Theory of Regge poles for $1/r^2$ potentials. I

Robert O. Mastalir

Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 3 June 1974)

In the following series of papers we give a detailed study of the theory of Regge poles for $1/r^2$ potentials with the behavior $r^2\,V(r) = -V_0$ at $r = 0$ and $r^2\,V(r) = -V_2$ at $r = \infty$. We give a complete description of the distribution of the Regge poles in the λ plane, which is cut from $-V_0^{1/2}$ to $V_0^{1/2}$ and study the behavior of the pole trajectories. We find that the high energy limit of the Regge poles is controlled by the parameter $p = (\lambda^2 - V_0)^{1/2}$ while at low energies the relevant parameter is $q = (\lambda^2 - V_2)^{1/2}$. This means that the point $\lambda = 0$ for the case of Yukawa potentials corresponds here to the point $q = 0$. We also find that the Regge trajectories $\lambda(E)$ may have branch points of the square root type at finite, in general complex, values of E at which points the pole passes the origin $\lambda = 0$. We further find that the kinematic singularity of the S matrix at $k = 0$ is more complicated than it is for Yukawa potentials and is here characterized by the Floquet parameter $\nu(\lambda, k)$ associated with the Schrödinger equation. We illustrate these and other results with some new exact solutions of the Schrödinger equation.

1. INTRODUCTION

Recently, Cheng and Wu[1] have shown that in quantum electrodynamics with massive photons the scattering amplitude from one-tower diagrams is proportional to $\beta(t)\,s^{\alpha(t)}(\ln s)^{-2}$ at infinite energy s, with $\alpha(0) > 1$, and that the leading singularity of the scattering amplitude in the J plane is a fixed Regge branch point at $J > 1$.

A comparatively simple and relevant model with the property that it introduces fixed branch points in the angular momentum plane is provided by the nonrelativistic scattering from $1/r^2$ potentials. It therefore seems desirable to investigate in detail the theory of Regge poles for such potentials.

The theory of Regge poles in potential scattering is widely known and has been extensively studied by many authors.[2] However, in most cases the investigations are based on the Schrödinger equation with a potential $V(r)$ that satisfies the regularity condition $r^2V(r) = 0$ at the origin. In the following papers we give a detailed study of the scattering and bound state properties of potentials with the behavior: $r^2V(r) = -V_0$ at $r = 0$ and $r^2V(r) = -V_2$ at $r = \infty$, with V_0, V_2 arbitrary constants. We also allow the possibility that $V(r)$ may have singularities at negative or complex values of r. In this paper we give the general theory of Regge poles for such potentials, while in the following papers we illustrate our results with some new exact solutions of the Schrödinger equation.

Some particular cases of $1/r^2$ potentials have been considered in the literature. The pure $1/r^2$ potential $V(r) = -V_0/r^2$ has been investigated by several authors.[3] Cornille[4] discussed the determination of the S matrix when $V(r)$ is of the form $\exp(-\mu r)/r^2$. Barut and Calogero[5] and Ferreira and Sesma[6] gave a detailed study of potentials with $1/r^2$ tails ($V_0 = 0$) including a numerical analysis of the pole trajectories in the λ plane. Do Amaral and Srivastava[7] studied the Regge trajectories for $V(r) = -V_0/r^2 - a/r$. Cheng[8] considered a particular $1/r^2$ potential with $V_0 = V_2 = 0$, but such that $V(r) = \infty$ for some complex values of r and studied its Regge pole structure at zero energy. Lastly, Challifour and Eden[9] investigated some of the properties of the Regge trajectories for attractive $1/r^2$ potentials with $V_0 = V_2$.

In Sec. 2 we define the S matrix and give its analytic properties. We find that S is a meromorphic function of λ in the whole λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$ and an analytic function of k with a kinematic branch point at $k = 0$ and the usual Yukawa cuts along the imaginary axis. We point out that the character of the branch point at $k = 0$ is different from that corresponding to Yukawa potentials and in Sec. 5 we show that it depends on the Floquet parameter $\nu(\lambda, k)$ associated with the Schrödinger equation, which is in general a very complicated function of λ, k, and the potential strength parameters. In Secs. 3, 4, and 6 we investigate the general properties, distribution, number and threshold behavior of the Regge poles. We find several interesting results, which are fully summarized in Sec. 7.

In subsequent papers we study the particular potential

$$V(r) = -\frac{1}{r^2}\left(\frac{r_0^2V_0 + r_0V_1r^\alpha + V_2r^{2\alpha}}{(r_0 + r^\alpha)^2}\right), \tag{1.1}$$

where r_0 and α are any positive numbers and V_0, V_1, and V_2 are arbitrary constants. We first give an exact solution of the Schrödinger equation at zero energy for this potential and study the properties of the corresponding zero energy Regge poles. Next we give exact solutions of the Schrödinger equation and derive the S matrix for arbitrary angular momentum and energy for the potential (1.1) in the special case $\alpha = 2$. We study the analytic structure of the S matrix in this case and investigate the properties and distribution of the Regge poles, particularly at low energies.

2. DEFINITION OF THE S MATRIX

We will be concerned with the radial Schrödinger equation

$$\frac{d^2y}{dr^2} + \left(k^2 - \frac{\lambda^2 - \frac{1}{4}}{r^2} - V(r)\right)y = 0, \tag{2.1}$$

where $\lambda = l + \frac{1}{2}$ with l the angular momentum and $k^2 = E$ is the energy. The potential $V(r)$ is assumed to be of the form

$$V(r) = -V_0/r^2 - V^a(r), \tag{2.2}$$

with $\lim r^2V^a(r) = 0$ at $r = 0$ and

$$V(r) = -V_2/r^2 - V^b(r), \quad r \to \infty. \tag{2.3}$$

with $\lim r^2V^b(r) = 0$ at $r = \infty$. In general, we take $V^a(r)$ and $V^b(r)$ to be Yukawa potentials of finite mass $m_0 \geq 0$.

The $1/r^2$ term in $V(r)$ may be absorbed into the angular momentum term in (2.1) by defining the "effective" angular momentum

$$p=(\lambda^2-V_0)^{1/2}, \tag{2.4}$$

which we define as an analytic function of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$. Similarly, (2.3) suggests the definition of the additional parameter

$$q=(\lambda^2-V_2)^{1/2}, \tag{2.5}$$

which we take as an analytic function of λ with a cut from $-V_2^{1/2}$ to $V_2^{1/2}$.

Solutions of (2.1) satisfying the boundary conditions

$$\phi(p,k,r)\to r^{1/2+p}, \qquad r\to 0, \tag{2.6}$$

$$F(q,\pm k,r)\to \exp(\mp ikr), \quad r\to\infty, \tag{2.7}$$

may be defined in terms of integral equations by the well-known method of variation of parameters. These will be identical to the integral equations found in the case of Yukawa potentials[2] with the exception that λ is everywhere replaced by p in the case of (2.6) and q in the case of (2.7). The method of successive approximations may then be used to obtain the appropriate iteration series.[2] We find the following results:

(1) When $V^a(r)$ in (2.2) is a Yukawa potential of mass $m_0\neq 0$ the iteration series for $\phi(p,k,r)$ converges absolutely for finite r, k when $\mathrm{Re}p>0$ [or $\mathrm{Re}p>-\frac{1}{2}\alpha$ when $V(r)$ is given by (1.1)]. $\phi(p,k,r)$ is analytic for all finite k and p in $\mathrm{Re}p>0$ (or $\mathrm{Re}p>-\frac{1}{2}\alpha$); in the left-hand plane of λ it has simple poles at $p=-\frac{1}{2}(1+n)$, $n=0,\ 1,\ 2\cdots$ [or $p=-\frac{1}{2}\alpha(1+n)$]. The following identities hold:

$$\phi(p,k,r)=\phi(p,-k,r)=\phi^*(p^*,k^*,r). \tag{2.8}$$

Furthermore, we find the symmetry property

$$\phi(p(\lambda_1),k,r)=\phi(p(-\lambda_2),k,r), \tag{2.9}$$

where λ_i is in the ith sheet of the λ plane. Thus, we may say that $\phi(p,k,r)$ is symmetric "across" the cut in the λ plane.

