus attention on the set of mappings Q_1. We assume Y to be any pathwise-connected manifold but shall consider the special case of $n = 3$. We shall investigate the conditions under which functionals may be defined on Q_1 which are double-valued under 2π rotation. The meaning of the expression "double-valued functional" is at first sight imprecise and perhaps a contradiction in terms. However, the concept may be formulated exactly by introducing the idea of universal covering space.[5,10] This involves labeling the functional by an additional parameter which describes the path by which the argument of the functional was reached, and it is in this sense that we understand double-valuedness. Suppose θ_1 is a mapping belonging to Q_1. If it is possible to define a double-valued functional on Q_1, then it must be possible to follow a path p in Q_1, starting and ending at θ_1, such that the value of the functional along the path changes continuously and does not return to its original value when the end of the path is reached. However, if the functional is evaluated after going around a path p^2 which is equivalent to going twice around the path p, then it must return to its original value. Clearly, p must not be deformable to a single point of Q_1 or else a contradiction is obtained. Paths which are deformable to a point are called trivial. Otherwise, they are called nontrivial. The path p^2 must be trivial. Now the quantity which contains the information about the path structure of Q_1 is the first homotopy group $\pi_1(Q_1)$. This is the set of different classes of closed paths in Q_1. A necessary and sufficient condition for the existence of double-valued functionals on Q_1 is that the group $\pi_1(Q_1)$ have an element of order 2. The existence of double-valued functionals alone does not imply the existence of spin properties. One must show that the double-valuedness arises through following a path, starting and ending at some $\theta_1 \in Q_1$, which corresponds to rotating the system through 2π. In summary, given a field theory which admits kinks, we say that the theory "admits spin" provided the following conditions hold:

(i) $\pi_1(Q_1)$ has an element of order 2.

(ii) Paths beginning and ending at some $\theta_1 \in Q_1$ and corresponding to rotation through 2π are nontrivial.

Condition (ii) implies (i), but (i) is usually easier to verify and can be used as a test for the possibility of (ii).

We now list a number of results useful in finding whether or not a given theory admits spin. First of all, condition (ii) holds or not simultaneously for all $\theta_1 \in Q_1$.[7] It can also be shown that, if condition (ii) holds for a particular 2π rotation, then it holds for all 2π rotations. This follows from the fact that all

2π rotations are homotopic to each other. Let us now consider how $\pi_1(Q_1)$ is to be evaluated. It has been proved[11] that there exists an isomorphism

$$\pi_1(Q_i) \simeq \pi_1(Q_j)$$

and, in particular,

$$\pi_1(Q_1) \simeq \pi_1(Q_0). \tag{2.3}$$

Thus, problems involving paths in Q_1 are transformed into problems involving paths in Q_0. One example of mapping belonging to Q_0 is the constant mapping θ_0, which maps the whole of R^3 into the fixed point y_0 of Y:

$$\theta_0(\mathbf{x}) = y_0, \quad \text{for all} \quad \mathbf{x} \in R^3.$$

Mappings which are homotopic to the constant mapping are called trivial. Let χ be a mapping

$$\chi: R^1 \to Q_0,$$

such that

$$\chi(-\infty) = \chi(+\infty) = \theta_0.$$

Clearly, χ represents a path in Q_0 beginning and ending at θ_0. We define a mapping

$$H: R^4 \to Y$$

by

$$H(\mathbf{x}, u) = [\chi(u)](\mathbf{x}),$$

and note that

$$H(\mathbf{x}, u) \to y_0,$$

as either of

$$|\mathbf{x}|, \quad |u| \to \infty.$$

Thus, we see that there is a correspondence between paths in Q_0 and mappings from R^4 into Y. The mapping H is a member of one of the homotopy classes which make up the group $\pi_4(Y)$. The triviality or nontriviality of the path χ depends upon the triviality or nontriviality of the mapping H, and so the groups $\pi_1(Q_0)$ and $\pi_4(Y)$ are isomorphic,