(2) The iteration series for $F(q,+k,r)$ $[F(q,-k,r)]$ converges absolutely for all $kr>0$ provided that k is not positive (negative) imaginary. $F(q,\pm k,r)$ are analytic in k in their domain of convergence except for a kinematic branch point at $k=0$. When $V^b(r)$ is a Yukawa potential of mass m_0 the domain of convergence extends up to $\mathrm{Im}k<m_0$. $F(q,\pm k,r)$ are analytic functions of λ in the whole λ plane. We note that the points $\lambda=\pm V_2^{1/2}$ (where $q=0$) are not branch points of $F(q,\pm k,r)$. The following identity holds:

$$F^*(q^*,-k^*,r)=F(q,k,r). \tag{2.10}$$

In order to define the S matrix we write

$$\phi(p,k,r)=f(p,q,k)F(q,-k,r)+f(p,q,-k)F(q,k,r). \tag{2.11}$$

and define S in terms of the Jost functions $f(p,q,\pm k)$ in the usual manner:

$$S=\exp[i\pi(\lambda+\tfrac{1}{2})][f(p,q,k)/f(p,q,-k)]. \tag{2.12}$$

When $V_0=V_2$ (and therefore $p=q$) and $V(r)$ has no finite singularities in r it is not difficult to determine the Jost functions explicitly. We simply calculate the Wronskians of $\phi(p,k,r)$ with $\exp(\pm ikr)$ at $r=\infty$. When $V_0\neq V_2$, however, the determination of the Jost functions becomes an extremely difficult task. This is due to the fact that in this case the branch point at $k=0$ is much more complicated than the simple "Bessel function" singularity of $\phi(p,k,r)$ and $F(q,\pm k,r)$. We discuss this question in more detail in Sec. 5 and give an explicit example in Paper III of this series.

The analytic properties of the Jost functions and the S matrix follow immediately from the above results. Thus, S is a meromorphic function of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$ and an analytic function of k with the usual Yukawa cuts and a kinematic branch point at $k=0$. Note that S is analytic at $q=0$. We easily obtain the identity

$$f^*(p^*,q^*,-k^*)=f(p,q,k), \tag{2.13}$$

and the extended unitarity relation

$$S^*(p^*,q^*,k^*)S(p,q,k)=1. \tag{2.14}$$

Additionally, as a consequence of (2.9) we find the symmetry property

$$S(p(\lambda_1),q,k)=\exp(2i\pi\lambda)S(p(-\lambda_2),q,k). \tag{2.15}$$

Thus, the S matrix is symmetric "across" the cut in the λ plane. Equation (2.15) is the result analogous to the well-known Mandelstam reflection property $S(-\lambda)=S(\lambda)$ for λ integer.[10] We also note that $S(-\lambda)=S(\lambda)$ identically for potentials more singular than $1/r^2$ at the origin.

Lastly, we state here the following useful identity satisfied by the Jost functions:

$$f(p,q,k)f(-p,q,-k)-f(-p,q,k)f(p,q,-k)=-4ipk. \tag{2.16}$$

3. GENERAL PROPERTIES OF THE REGGE POLES

The Regge poles are defined as the zeroes of the Jost function $f(p,q,-k)$. A very general symmetry in the distribution of the Regge poles follows from the observation that the S matrix and the Jost functions are symmetric "across" the cut in the λ plane [see (2.15)]. It follows that a pole at $\lambda(k)$ in the first sheet must also appear at $-\lambda(k)$ in the second sheet. Other results may be obtained by means of well-known methods directly from equation (2.1).[2]

When $\lambda(k)$ is a Regge pole with $\mathrm{Re}p>0$ and $\mathrm{Im}k>0$ it follows from (2.1) and (2.11) that

$$\mathrm{Re}k\,\mathrm{Im}k\int_0^\infty|\phi|^2\,dr-\mathrm{Re}\lambda\,\mathrm{Im}\lambda\int_0^\infty(|\phi|^2/r^2)\,dr=0, \tag{3.1}$$

and a similar equation may be written down with λ replaced by p. We conclude from (3.1) that the S matrix has no poles in the domains: $\mathrm{Re}k\gtrless 0$, $\mathrm{Re}\lambda\,\mathrm{Im}\lambda\lesseqgtr 0$, $\mathrm{Im}p\lesseqgtr 0$.

If $\mathrm{Re}k=0$ in (3.1) we see that λ may be either real or pure imaginary. Since we must have $\mathrm{Re}p>0$ the latter possibility may only occur if $V_0<0$ and $p=(|V_0|-(\mathrm{Im}\lambda)^2)^{1/2}$ is greater than zero. This corresponds to a potential $V(r)$ repulsive near the origin. The possibility of the existence of Regge poles with λ pure imaginary

and on the cut is quite interesting and is a unique property of $1/r^2$ potentials repulsive near $r=0$.

If $\mathrm{Im}k=0$ we find from (2.1) and (2.11) that

$$\mathrm{Re}k\,|f(p,q,k)|^2-2\mathrm{Re}\lambda\,\mathrm{Im}\lambda\int_0^\infty(|\phi|^2/r^2)\,dr=0, \tag{3.2}$$

and a similar equation with λ replaced by p. These equations imply the existence of positive energy poles in the domains: $\mathrm{Re}k\gtrless 0$, $\mathrm{Re}\lambda\mathrm{Im}\lambda\gtrless 0$, $\mathrm{Im}p\gtrless 0$. Consequently, as E becomes positive a Regge pole $\lambda(E)$ must leave the real axis with a positive imaginary part, as expected. Similarly, if $\lambda(E)$ is pure imaginary with $\mathrm{Im}\lambda>0$, the pole must emerge from the cut and enter the first quadrant in the first sheet as E becomes positive with $\mathrm{Re}k>0$.

Additional information may be obtained by differentiating (2.1) with respect to E. If $\mathrm{Re}p>0$ with λ^2 real and $\mathrm{Im}k>0$, we find

$$\frac{d\lambda}{dE}=\left(\frac{1}{2\lambda}\right)\left(\frac{\int_0^\infty|\phi|^2\,dr}{\int_0^\infty(|\phi|^2/r^2)\,dr}\right). \tag{3.3}$$

and a similar equation with λ replaced by p. Thus we see that both $\mathrm{Re}\lambda$ and $\mathrm{Re}p$ are increasing functions of E. Similarly, when λ is pure imaginary with $\mathrm{Im}\lambda>0$, $\mathrm{Im}\lambda(E)$ is a decreasing function of E. That is, as $E\to 0^-$ the pole $\mathrm{Im}\lambda(E)$ moves along the cut toward the origin $\lambda=0$. Upon reaching the point $\lambda=0$ the pole turns to the right and moves along the positive real axis in the first sheet.

We now derive some results on the behavior of Regge poles when $\mathrm{Re}p=0$. The Jost functions may be analytically continued into the region $\mathrm{Re}p\leqslant 0$ using standard methods.[2] Thus, from the observation that $\phi(p,k,r)$ has simple poles at $p=-\frac{1}{2}(1+n)$, $n=0,1,2\cdots$ we may obtain the analytically continued Jost functions

$$\bar f(p,q,\pm k)=f(p,q,\pm k)/\Gamma(2p+1). \tag{3.4}$$

Using (3.4) in (2.16), we find

$$\bar f(p,q,k)\bar f(-p,q,-k)-\bar f(-p,q,k)\bar f(p,q,-k)=-2ik\frac{\sin(2\pi p)}{\pi}. \tag{3.5}$$

If k is real and p pure imaginary we find from (3.5) that

$$|\bar f(-p,q,-k)|^2-|\bar f(p,q,-k)|^2=2k\frac{\sinh[2\pi(\mathrm{Im}p)]}{\pi}. \tag{3.6}$$

Since a Regge pole in this case satisfies $\bar f(p,q,-k)=0$, we conclude that there are no poles with k real and p pure imaginary in the domains: $\mathrm{Re}k\lessgtr 0$, $\mathrm{Im}p\gtrless 0$.

If k and p are both pure imaginary, it follows from (2.13) and (3.5) that

$$\frac{1}{2}\left(\frac{\bar f(p,q,k)}{\bar f^*(p,q,k)}-\frac{\bar f(p,q,-k)}{\bar f^*(p,q,-k)}\right)=\frac{i\,\mathrm{Im}k\sinh[2\pi(\mathrm{Im}p)]}{\pi\bar f^*(p,q,k)\bar f^*(p,q,-k)}. \tag{3.7}$$

Taking the absolute value of (3.7), we find the result

$$|\bar f^*(p,q,k)\bar f^*(p,q,-k)|\geqslant\left|\mathrm{Im}k\frac{\sinh[2\pi(\mathrm{Im}p)]}{\pi}\right|. \tag{3.8}$$

It follows from this that $\bar f^*(p,q,-k)=\bar f(-p,q,-k)$ cannot vanish for p pure imaginary unless $p=0$. Consequently, if $V_0>0$ there can be no Regge poles with λ real and on the cut for $E<0$. Similarly, if $V_0<0$ there are no Regge poles with λ pure imaginary and away from the cut for $E<0$.

In order to find the locations of the Regge poles at infinite energy we observe that if we set $z=kr$ and let $|k|\to\infty$ while keeping z fixed, Eq. (2.1) reduces in this limit to the Schrödinger equation with a Coulomb potential and angular momentum p. We conclude that as $|E|\to\infty$ the Regge poles approach the locations $p=-(\frac{1}{2}+n)$, $n=0,1,2\cdots$.[11] The same result follows from known general results on the high energy scattering from Yukawa potentials,[12] since we assumed at the outset $V^a(r)$ was a superposition of Yukawa potentials. Thus, as $|E|\to\infty$, the trajectory $\lambda(E)$ tends to the values $-(V_0+(\frac{1}{2}+n)^2)^{1/2}$ in the first sheet and $(V_0+(\frac{1}{2}+n)^2)^{1/2}$ in the second sheet, with one exception. If $V_0<0$ and we further have that $(n+\frac{1}{2})^2-|V_0|$ is negative then it follows that for these values of n the trajectory $\lambda(E)$ tends to the values $\pm i(|V_0|-(\frac{1}{2}+n)^2)^{1/2}$ as $|E|\to\infty$. The meaning of this is that some of the imaginary poles start from the cut at $E=-\infty$, while others terminate at the cut when $E=+\infty$.