$$\pi_1(Q_0) \simeq \pi_4(Y).$$

It follows from Eq. (2.3) that

$$\pi_1(Q_1) \simeq \pi_4(Y). \tag{2.4}$$

3. CONNECTIVITY OF Q_1 AND THE ROTATION GROUP

Consider the 3-dimensional theory given by Eqs. (1.1) and (1.2). In seeking to discover whether or not this theory admits spin, the first thing is to check whether $\pi_1(Q_1)$ has an element of order 2. It is well known[9] that

$$\pi_4(S^3) = Z_2, \tag{3.1}$$

where Z_2 is the group of integers modulo 2. From Eq. (2.4), it follows that condition (i) is satisfied. In Sec. 5, we check condition (ii), namely that a path in Q_1 corresponding to a 2π rotation is nontrivial and so belongs to the member of $\pi_1(Q_1)$, which is of order 2. However, to get an intuitive understanding of how this could arise, let us consider a field theory in which the domain of the mappings is R^2 and the range is S^2. By analogy with the 3-dimensional case, it follows that

$$\pi_1(Q_1) \simeq \pi_3(S^2).$$

From tables,[9] we find

$$\pi_3(S^2) = Z. \tag{3.2}$$

Hence, in the 2-dimensional theory, $\pi_1(Q_1)$ does not have an element of order 2, and so the theory does not admit spin. This is not surprising. The 2-dimensional theories never involve spin because the 2-dimensional rotation group $SO(2)$ is not doubly connected. It is infinitely multiply connected:

$$\pi_1(SO(2)) = Z.$$

Spin wavefunctions arise because of the doubly connectedness of $SO(3)$:

$$\pi_1(SO(3)) = Z_2.$$

This illustrates a relationship between the connectivity of Q_1 (when $Y = S^n$) and that of the corresponding rotation group. The relationship holds for any dimension, and a list of results may be drawn up as shown in Table I. The proofs of the last entries in the second and third columns of the table are given by Hilton[12] and Borel,[13] respectively. Table I strongly suggests that the connectivity of Q_1 (when $Y = S^n$) is directly related to the connectivity of the n-dimensional rotation group, and that the triviality or nontriviality of a path in $SO(n)$ determines the triviality or nontriviality of the corresponding path in Q_1. In what follows, we prove that this is so for the 3-dimensional case. First, however, it is convenient to introduce the concept of the Hopf mapping.

TABLE I. Connectivity of Q_1 and $SO(n)$.

n	$\pi_1(Q_1)$	$\pi_1(SO(n))$
1	0	0
2	Z	Z
$n \geq 3$	Z_2	Z_2

4. THE HOPF MAPPING

We are interested in the path structure of Q_1 for the 3-dimensional theory. We have explained how this problem can be reduced to that of studying mappings from R^4 into S^3. Before investigating such

mappings, it is convenient to examine the lower-dimensional problem of mappings from R^3 into S^2.

Let g be any mapping

$$g: R^3 \to S^2$$

subject to the boundary condition

$$g(\mathbf{x}) \to (0, 0, 1), \quad \text{as} \quad |\mathbf{x}| \to \infty.$$

Because of the boundary condition on g, it is possible to deform the domain R^3 into the 3-sphere, and so we consider mappings

$$\tilde{g}: S^3 \to S^2.$$

The topological properties of $\tilde{g}$ are identical with those of g. It follows from Eq. (3.2) that the homotopy classes of the mappings g (or $\tilde{g}$) can be labeled by a single integer i. We denote them by Q_i'. To agree with previous notation, Q_0' denotes the homotopy class of the constant mapping which takes the whole of R^3 (or S^3) into a single point of S^2, and Q_1' denotes the first homotopy class [which is one of the two generators of the group $\pi_3(S^2)$]. An example of a mapping belonging to Q_1' is given by Steenrod.[14] Denoting a point of S^2 by (ϕ_1, ϕ_2, ϕ_3) and a point of S^3 by $(\psi_1, \psi_2, \psi_3, \psi_4)$, the mapping is defined by the following equations:

$$\phi_1 = -2(\psi_4\psi_1 - \psi_3\psi_2), \tag{4.1a}$$

$$\phi_2 = -2(\psi_4\psi_2 + \psi_3\psi_1), \tag{4.1b}$$

$$\phi_3 = 1 - 2(\psi_1^2 + \psi_2^2). \tag{4.1c}$$

It is called the Hopf mapping, and it maps great circles in S^3 into single points of S^2. Having found an example of a mapping $\tilde{g}$ which belongs to the first homotopy class, we now look for an example of a mapping

$$\tilde{f}: S^4 \to S^3,$$

which also belongs to the first homotopy class. For this case, it follows from Eq. (3.1) that there are only two homotopy classes, Q_0' and Q_1'. Thus, all the nontrivial examples of $\tilde{f}$ belong to Q_1'.

Let us define the suspension of a mapping. Suppose that λ is a mapping between two spheres

$$\lambda: S^m \to S^n.$$

S^m and S^n can be regarded as equators of the higher-dimensional spheres S^{m+1} and S^{n+1}. A mapping

$$E(\lambda): S^{m+1} \to S^{n+1}$$

can be defined which reduces to λ on the equator and maps the northern hemisphere of S^{m+1} into the northern hemisphere of S^{n+1}, and the southern hemisphere of S^{m+1} into the southern hemisphere of S^{n+1}. For a given λ, many examples of such a mapping $E(\lambda)$ can be chosen and any one of them is called a suspension of λ. It is a well-known theorem[12] that a suspension of the Hopf mapping is nontrivial and so belongs to the homotopy class Q_1'. We now mention a useful special case. Let us denote the outer product of S^3 and I^1 by $S^3 \times I^1$. A typical point of $S^3 \times I^1$ is written $(\phi_1, \phi_2, \phi_3, \phi_4, s)$, where $(\phi_1, \phi_2, \phi_3, \phi_4) \in S^m$ and $s \in I^1$. Consider a mapping

$$F: S^3 \times I^1 \to S^3,$$

such that

$$F(\phi_1, \phi_2, \phi_3, \phi_4, 0) = y_0,$$

$$F(\phi_1, \phi_2, \phi_3, \phi_4, 1) = y_0,$$

$$\text{for all} \quad (\phi_1, \phi_2, \phi_3, \phi_4) \in S^3,$$

and

$$F(\phi_1^0, \phi_2^0, \phi_3^0, \phi_4^0, s) = y_0, \quad \text{for all} \quad s \in I^1,$$

where y_0 denotes a fixed point of the range sphere S^3 and $(\phi_1^0, \phi_2^0, \phi_3^0, \phi_4^0)$ denotes a fixed point of the domain sphere S^3. Because of the boundary conditions, the domain $S^3 \times I^1$ may be continuously deformed into S^4 and the mapping F replaced by a mapping $\tilde{F}$ between two spheres:

$$\tilde{F}: S^4 \to S^3.$$

One may then try to find a mapping

$$\tilde{\lambda}: S^3 \to S^2$$

such that

$$E(\tilde{\lambda}) = \tilde{F}.$$

Thus, $\tilde{F}$ is a suspension of $\tilde{\lambda}$. In a similar way, one may seek a mapping

$$\lambda: S^3 \to S^2$$

which can be extended to form a mapping

$$F: S^3 \times I^1 \to S^3,$$

such that F reduces to λ when a particular point $s_0 \in I^1$ is chosen. Clearly, $s_0 \neq 0, 1$ if λ is to be the Hopf mapping. We shall shortly see an example in which $s_0 = \frac{1}{2}$. The process by which F is obtained from λ is equivalent topologically to taking the suspension of λ. We shall, in fact, use the word "suspension" in this sense.