Lastly, we note that the Regge trajectories $\lambda(E)$ may be multivalued functions of E with branch points at various, generally complex, values of E. This observation follows simply by noting that the Jost function $f(p,q,-k)$ depends on λ only through p and q and the Regge poles are in effect given by an equation of the form $q(\lambda(E))=g(E)$ or $p(\lambda(E))=h(E)$, where g and h are some functions of E. Further, if $\lambda(E)$ does have a branch point, it will be of the square root type, $\lambda(E)=(E-E_0)^{1/2}f(E)$, with $f(E)$ analytic at $E=E_0$. Clearly, at any such branch point the Regge trajectory $\lambda(E)$ passes through the origin $\lambda=0$. We see that these branch points are characteristic of $1/r^2$ potentials and are not related to the square root type branch points associated with the crossing of Regge trajectories found by Cheng.[13]

4. THE NUMBER OF TRAJECTORIES

We now determine the number of Regge poles in the right half-plane of the first sheet of λ for $E\leqslant 0$. These include the physical bound states of the system.

In Sec. 3 we proved that when $V_0>0$ there are no negative energy Regge poles with λ real and on the cut. In this case p is pure imaginary and the solutions of (2.1) are of the form $r^{1/2\pm i|p|}$ near the origin for $E\leqslant 0$. They both vanish at $r=0$ while oscillating infinitely rapidly. There are no bound states and a particle in this case would "fall to the center" while seeking its ground state at $E=-\infty$. We therefore need only consider p real and positive. Thus, we have either $\lambda>(V_0)^{1/2}$ or $-iV_0^{1/2}<\lambda<iV_0^{1/2}$. With no loss in generality in what follows we also set $E=0$.

Given any "regular" potential $V(r)$ the number of bound states at zero energy may be estimated by means of Bargmann's inequality[14]:

$$N_\lambda\leqslant\frac{1}{2|\lambda|}\int_0^\infty rU(r)\,dr, \tag{4.1}$$

where N_λ is the number of bound states of angular mo-

mentum $\lambda = l + \frac{1}{2}$ and

$$U(r) = \begin{cases} |V(r)|, & V(r) < 0, \\ 0, & V(r) \geq 0. \end{cases} \tag{4.2}$$

When $V(r)$ is of the form of (2.2), (2.3) with $V_0 = V_2$, (4.1) may still be used to estimate N_λ provided that we replace λ with p and $V(r)$ with $V^a(r)$. Clearly, N_λ is finite provided that $V^a(r)$ is nonsingular in $0 < r < \infty$ and $\lambda > V_0^{1/2}$.

When $V_0 \neq V_2$ (4.1) is no longer applicable. An expression similar to (4.1) may nevertheless be derived by using the methods of Ref. 14 with the result that N_λ is likewise finite provided that $V(r)$ has no singularities in $0 < r < \infty$ and that $\lambda > V_2^{1/2} > V_0^{1/2}$.

When λ is in the range $V_0^{1/2} < \lambda < V_2^{1/2}$, however, p is real but $q = i(V_2 - \lambda^2)^{1/2}$ is pure imaginary. The zero energy wavefunction has the asymptotic form $r^{1/2 \pm i|q|}$ and oscillates infinitely rapidly near $r = \infty$. This suggests that there must be an infinite number of bound states in $V_0^{1/2} < \lambda < V_2^{1/2}$. In Sec. 6 we show that this is indeed the case and that an infinite number of Regge poles emerge from the branch point $V_0^{1/2}$ near threshold and move to the right along the real axis converging on the point $\lambda = V_2^{1/2}$ as $E \to 0^-$.

5. SINGULARITY OF THE S MATRIX AT $k = 0$

It is well known that the S matrix has a fixed kinematic branch point at $k = 0$ in the case of Yukawa potentials.[2] This remains true in the case of $1/r^2$ potentials. However, the nature of the singularity at $k = 0$ is modified according to whether $V(r)$ has a $1/r^2$ core, tail, or both.

When $V(r)$ is given by (2.2), (2.3) with $V_0 = V_2$ and $V^a(r)$ is an arbitrary superposition of Yukawa potentials, the S matrix may be written in the form

$$S = \exp i\pi(\lambda - p)\left(\frac{Y(p,k) + k^{2p}\exp(i\pi p)}{Y(p,k) + k^{2p}\exp(-i\pi p)}\right). \tag{5.1}$$

When $V^a(r)$ is a Yukawa potential of mass m_0, we find that

$$Y(p,k) = Y(p, k\exp(-i\pi)). \tag{5.2}$$

Indeed, $Y(p,k)$ is an analytic function of k in the whole k plane with the usual Yukawa cuts starting at $k = \pm im_0$ and a meromorphic function of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$.

It follows from (5.1) and (5.2) that S satisfies

$$S(p, k\exp(-i\pi)) = \exp(2i\pi l)[S(p,k) + 2i\cos\pi p\exp(i\pi l)]^{-1}, \tag{5.3}$$

from which its circuital behavior about the singularity at $k = 0$ may be easily determined.

When $V(r)$ is given by (2.2), (2.3) but $V_0 \neq V_2$, the above expressions are no longer applicable. The presence of a $1/r^2$ tail in $V(r)$ modifies considerably the character of the branch point at $k = 0$ and an entirely new procedure must be used in the derivation of the S matrix.

Let us consider the Schrödinger equation (2.1) with a potential $V(r)$ satisfying (2.2), (2.3). In the limit $k = 0$ it follows from (2.3) and the theory of differential equations that for large r this equation must have two solutions of the form

$$y_{1,2}^{(0)}(r) = r^{1/2 \pm q} g_{1,2}^{(0)}(r), \tag{5.4}$$

where $g_{1,2}^{(0)}(r)$ are single-valued functions of r. This suggests that when $k \neq 0$ Eq. (2.1) has solutions of the form

$$y_{1,2}(r) = (kr)^{1/2 \pm \nu(k)} g_{1,2}(kr), \tag{5.5}$$

where $g_{1,2}(kr)$ are single-valued functions of kr and $\nu(k)$ is some function of k satisfying $\nu(0) = q = (\lambda^2 - V_2)^{1/2}$.

The existence of solutions of the form of (5.5) for an equation of the type of the radial Schrödinger equation may be generally established by means of Floquet's theorem[15] provided that $r^2V(r)$ is a single-valued function of r. The parameter ν is then the so-called Floquet parameter and is in general a very complicated function of k, λ and the potential strenth and range parameters. More precisely, if $r^2V(r) = \sum_{n=-\infty}^{+\infty} u_n r^n$, then it follows from the work of Fubini and Stroffolini[16] that (1) if $u_n \neq 0$ for some negative n (singular potentials), then $\nu(\lambda, k)$ is an even analytic transcendental function of k and a meromorphic function of λ; and (2) if $u_n = 0$ for all negative n (regular potentials), then $\nu(\lambda, k) = \lambda$. The case $u_0 \neq 0$ which applies for the "transitionally" singular $1/r^2$ potentials is a special case. Using either the methods of Ref. 16 or other available methods,[17] it may be shown that (1) if $V(r) = -V_0/r^2 + V_Y(r)$ and $V_Y(r)$ is a Yukawa potential of finite mass, then $\nu(\lambda, k) = p = (\lambda^2 - V_0)^{1/2}$; (2) if $V(r) = V_Y(r)$ for $r < r_0$ and $V(r) = -V_2/r^2$ for $r > r_0$ for some finite r_0, then $\nu(\lambda, k) = q = (\lambda^2 - V_2)^{1/2}$; and (3) lastly, when $V(r)$ has both a $1/r^2$ core and tail then $\nu(\lambda, k)$ is an even analytic transcendental function of k and a meromorphic function of λ.

An immediate implication of the above observations is that the branch point at $k = 0$ is more complicated than the "Bessel function" singularity of Yukawa potentials and is now characterized by the Floquet parameter $\nu(\lambda, k)$. Indeed, as a direct consequence of (5.5) we find that the S matrix is correctly given by the expression

$$S = \exp i\pi(\lambda - \nu)\left(\frac{Y(p,\nu,k) + k^{2\nu}\exp(i\pi\nu)}{Y(p,\nu,k) + k^{2\nu}\exp(-i\pi\nu)}\right). \tag{5.6}$$

where $\nu = \nu(\lambda, k)$. Clearly, ν is of the nature of an "effective" angular momentum. Elsewhere we show explicitly that the representation (5.6) applies when $V(r)$ is given by (1.1) with $\alpha = 2$ plus an arbitrary superposition of Yukawa potentials of finite mass m_0.[18] In addition to this, we have also verified (5.6) exactly when $V(r)$ is given by (1.1) with $\alpha = 1$.[19]

For the cases indicated above we find that the S matrix satisfies the identities[18]

$$S(-\nu) = S(\nu), \tag{5.7}$$

$$S(\nu, k\exp(-i\pi)) = \exp(2i\pi l)]S(\nu,k) + 2i\cos\pi\nu\exp(i\pi l)]^{-1}. \tag{5.8}$$

The circuital behavior of S about the point $k = 0$ follows immediately from (5.8), while (5.7) is a restatement of the fact that the S matrix is analytic at $\lambda = \pm V_2^{1/2}$.