5. PROOF OF THE ADMISSION OF SPIN

As mentioned before, to prove that the 3-dimensional theory admits spin, we need only consider a particular mapping belonging to Q_1 and a particular 2π rotation. For the latter, we consider a 2π rotation

about the z axis:

$$x_i \to x_i' = R_{ij}(s)x_j,$$
$$\|R_{ij}(s)\| = \begin{pmatrix} \cos 2\pi s & \sin 2\pi s & 0 \\ -\sin 2\pi s & \cos 2\pi s & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

As an example of a mapping, we choose

$$\varphi_1 : R^3 \to S^3$$

defined by

$$\varphi_1(\mathbf{x}) = (\phi_1, \phi_2, \phi_3, \phi_4),$$

where

$$\phi_i = 2ax_i/(r^2 + a^2), \quad i = 1, 2, 3,$$
$$\phi_4 = (r^2 - a^2)/(r^2 + a^2).$$

This is the usual stereographic projection. It is of degree 1 and so belongs to Q_1. As s varies between 0 and 1, the rotation $R_{ij}(s)$ gives rise to a path in Q_1, which we denote by $P(s)\varphi_1$. This constitutes a sequence of mappings defined by

$$P(s)\varphi_1(\mathbf{x}) = (\phi_1, \phi_2, \phi_3, \phi_4),$$

where

$$\phi_i = 2aR_{ij}(s)x_j/(r^2 + a^2), \quad i = 1, 2, 3,$$
$$\phi_4 = (r^2 - a^2)/(r^2 + a^2).$$

To show that this path is nontrivial, it is convenient to express φ_1 as a mapping between two spheres. φ_1 is topologically equivalent to the identity mapping

$$\tilde{\varphi}_1 : S^3 \to S^3$$

given by

$$\phi_i = \psi_i, \quad i = 1, 2, 3,$$
$$\phi_4 = \psi_4,$$

where $(\psi_1, \psi_2, \psi_3, \psi_4)$ denotes a point of the domain sphere. Thus, $P(s)\varphi_1$ corresponds to the path defined by

$$P(s)\tilde{\varphi}_1(\psi_1, \psi_2, \psi_3, \psi_4) = (\phi_1, \phi_2, \phi_3, \phi_4),$$

where

$$\phi_i = R_{ij}(s)\psi_i, \quad i = 1, 2, 3,$$
$$\phi_4 = \psi_4. \tag{5.1}$$

At this point, we remark that the space Q of mappings may be topologized using the compact-open topology.[10] Now the range S^3 of the mappings is a group, having the group structure of $SU(2)$. It follows that Q is a topological group. It is a well-known fact[15] that the pathwise-connected components of a topological group are homeomorphic, and so the homotopy classes Q_i are all homeomorphic to each other.[16] Let us write the path of Eq. (5.1) in the form of a unitary matrix

$$\begin{pmatrix} \phi_4 + i\phi_3 & \phi_2 + i\phi_1 \\ -\phi_2 + i\phi_1 & \phi_4 - i\phi_3 \end{pmatrix}$$
$$= \begin{pmatrix} \psi_4 + iR_{3j}(s)\psi_j & R_{2j}(s)\psi_j + iR_{1j}(s)\psi_j \\ -R_{2j}(s)\psi_j + iR_{1j}(s)\psi_j & \psi_4 - iR_{3j}(s)\psi_j \end{pmatrix}$$
$$\equiv U(s).$$

This is a path in Q_1. It may be transformed into a path in Q_0 by a suitable homeomorphism. A convenient choice of a homeomorphism is obtained by multiplying $U(s)$ from the left by $U^{-1}(0)$. A proof that such a unitary quantity represents a homeomorphism between different homotopy classes is given by Skyrme[3] [Eq. (27)] and is a special case of a theorem given by Hilton.[12] We obtain

$$\begin{pmatrix} \phi_4 + i\phi_3 & \phi_2 + i\phi_1 \\ -\phi_2 + i\phi_1 & \phi_4 - i\phi_3 \end{pmatrix} = U^{-1}(0)U(s). \tag{5.2}$$

This describes a path in Q_0. When $s = 0, 1$,

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

and so the mapping becomes

$$\phi_i = 0, \quad i = 1, 2, 3,$$
$$\phi_4 = 1.$$

This is the constant mapping $\tilde{\varphi}_0$. Writing out Eq. (5.2) explicitly, we can calculate the quantities ϕ_1, ϕ_2, ϕ_3, and ϕ_4:

$$\phi_1 = \psi_4[\psi_1(\cos 2\pi s - 1) + \psi_2 \sin 2\pi s] - \psi_3[-\psi_1 \sin 2\pi s + \psi_2(\cos 2\pi s - 1)],$$
$$\phi_2 = \psi_4[-\psi_1 \sin 2\pi s + \psi_2(\cos 2\pi s - 1)] + \psi_3[\psi_1(\cos 2\pi s - 1) + \psi_2 \sin 2\pi s],$$
$$\phi_3 = -(\psi_1^2 + \psi_2^2) \sin 2\pi s,$$
$$\phi_4 = 1 + (\psi_1^2 + \psi_2^2)(\cos 2\pi s - 1).$$