6. BEHAVIOR OF THE REGGE POLES NEAR THRESHOLD

Detailed investigations about the threshold motion of the Regge poles are available for the case of Yukawa potentials.[20] In particular, it is known that an infinite number of trajectories converge on $\lambda=0$ as $E\to 0$. In our case we find that the points $\lambda=\pm V_2^{1/2}$ assume the role of the point $\lambda=0$, and an infinite number of trajectories converge on these points as $E\to 0$. Physically this is not surprising as it is well known that the low energy behavior of the S matrix and the Regge trajectories is determined by the asymptotic tail of the potential. Here $V(r)\sim -V_2/r^2$ and, therefore, the relevant parameter for very low energy phenomena is just $q=(\lambda^2-V_2)^{1/2}$.

From Eq. (5.6) we see that the Regge poles are given by the solutions of the equation

$$Y(p,\nu,E)+E^{\nu}\exp(-i\pi\nu)=0, \tag{6.1}$$

where $\nu=\nu(p,q,E)$ is the Floquet parameter. Near $E=0$, $\nu(p,q,E)$ has the expansion[17,18]

$$\nu(p,q,E)=q+E^{m}[\nu_1(p,q)+O(E^{m})], \tag{6.2}$$

where m is a positive integer and $\nu_1(p,q)$ is some function of p,q. Using (6.2), we find, similarly,

$$Y(p,\nu,E)=Y(p,q,0)+E\left[\left.\frac{\partial Y}{\partial E}\right|_{\substack{E=0\\ \nu=q}}+A\left.\frac{\partial Y}{\partial \nu}\right|_{E=0}\right]+O(E)^2, \tag{6.3}$$

where $A=\nu_1(p,q)$ for $m=1$ and $A=0$ if $m\neq 1$. Using these results in (6.1), we readily obtain low energy expansions for the Regge poles $\bar{\lambda}(E)$. As expected, when $E<0$ and $V_2>0$ the Regge poles are real. As E becomes positive, $\bar{\lambda}(E)$ acquires a positive imaginary part. When $V_2<0$, a trajectory $\bar{\lambda}(E)$ may reach threshold on the imaginary axis with $\bar{\lambda}(E)<i|V_2|^{1/2}$ if $|V_0|>|V_2|$ or $\bar{\lambda}(E)<i|V_0|^{1/2}$ if $|V_2|>|V_0|$. Additional information, such as the angle at which the trajectories meet the real axis as $E\to 0^+$, may be easily obtained from (6.1)–(6.3).

The above results are not valid at $q=0$. Indeed, using the result[18]

$$Y(p,0,E)=-1, \tag{6.4}$$

which holds for any energy E, we see that when $\nu(E)=0$ Eq. (6.1) is satisfied identically. At this point the S matrix is of the form $0/0$ for all E and must be defined using L'Hopital's rule. In order to determine the threshold behavior of the Regge poles when $\nu(E)\to 0^+$, that is, when $\lambda\to\pm V_2^{1/2}$ from the right, we proceed as follows: Near $|E|\sim 0$ and $\nu(E)\sim q\sim 0$ we expand $Y(p,\nu,E)$ to find

$$Y(p,\nu,E)=-1+q\left.\frac{\partial Y}{\partial \nu}\right|_{\substack{E=0\\ \nu=0}}+O(q^2). \tag{6.5}$$

A solution $\bar{q}(E)$ of (6.1) is then obtained with

$$\mathrm{Re}\,\bar{q}(E)\approx(\pi-\gamma)\frac{2n\pi}{|\ln|E||^2}-\frac{2n^2\pi^2Y_{00}^2}{|\ln|E||^3},$$

$$\mathrm{Im}\,\bar{q}(E)\approx\frac{2n\pi}{|\ln|E||}, \tag{6.6}$$

where $n=\pm 1,\ \pm 2\cdots$, $Y_{00}=(\partial Y/\partial\nu)_{E=0,\nu=0}$ and $E=|E|\times\exp(i\gamma)$ with $|E|\sim 0$. Note that Y_{00} is real.

It follows from (6.6) that an infinite number of trajectories approach the point $q=0$ as E approaches the threshold from any direction in the complex energy plane.

When $V_2>0$, $V_2>V_0$ we find from (6.6) that an infinite number of complex conjugate trajectories converge on $\lambda=-V_2^{1/2}$ from the right as $E\to 0^-$. The angle of approach is proportional to $(\ln|E|)^{-2}$. Similarly, an infinite number of trajectories converge on $\lambda=\pm V_2^{1/2}$ as $E\to 0^+$. The angle at which they meet the real axis is proportional to $(\ln|E|)^{-1}$.

When $V_2>0$, but $V_2<V_0$, the points $\lambda=\pm V_2^{1/2}$ are located within the cut. We find from (6.6) that an infinite number of trajectories approach the point $\lambda=V_2^{1/2}$ on the second sheet of λ as $E\to 0^-$. At $E=0$ these poles accumulate at $\lambda=V_2^{1/2}$ on the lower lip of the cut. Thus, these poles are never physical.

When V_2 and V_0 are both negative and the cut is on the imaginary axis the analysis and results are entirely analogous to the above. For example, an infinite number of trajectories is found to converge on the point $\lambda=i|V_2|^{1/2}$ from above, and $\lambda=-i|V_2|^{1/2}$ from below both as $E\to 0^+$ and $E\to 0^-$, when $|V_2|<|V_0|$.

Suppose now that V_0, V_2 are both positive and λ is real with $V_0^{1/2}<\lambda<V_2^{1/2}$. We recall that in Sec. 4 we concluded that there must be an infinite number of Regge poles in this region for $E\lesssim 0$. In this case, $\nu(0)=q$ is pure imaginary and (6.1) is not well defined in the limit $E\to 0$. Using the result $Y(\nu)=1/Y(-\nu)$ (Ref. 18) and (2.14), we see that for any energy E and imaginary $\nu(E)$ we may write

$$Y(p,i|\nu|,E)=\exp[iy(p,|\nu|,E)], \tag{6.7}$$

where $y(p,|\nu|,E)$ is a real function. As $E\to 0^-$ and $q\sim 0$, we find, using (6.1)–(6.3), that the Regge poles $\bar{\lambda}(E)$ in $V_0^{1/2}<\lambda<V_2^{1/2}$ are given by

$$(V_2-\bar{\lambda}_n^2(E))^{1/2}\approx\frac{2n\pi}{|\ln|E||}+\left(\frac{2n\pi}{|\ln|E||^2}\right)Y_{00}+\cdots, \tag{6.8}$$

where $n=\pm 1,\ \pm 2,\cdots$ and $Y_{00}=(\partial Y/\partial\nu)_{E=0,\nu=0}$.

We conclude from (6.8) that an infinite number of Regge poles must pass through every point in $V_0^{1/2}<\lambda<V_2^{1/2}$ for $E\lesssim 0$. As $E\to 0^-$ these poles approach the point $\lambda=V_2^{1/2}$ along the real axis. Evidently, the above discussion may be immediately extended to the case in which V_0, V_2 are both negative and $i|V_2|^{1/2}<\pm\lambda<i|V_0|^{1/2}$. Again, we find an infinite number of Regge poles converging on the points $\lambda=\pm i|V_2|^{1/2}$ along the cut as $E\to 0^-$.

7. CONCLUSION AND SUMMARY OF RESULTS

When $V(r)$ is a $1/r^2$ potential of the type defined in (2.2), (2.3), we have found that the S matrix is a meromorphic function of λ with a cut from $-V_0^{1/2}$ to $V_0^{1/2}$ and an analytic function of k with a kinematic branch point at $k=0$ and the usual Yukawa cuts along the imaginary axis. We also found that the branch point at $k=0$ is now characterized by a Floquet parameter $\nu(\lambda,k)$ which is a transcendental function of λ and k and plays the role of an "effective angular momentum" of the system.

We also investigated in detail the properties and distribution of the Regge poles. The principal results for $E \leq 0$ with λ in the first sheet and $\mathrm{Re}\lambda \geq 0$ are as follows:

(1) $V_0 > 0$. $V(r)$ is attractive at the origin and the cut in the λ plane is on the real axis. We find:

(i) There are no Regge poles on the cut.
(ii) If $V_2 > 0$ there is a finite number of Regge poles located to the right of $V_0^{1/2}$ or $V_2^{1/2}$, whichever is greater. If $V_2 > V_0$ an infinite number of poles emerge from the branch point $V_0^{1/2}$ and approach the point $V_2^{1/2}$ as $E \to 0^-$. If $V_2 < V_0$ there is an infinite number of poles which approach the point $V_2^{1/2}$ from the second sheet of λ. At threshold these poles are located at $V_2^{1/2}$ on the lower lip of the cut and are therefore never physical.
(iii) If $V_2 < 0$ we find a finite number of Regge poles to the right of $V_0^{1/2}$. There are no poles on the cut or the imaginary axis.

(2) $V_0 < 0$. $V(r)$ is repulsive at the origin and the cut is on the imaginary axis. We find:

(i) If $V_2 > 0$ there is a finite number of Regge poles to the right of $V_2^{1/2}$. An infinite number of poles emerge from the branch points $\pm i|V_0|^{1/2}$, move along the cut and enter the positive real axis approaching the point $V_2^{1/2}$ as $E \to 0^-$.
(ii) If $V_2 < 0$ there is a finite number of Regge poles on the positive real axis $\lambda > 0$. If $|V_2| < |V_0|$ a finite number of poles is located in $-i|V_2|^{1/2} < \lambda < i|V_2|^{1/2}$ (on the cut). Furthermore, an infinite number of poles emerge from the branch points $\pm i|V_0|^{1/2}$ and approach the points $\pm i|V_2|^{1/2}$ as $E \to 0^-$. If $|V_2| > |V_0|$ there is a finite number of poles both on the positive real axis and on the cut. There are no poles on the imaginary axis outside of the cut.

(3) The Regge trajectories $\lambda(E)$ are multivalued functions of E. In addition to the usual branch points at $E = 0$, there may be additional branch points at finite, in general complex, values of E. When such branch points exist, they are of the square root type. That is, $\lambda(E) = (E - E_0)^{1/2} g(E)$ near the branch point $E = E_0$, with $g(E)$ analytic at $E = E_0$. Evidently, at the branch point $E = E_0$ the Regge pole passes through the origin $\lambda = 0$. These branch points do not appear in the scattering amplitude. These singularities are characteristic of $1/r^2$ potentials and are not related to the square root branch points associated with the crossing of Regge trajectories.[13]

ACKNOWLEDGMENT

The author wishes to thank Professor Hung Cheng for his help and advice in the preparation of this work.

[1]H. Cheng and T.T. Wu, Phys. Rev. **D 1**, 2775 (1970).
[2]T. Regge, Nuovo Cimento **14**, 951 (1959); A. Bottino, A.M. Longoni, and T. Regge, Nuovo Cimento **23**, 954 (1962); H. Cheng, Phys. Rev. **127**, 647 (1962); E.J. Squires, Nuovo Cimento **25**, 242 (1962).
[3]K.M. Case, Phys. Rev. **80**, 797 (1950); F.L. Scarf, Phys. Rev. **109**, 2170 (1958); T. Tietz, Nuovo Cimento **11**, 126 (1959).
[4]H. Cornille, Nuovo Cimento **33**, 434 (1964).
[5]A.O. Barut and F. Calogero, Phys. Rev. **128**, 1383 (1962).
[6]E. Ferreira and J. Sesma, J. Math. Phys. **11**, 3245 (1970).
[7]C.M. Do Amaral and P.P. Srivastava, Nuovo Cimento **32**, 237 (1964).
[8]H. Cheng, Nuovo Cimento **44**, 487 (1966).
[9]J. Challifour and R.J. Eden, J. Math. Phys. **4**, 359 (1962).
[10]S. Mandelstam, Ann. Phys. (N.Y.) **19**, 254 (1962).
[11]V. Singh, Phys. Rev. **127**, 632 (1962).
[12]H.J.W. Müller and K. Schilcher, J. Math. Phys. **9**, 255 (1968).
[13]H. Cheng, Phys. Rev. **130**, 1283 (1963).
[14]V. Bargmann, Proc. Natl. Acad. Sci. **38**, 961 (1952); J. Schwinger, Proc. Natl. Acad. Sci. **47**, 122 (1961).
[15]E.L. Ince, *Ordinary Differential Equations* (Dover, New York, 1956), Chap. 15; W. Magnus and S. Winkler, *Hill's Equation* (Interscience, New York, 1966), Chap. 1.
[16]S. Fubini and R. Stroffolini, Nuovo Cimento **37**, 1812 (1965).
[17]See, for example, E.L. Ince, Ref. 15, pp. 382—384.
[18]R.O. Mastalir, J. Math. Phys. **15**, 000 (1974), Paper III of this series.
[19]R.O. Mastalir, *Theory of Confluent Heun Functions* (to be published).
[20]B.R. Desai and R.G. Newton, Phys. Rev. **130**, 2109 (1963); H. Cheng, Ref. 8.

Theory of Regge poles for $1/r^2$ potentials. II. An exactly solvable example at zero energy

Robert O. Mastalir

Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 3 June 1974)

We give the exact solution of the Schrödinger equation at zero energy and derive an expression in closed form for the Regge poles for a particular $1/r^2$ potential with the behavior $r^2V(r) = -V_0$ at $r = 0$ and $r^2V(r) = -V_2$ at $r = \infty$. We give detailed results on the properties and distribution of the Regge poles in the λ plane and find them to be in agreement with the predictions of a previous paper in this series.

1. INTRODUCTION

In a previous paper we discussed in detail the theory of Regge poles for $1/r^2$ potentials satisfying $\lim r^2V(r) = -V_0$ at $r=0$ and $\lim r^2V(r) = -V_2$ at $r=\infty$.[1] In the present paper we give the exact solution of the Schrödinger equation at zero energy and study the properties of the Regge poles for arbitrary angular momentum and zero energy for the particular potential

$$V(r) = -\frac{1}{r^2}\left(\frac{r_0^2V_0 + r_0V_1r^\alpha + V_2r^{2\alpha}}{(r_0 + r^\alpha)^2}\right). \tag{1.1}$$

where r_0, α are any positive numbers and V_0, V_1, V_2 are arbitrary constants.

A potential of the form of (1.1) was first considered by Eckart.[2] A particular case of (1.1) corresponding to $V_0 = V_2 = 0$ was investigated in detail by Cheng,[3] who obtained an expression in closed form for the zero energy Regge poles and gave a formula for the asymptotic behavior of the S matrix for $|\lambda| \to \infty$.

In Sec. 2 we recall some relevant results on the theory of Regge poles at zero energy. In Sec. 3 we solve the Schrödinger equation while in Sec. 4 we discuss in detail the properties of the Regge poles. The results obtained are summarized in Sec. 5 and are found to be in agreement with the general results obtained in I in the limit $E=0$.

2. THEORY OF REGGE POLES AT ZERO ENERGY

The behavior of Regge poles at zero energy has been the subject of detailed investigation.[1,3,4] In the present section we recall from I some of the principal results for the case of $1/r^2$ potentials.

The S matrix may be written in the form[1,5]

$$S = \exp[i\pi(\lambda - \nu)]\left(\frac{Y(p,\nu,k) + k^{2\nu}\exp(i\pi\nu)}{Y(p,\nu,k) + k^{2\nu}\exp(-i\pi\nu)}\right), \tag{2.1}$$

where $p = (\lambda^2 - V_0)^{1/2}$, $q = (\lambda^2 - V_2)^{1/2}$, and $\nu = \nu(p,q,k)$ is the Floquet parameter of the Schrödinger equation. When $V(r)$ is given by (1.1) the zero energy Floquet parameter is given by $\nu(p,q,0) = q/\alpha$. The following results follow from (2.1) and the discussion in Sec. 6 of I.

(1) If $\nu(p,q,k)$ is not zero or an integer the zero energy Regge poles in the first sheet of λ are given by the solutions of the equation:

$$Y(p,\nu,0) = \begin{cases} 0, & \mathrm{Re}\nu(p,q,0) > 0, \quad \mathrm{Re}\lambda > 0, \\ \infty, & \mathrm{Re}\nu(p,q,0) < 0, \quad \mathrm{Re}\lambda < 0. \end{cases} \tag{2.2}$$

(2) If $\nu(p,q,k)$ is an integer, $\nu = n$, a Regge pole at $\lambda = \lambda_0$, $E=0$ may only occur if S has a double pole at λ_0, $E=0$.

(3) If $\nu(p,q,k)$ is pure imaginary, we have $Y(p, i|\nu|, k) = \exp[iy(p, |\nu|, k)]$ for all k, where $y(p, |\nu|, k)$ is a real function of p, k which approaches a finite, nonzero limit as $k \to 0$. Therefore, the denominator in (2.1) does not have a well-defined limit as $k \to 0$. There are no Regge poles at $E=0$ in this case.

(4) There are no zero energy Regge poles on the cut.