These equations specify a path in Q_0. We can associate a mapping $\tilde{f}_0$ with this path:

$$\tilde{f}_0 : S^4 \to S^3.$$

The parameter s plays the role of the extra variable needed to describe S^4 rather than S^3. The path in Q_0 is nontrivial if and only if the mapping $\tilde{f}_0$ is nontrivial. Now $\tilde{f}_0$ is a suspension of the mapping obtained by choosing $s = \frac{1}{2}$. To see this, we put $s = \frac{1}{2}$ and we find

$$\phi_1 = -2(\psi_4\psi_1 - \psi_3\psi_2),$$
$$\phi_2 = -2(\psi_4\psi_2 + \psi_3\psi_1),$$
$$\phi_4 = 1 - 2(\psi_1^2 + \psi_2^2).$$

This defines a mapping from S^3 into S^2. Reference to Eq. (4.1) shows that it is precisely the Hopf mapping. Hence, $\tilde{f}_0$ is a suspension of the Hopf mapping and is consequently nontrivial. This is the desired result.

6. SUMMARY

In this paper, we considered a particular 3-dimensional nonlinear field theory and set out to show that this theory "admitted spin," in the sense that it was possible to define 1-particle wavefunctionals which were double-valued under 2π rotation. The space Q_1 on which these wavefunctionals are defined was shown to admit two and only two inequivalent types of path. We then showed that a 2π rotation path in Q_1 was a nontrivial path. To do this, we showed that the nontriviality of this path depended on that of a corresponding path in Q_0. The nontriviality of this latter path was related to that of a mapping from S^4 into S^3. This mapping proved to be nontrivial because it was shown to be a suspension of the Hopf mapping. This completed the proof.

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[1] T. H. R. Skyrme, Proc. Roy. Soc. **A262**, 237 (1961).
[2] T. H. R. Skyrme, Proc. Roy. Soc. **A260**, 127 (1961).
[3] T. H. R. Skyrme, Nucl. Phys. **31**, 556 (1962).
[4] D. Finkelstein and C. W. Misner, Ann. Phys. (N.Y.) **6**, 230 (1959); U. Enz, Phys. Rev. **131**, 1392 (1963).
[5] D. Finkelstein, J. Math. Phys. **7**, 1218 (1966).
[6] D. Finkelstein and J. Rubinstein, J. Math. Phys. **9**, 1762 (1968).
[7] J. Rubinstein, Ph.D. thesis, Yeshiva University, New York, 1967.
[8] A mapping is defined to be a continuous function.
[9] H. Toda, *Composition Methods in Homotopy Groups of Spheres* (Princeton U.P., Princeton, N.J., 1962).
[10] J. G. Hocking and G. S. Young, *Topology* (Addison-Wesley, Reading, Mass., 1961).
[11] G. W. Whitehead, Ann. Math. **47**, 460 (1946).
[12] P. J. Hilton, *An Introduction to Homotopy Theory* (Cambridge U.P., London, 1966).
[13] A. Borel, Bull. Am. Math. Soc. **61**, 397 (1955).
[14] N. Steenrod, *The Topology of Fibre Bundles* (Princeton U.P., Princeton, N.J., 1951), p. 126.
[15] D. Montgomery and L. Zippin, *Topological Transformation Groups* (Interscience, New York, 1955), p. 39.
[16] This does not mean that either all or none of the Q_i have spin properties. A nontrivial 2π rotation path in Q_i, say, will be mapped by the homeomorphism into a nontrivial path in Q_j, say. However, this latter path will not correspond to rotating the system through 2π.