3. SOLVABLE EXAMPLE OF REGGE POLES AT ZERO ENERGY

The radial Schrödinger equation at zero energy is

$$\frac{d^2\psi}{dr^2} + \left(\frac{\frac{1}{4} - \lambda^2}{r^2} - V(r)\right)\psi = 0. \tag{3.1}$$

We wish to solve (3.1) when $V(r)$ is given by (1.1). We readily find that (3.1) may be reduced to a hypergeometric equation by means of the transformations

$$x = -(r^\alpha/r_0), \quad \psi = x^{(1-\alpha)/2\alpha}\phi. \tag{3.2}$$

The general solution of (3.1) is found to be[6]

$$\psi(r) = r^{1/2}(1-x)^{(1+\delta)/2}[C_1x^{-\sigma/2}{}_2F_1(a,b;c;x) + C_2x^{\sigma/2}{}_2F_1(a+1-c,\ b+1-c;\ 2-c;x)], \tag{3.3}$$

where

$$a = \tfrac{1}{2}(1-\sigma-\delta-\mu), \quad b = \tfrac{1}{2}(1-\sigma-\delta+\mu), \quad c = 1-\sigma, \tag{3.4}$$

$$\sigma = (2/\alpha)(\lambda^2 - V_0)^{1/2}, \quad \mu = (2/\alpha)(\lambda^2 - V_2)^{1/2}, \quad \delta = [1 + (4/\alpha^2)(V_1 - V_0 - V_2)]^{1/2}, \tag{3.5}$$

and C_1, C_2 are arbitrary constants. Here ${}_2F_1(a,b;c;x)$ is the hypergeometric series and we define σ and μ as analytic functions of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$ and $-V_2^{1/2}$ to $V_2^{1/2}$, respectively. With reference to the notation of I, we note that $\sigma = (2/\alpha)p$, $\mu = (2/\alpha)q$.

From (3.5) we see that when λ is real and positive and away from the cut σ is also real and positive. Thus, for sufficiently large λ a unique physical solution of (3.1) that vanishes at the origin may be obtained by setting

$C_1=0$ and $C_2=1$. For other values of λ, the function $\psi(r)$ is then defined by analytic continuation.

From (3.3) we find that, for large r,[6]

$$\psi(r)\simeq a_1(\sigma,\mu)r^{1/2+(\alpha^2-V_2)^{1/2}}+a_2(\sigma,\mu)r^{1/2-(\alpha^2-V_2)^{1/2}}, \quad (3.6)$$

where σ and μ are given by (3.5) and

$$a_1(\sigma,\mu)=r_0^{-\mu/2}\left(\frac{\Gamma(\mu)\Gamma(1+\sigma)\exp(\frac{1}{2}i\pi\sigma)}{\Gamma(\frac{1}{2}(1+\sigma+\mu+\delta))\Gamma(\frac{1}{2}(1+\sigma+\mu-\delta))}\right). \quad (3.7)$$

$$a_2(\sigma,\mu)=r_0^{\mu/2}\left(\frac{\Gamma(-\mu)\Gamma(1+\sigma)\exp(\frac{1}{2}i\pi\sigma)}{\Gamma(\frac{1}{2}(1+\sigma-\mu+\delta))\Gamma(\frac{1}{2}(1+\sigma-\mu-\delta))}\right). \quad (3.8)$$

From (3.6) we see that when λ is real and sufficiently large $\psi(r)$ vanishes at infinity provided that

$$a_1(\sigma,\mu)=0. \quad (3.9)$$

We conclude that a Regge pole occurs if (3.9) is satisfied. Furthermore, this must be true for all λ in the right half-plane as a consequence of analytic continuation. More precisely, let us introduce the function $Y(\lambda,k)$, which at zero energy is given by[5]

$$Y(\lambda,0)=2^{2\mu}\frac{\Gamma(1+\mu)}{\Gamma(1-\mu)}\left(\frac{a_1(\sigma,\mu)}{a_2(\sigma,\mu)}\right). \quad (3.10)$$

Thus, (3.7)—(3.10) give

$$Y(\lambda,0)=-2^{2\mu}r_0^{-\mu}\left(\frac{\Gamma(1+\mu)}{\Gamma(1-\mu)}\right)^2 \times\left(\frac{\Gamma(\frac{1}{2}(1+\sigma+\delta-\mu))\Gamma(\frac{1}{2}(1+\sigma-\delta-\mu))}{\Gamma(\frac{1}{2}(1+\sigma+\delta+\mu))\Gamma(\frac{1}{2}(1+\sigma-\delta+\mu))}\right). \quad (3.11)$$

The Regge poles in the right half-plane may be found by setting $Y(\lambda,0)=0$ with $\mathrm{Re}\lambda>0$. Thus, they are given by the solutions of the equations

$$1+\sigma+\mu\pm\delta=-2n, \quad n=0,\ 1,\ 2\cdots, \quad \mathrm{Re}\lambda>0. \quad (3.12)$$

Equation (3.11) also has double zeroes at $\mu=1,\ 2\cdots$. However, these are not locations of zero energy Regge poles. In this case the continuation of the hypergeometric series in (3.4) contains logarithmic terms and is no longer given by (3.6). Reference to the appropriate continuation formulas[6] shows that the points $\mu=1,\ 2\cdots$ are locations of zero energy Regge poles only when (3.12) is also satisfied at these points. Thus, (3.12) gives all the Regge poles at zero energy.

4. DISTRIBUTION AND PROPERTIES OF THE REGGE POLES

We now study Eq. (3.12) in some detail. We limit our discussion to the solutions of (3.12) in $\mathrm{Re}\lambda\geq 0$ with λ in the first sheet. In what follows we assume that V_0, V_1, V_2 are real numbers. Consequently, we may take δ, σ, μ to be nonnegative real numbers.

Equation (3.12) may be rewritten in the form

$$(\lambda^2-V_0)^{1/2}+(\lambda^2-V_2)^{1/2}=N, \quad \mathrm{Re}\lambda\geq 0, \quad (4.1)$$

where

$$N=(\alpha/2)(\delta-2n-1), \quad n=0,\ 1,\ 2\cdots. \quad (4.2)$$

Clearly, (4.1) has at least one solution provided that

$$\mathrm{Re}N>0. \quad (4.3)$$

That is, using (3.5),

$$V_1-V_0-V_2>\alpha^2 n(n+1), \quad n=0,\ 1,\ 2\cdots. \quad (4.4)$$

Since $\alpha>0$, it follows that there are no Regge poles with $\mathrm{Re}\lambda\geq 0$ in the first sheet of λ unless $V_1>V_0+V_2$.

The solution of (4.1) is found to be

$$\lambda_n=\frac{1}{2N}\left[N^2+(V_0^{1/2}+V_2^{1/2})^2\right]^{1/2}\left[N^2+(V_0^{1/2}-V_2^{1/2})^2\right]^{1/2}. \quad (4.5)$$

It follows from (4.2)—(4.3) that there can be at most a finite number of poles λ_n for arbitrary V_0, V_1, V_2, and α. Indeed, the number of poles is given by the closest integer less than $\frac{1}{2}(\delta-1)$.

From (4.5) we see that λ_n may be either real or pure imaginary. If V_0 and V_2 are positive or have opposite signs, λ_n is always real. The possibility that λ_n be pure imaginary can only arise if both V_0, V_2 are negative and N satisfies the inequality

$$|V_0|^{1/2}-|V_2|^{1/2}<N<|V_0|^{1/2}+|V_2|^{1/2}. \quad (4.6)$$

When $V_0>0$ and $V_2>0$, we find from (4.5) that λ_n is real and to the right of $V_0^{1/2}$ or $V_2^{1/2}$, whichever is greater. Indeed, $\lambda_n(N)$ has a local minimum at

$$N=N^*=(|V_0-V_2|)^{1/2}, \quad (4.7)$$

at which

$$\lambda_n(N^*)=\begin{cases} V_0^{1/2}, & V_0>V_2,\\ V_2^{1/2}, & V_2>V_0.\end{cases} \quad (4.8)$$

That is, if for some nonnegative integer $n=n^*$ equation (4.7) happens to be satisfied, then $\lambda_{n^*}(N^*)$ corresponds to the leftmost Regge pole and is given by (4.8). For any other allowed value of n (such that $N>0$) λ_n will be to the right of $\lambda_{n^*}(N^*)$. In particular, we see from (4.8) that there are no zero energy Regge poles in the segment $V_0^{1/2}<\lambda<V_2^{1/2}$.

Similarly, when $V_0>0$ and $V_2<0$ we find from (4.5) that λ_n is real and to the right of $V_0^{1/2}$, except when $N=(V_0+|V_2|)^{1/2}$ in which case λ_n is precisely at the branch point $V_0^{1/2}$. When $V_0<0$ and $V_2>0$, λ_n is likewise real and to the right of $V_2^{1/2}$ except when $N=(V_2+|V_0|)^{1/2}$, in which case $\lambda_n=V_2^{1/2}$.

When $V_0<0$ and $V_2<0$, the Regge poles λ_n may be either real or pure imaginary. If N is not in the range specified by (4.6), the poles λ_n are real and located on the positive real axis $\mathrm{Re}\lambda>0$. If N satisfies (4.6), λ_n becomes pure imaginary. If $|V_0|>|V_2|$, the poles are located in $-i|V_2|^{1/2}<\lambda_n<i|V_2|^{1/2}$, that is, on the cut. We note that there are no poles in the segments $i|V_2|^{1/2}<\pm\lambda_n<i|V_0|^{1/2}$ or elsewhere on the imaginary axis. If $|V_2|>|V_0|$ the Regge poles are located in $-i|V_0|^{1/2}<\lambda_n<i|V_0|^{1/2}$ which comprises the whole cut.

The above discussion exhausts all the possibilities for the existence of zero energy Regge poles with $\mathrm{Re}\lambda>0$ and λ on the first sheet. We have found only a finite

number of such poles. We note, however, that an infinite number of poles with $\mathrm{Re}\lambda > 0$ do exist in the second sheet, where $\mathrm{Re}\sigma < 0$ and $\mathrm{Re}\mu < 0$. Indeed, in this case equation (3.12) reads

$$1 - \sigma - \mu \pm \delta = -2n, \quad n = 0, 1, 2 \cdots, \tag{4.9}$$

which evidently has an infinite number of solutions with $\mathrm{Re}\lambda > 0$.

5. SUMMARY

We have derived an expression in closed form for the Regge poles at zero energy for the potential defined in (1.1) and studied in detail their properties and distribution in the λ plane, which is cut from $-V_0^{1/2}$ to $V_0^{1/2}$. Our results agree with those predicted in a previous paper.[1] Briefly, we have found that:

(1) There is a finite number of zero energy Regge poles with $\mathrm{Re}\lambda \geq 0$ in the first sheet of λ. There are no poles on the cut. If V_0 and V_2 are both positive or have opposite signs, the poles are real and to the right of $V_0^{1/2}$ or $V_2^{1/2}$, whichever is greater. If V_0 and V_2 are both negative the poles may be either real and located in $\mathrm{Re}\lambda > 0$ or pure imaginary and within the cut. The total number of poles is given by the nearest integer less than $\frac{1}{2}(\delta - 1)$, where δ is defined in (3.5).

(2) There is an infinite number of zero energy Regge poles with $\mathrm{Re}\lambda > 0$ in the second sheet of λ.

[1] R. O. Mastalir, J. Math. Phys. **16**, 743 (1974), preceding paper. Hereafter referred to as I.
[2] C. Eckart, Phys. Rev. **35**, 1303 (1930).
[3] H. Cheng, Nuovo Cimento **44**, 487 (1966).
[4] B. P. Desai and R. G. Newton, Phys. Rev. **130**, 2109 (1963).
[5] R. O. Mastalir, J. Math. Phys. **16**, 752 (1974), following paper, III in this series.
[6] *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. 1, Chap. 2.

Theory of Regge poles for $1/r^2$ potentials. III. An exact solution of Schrödinger's equation for arbitrary l and E

Robert O. Mastalir

Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 3 June 1974)

We give the exact solution of the radial Schrödinger equation and derive the S matrix for arbitrary energy and angular momentum for a particular $1/r^2$ potential with the behavior $r^2V(r) = -V_0$ at $r = 0$ and $r^2V(r) = -V_2$ at $r = \infty$. We obtain an expression for the Regge poles and study their properties and distribution at low energy. The present results are in agreement with those obtained in a previous paper in this series.

1. INTRODUCTION

In previous papers[1] (referred to as Papers I and II) we studied in detail the general theory of Regge poles for $1/r^2$ potentials with the behavior $r^2\ V(r) = -V_0$ at $r=0$ and $r^2\ V(r)=-V_2$ at $r=\infty$ and we discussed the exact solution and the Regge pole structure at zero energy for a particular $1/r^2$ potential with the above characteristics. In the present paper we give the exact solution of the radial Schrödinger equation for arbitrary energy and angular momentum for the potential

$$V(r)=-\frac{1}{r^2}\left(\frac{r_0^2V_0+r_0V_1r^2+V_2r^4}{(r^2+r_0)^2}\right), \tag{1.1}$$

where r_0 is positive and V_0, V_1, V_2 are arbitrary constants.

We give the solution of the Schrödinger equation in terms of a set of new functions which are generalizations of the spheroidal wave functions.[2] We give the theory of these functions elsewhere[3] and only state results here.

In Sec. 2 we obtain the exact S matrix and discuss its analytic properties. In Sec. 3 we study the properties and distribution of the Regge poles at low energy. In each case the results obtained agree with the general results predicted in I.

Lastly, in Appendix B we consider the problem of deriving the S matrix for a potential which is a superposition of (1.1) and an arbitrary Yukawa potential of finite mass m_0.

2. DERIVATION OF THE S MATRIX

We wish to solve the radial Schrödinger equation

$$\frac{d^2y}{dr^2}+\left[k^2-\frac{\lambda^2-\frac{1}{4}}{r^2}-V(r)\right]y=0, \tag{2.1}$$

where $k^2=E$ is the energy and $\lambda=l+\frac{1}{2}$ with l the angular momentum and $V(r)$ is given by (1.1).

Setting

$$p=(\lambda^2-V_0)^{1/2},\quad q=(\lambda^2-V_2)^{1/2},\quad \rho=(1+V_1-V_0-V_2)^{1/2}, \tag{2.2}$$

we find that (2.1) may be rewritten in the form

$$\frac{d^2y}{dr^2}+\left(k^2-\frac{(1-p^2-\rho^2+q^2)}{(r^2+r_0)}+\frac{(1-\rho^2)r^2}{(r^2+r_0)^2}-\frac{p^2-\frac{1}{4}}{r^2}\right)y=0, \tag{2.3}$$

which is identical to the equation of Generalized Spheroidal functions (of the second type).[3]

A solution of (2.3) satisfying the boundary condition

$$y(r)\approx r^{1/2+p},\quad r\to 0, \tag{2.4}$$

is given by the function[3]

$$Ps_\nu^{(3)}(r)=r^{1/2+p}(r^2+r_0)^{(1+\rho)/2}$$

$$\times\sum_{m=-\infty}^{+\infty}Ds_m{}^\nu Ps_{\nu,m}^{(3)}(r), \tag{2.5}$$

where

$$Ps_{\nu,m}^{(3)}(r)=(-1)^{-m-\nu-(p+\rho)/2-1}\frac{(\nu+1+\frac{1}{2}(p-\rho))_m}{(\nu+1-\frac{1}{2}(p-\rho))_m}$$

$$\times {}_2F_1(A+1-C,\ B+1-C;\ 2-C;-(r^2/r_0)), \tag{2.6}$$

and

$$A=m+\nu+1-\tfrac{1}{2}(p-\rho),\quad B=-m-\nu-\tfrac{1}{2}(p-\rho),\quad C=1-p. \tag{2.7}$$

Here ${}_2F_1(a,\ b;\ c;\ z)$ is the hypergeometric function and $(z)_m$ is the Pochhammer symbol:

$$(z)_m=\frac{\Gamma(z+m)}{\Gamma(z)},\quad (z)_0=1. \tag{2.8}$$

The coefficients Ds_m^ν in (2.5) satisfy the three term recurrence relation[3]

$$\eta Ks_m^\nu Ds_{m-1}^\nu+Ls_m^\nu Ds_m^\nu+\eta Ms_m^\nu Ds_{m+1}^\nu=0,\quad m=0,\pm1,\pm2\cdots, \tag{2.9}$$

where

$$Ks_m^\nu=-\frac{(m+\nu-\frac{1}{2}(p-\rho))(m+\nu+\frac{1}{2}(p+\rho))}{(2m+2\nu)(2m+2\nu-1)}, \tag{2.10a}$$

$$Ls_m^\nu=-\lambda s_\nu+\tfrac{1}{2}\eta-\tfrac{1}{8}\eta\left(\frac{(p^2-\rho^2)}{(m+\nu)(m+\nu+1)}\right)$$

$$+(m+\nu+1+\tfrac{1}{2}(p+\rho))(m+\nu-\tfrac{1}{2}(p+\rho)), \tag{2.10b}$$

$$Ms_m^\nu=-\frac{(m+\nu+1-\frac{1}{2}(p+\rho))(m+\nu+1+\frac{1}{2}(p-\rho))}{(2m+2\nu+2)(2m+2\nu+3)}. \tag{2.10c}$$

and we have introduced the parameters

$$\eta=(r_0k^2)/4, \tag{2.11}$$

and

$$\lambda s_\nu=[\tfrac{1}{2}(q-1)-\tfrac{1}{2}(p+\rho)][\tfrac{1}{2}(q-1)+\tfrac{1}{2}(p+\rho)+1]. \tag{2.12}$$

In the above expressions the parameter ν is the Floquet parameter associated with Eq. (2.3). It is a complicated transcendental function of λ, k, r_0, V_0, V_1, and V_2. It is an even analytic function of k and a meromorphic function of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$. In general, ν may be obtained as the result of a consistency condition in the process of solving the recurrence relation (2.9). In practice one can derive an expansion for λs_ν in powers of η which serves as an implicit definition of ν, together with the initial condition at zero energy (see Appendix 1)[4]

$$\nu(k=0)=\tfrac{1}{2}(q-1). \tag{2.13}$$

It can be shown that λs_ν and Ds_m^ν satisfy the following identities[3]:

$$\lambda s_\nu(k)=\lambda s_{-\nu-1}(k)=\lambda s_\nu(k\exp(-i\pi)), \tag{2.14}$$

$$Ds_m^\nu(k)=Ds_{-m}^{-\nu-1}(k)=Ds_m^\nu(k\exp(-i\pi)), \quad m=0,\ \pm1,\ \cdots. \tag{2.15}$$

Proofs of the convergence of (2.5) and (2.9) as well as (2.16) below and a more detailed description of the computational aspects relevant to the present problem can be found in Ref. 3. We note that the above treatment is not adequate when ν is integral or half-integral. These are exceptional cases which require a slightly modified treatment [briefly, the functions $Ps^\nu(r)$ and $\Psi s^\nu(r)$ include logarithmic terms in these cases]. A short list of relevant results is given in Appendix A.

A pair of solutions of (2.3) with the behavior $\exp(\pm ikr)$ at infinity is given by[3]

$$\Psi s_\nu^{(j)}(r)=r^{1/2+\rho}(r^2+r_0)^{(1+\rho)/2} \times\sum_{m=-\infty}^{+\infty}Ds_m^\nu\psi s_{\nu,m}^{(j)}(r), \quad j=3,\ 4, \tag{2.16}$$

where

$$\psi s_{\nu,m}^{(3)}(r)=-i\pi(\tfrac{1}{2}k)^{-2\nu-1}\exp[-i\pi(m+2\nu+1)] \times r^{-1-\rho-\rho}H_{2m+2\nu+1}^{(2)}(kr), \tag{2.17}$$

$$\psi s_{\nu,m}^{(4)}(r)=i\pi(\tfrac{1}{2}k)^{-2\nu-1}\exp[i\pi(m+2\nu+1)] \times r^{-1-\rho-\rho}H_{2m+2\nu+1}^{(1)}(kr). \tag{2.18}$$

The coefficients Ds_m^ν and the Floquet parameter ν in (2.16) are identical to the ones appearing in (2.5). Here $H_{2m+2\nu+1}^{(1),(2)}(kr)$ are the Hankel functions of the first and second kind.

At $r=\infty$ the following results hold[3]:

$$\Psi s_\nu^{(3)}(r)\sim\pi^{1/2}\exp[\mp i\pi(\nu+3/4)](\tfrac{1}{2}k)^{-2\nu-3/2}\exp(\mp ikr) \times\left(\sum_{m=-\infty}^{+\infty}Ds_m^\nu\right)\left[1+O\left(\frac{1}{|kr|}\right)\right], \quad |kr|\to\infty, \tag{2.19}$$

where

$$-3\pi/2<\arg(kr)<3\pi/2 \quad \text{for } \Psi s_\nu^{(3)}(r),$$
$$-3\pi/2<\arg(-kr)<3\pi/2 \quad \text{for } \Psi s_\nu^{(4)}(r). \tag{2.20}$$

In order to find the S matrix we must obtain connection formulas between the function $Ps_\nu^{(3)}(r)$ and the functions $\Psi s_\nu^{(3)}(r)$ and $\Psi s_\nu^{(4)}(r)$. These are derived in Ref. 3.

As $r\to\infty$, we may write

$$Ps_\nu^{(3)}(r)\approx f_+\exp(ikr)-f_-\exp(-ikr), \quad r\to\infty, \tag{2.21}$$

from which the S matrix is obtained as $S=(f_+/f_-)\exp(i\pi l)$. The final result is[3]

$$S=\exp i\pi(\lambda-2\nu)\left(\frac{Y_\nu(k)+k^{4\nu+2}\exp[i\pi(2\nu+1)]}{Y_\nu(k)+k^{4\nu+2}\exp[-i\pi(2\nu+1)]}\right), \tag{2.22}$$

where

$$Y_\nu(k)=-(4/r_0)^{2\nu+1}\left(\frac{\Gamma(2\nu+1)}{\Gamma(-2\nu-1)}\right)^2 Rs_\nu(k) \times\left(\frac{\Gamma(-\nu+\frac{1}{2}(p-\rho))\Gamma(-\nu+\frac{1}{2}(p+\rho))}{\Gamma(\nu+1+\frac{1}{2}(p-\rho))\Gamma(\nu+1+\frac{1}{2}(p+\rho))}\right), \tag{2.23}$$

and

$$Rs_\nu(k)=\frac{Rs_\nu^{(1)}Rs_\nu^{(2)}}{Rs_{-\nu-1}^{(1)}Rs_{-\nu-1}^{(2)}}, \tag{2.24}$$

with

$$Rs_\nu^{(1)}=\sum_{m=0}^{\infty}Ds_m^\nu(-1)^m\frac{(2\nu+1)_m}{m!}, \tag{2.25}$$

$$Rs_\nu^{(2)}=\sum_{m=0}^{\infty}Ds_m^\nu(-1)^m\frac{(2\nu+1)_m}{m!} \times\left(\frac{(\nu+1-\frac{1}{2}(p+\rho))_m(\nu+1+\frac{1}{2}(p-\rho))_m}{(\nu+1-\frac{1}{2}(p-\rho))_m(\nu+1+\frac{1}{2}(p+\rho))_m}\right). \tag{2.26}$$

Since ν is an even analytic function of k, we find, using (2.14), (2.15), that

$$Y_\nu(k)=Y_\nu(k\exp(-i\pi))=[Y_{-\nu-1}(k)]^{-1}. \tag{2.27}$$

We see that $Y_\nu(k)$ is likewise an even analytic function of k with no singularity at $k=0$ and a meromorphic function of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$. Evidently, $Y_\nu(k)$ is regular at $\lambda=\pm V_2^{1/2}$.

From (2.22) and (2.27) we find

$$S_\nu(k)=S_{-\nu-1}(k), \tag{2.28}$$

$$S_\nu(k\exp(-i\pi))=\exp(2i\pi l)[S_\nu(k)-2\cos(2\pi\nu)\exp(i\pi\lambda)]^{-1}. \tag{2.29}$$

Thus, the S matrix is regular at $\lambda=\pm V_2^{1/2}$. The circuital relation for S about the branch point at $k=0$ follows immediately from (2.29).

3. REGGE POLES AT LOW ENERGY

Due to the complicated nature of the results (2.22)–(2.26), we restrict our discussion of the Regge poles of (1.1) to the low energy limit. In what follows we restrict λ to the right-hand plane of the first sheet.

The Regge poles $\lambda_n(E)$ are given by the solutions of

$$Y_\nu(E)+E^{2\nu+1}\exp[-i\pi(2\nu+1)]=0. \tag{3.1}$$

Using (2.13) and (A6), we find that in the low energy limit (3.1) reduces to

$$Y_q(0)\left[1+\tfrac{1}{2}r_0E\left(\frac{q(p^2-\rho^2)}{(q^2-1)^2}\right)+O(r_0^2E^2)\right]+E^q\exp(-i\pi q), \quad +O(E^2\ln E), \quad E\to0, \tag{3.2}$$

where $Y_q(0)$ is just (2.23) with $E=0$. We see that the Regge poles at zero energy $\lambda_n(0)$ are given by

$$(\lambda_n^2(0)-V_2)^{1/2}+(\lambda_n^2(0)-V_0)^{1/2}=N(0),\quad \mathrm{Re}\lambda_n(0)>0, \tag{3.3}$$

where

$$N(0)=\rho-2n-1,\quad n=0,\ 1,\ 2\cdots, \tag{3.4}$$

and ρ is given by (2.2). The solutions of (3.3) were studied in detail in II.

When $q<1$ we find from (3.2) that the Regge poles $\lambda_n(E)$ in the right-hand plane are given by, to the leading order in E

$$(\lambda_n^2(E)-V_2)^{1/2}+(\lambda_n^2(E)-V_0)^{1/2}=N(E),\quad \mathrm{Re}\lambda_n(E)>0, \tag{3.5}$$

where

$$N(E)=N(0)-M\sin[\pi q(0)](r_0E/4)^{q(0)}\exp[-i\pi q(0)], \tag{3.6}$$

with

$$M=(2/\pi)\frac{\Gamma(\rho-n)}{n!}\left(\frac{\Gamma(-q(0))}{\Gamma(q(0))}\right)^2\frac{\Gamma(1+n+q(0))}{\Gamma(1+n+p(0))}, \tag{3.7}$$

and

$$q(0)=(\lambda_n^2(0)-V_2)^{1/2}=[N^2(0)+V_0-V_2]/2N(0), \tag{3.8}$$

$$p(0)=(\lambda_n^2(0)-V_0)^{1/2}=[N^2(0)+V_2-V_0]/2N(0). \tag{3.9}$$

The solution of (3.5) is given by

$$\lambda_n(E)=\frac{1}{2N(E)}[N^2(E)+(V_0^{1/2}+V_2^{1/2})^2]^{1/2}\times[N^2(E)+(V_0^{1/2}-V_2^{1/2})^2]^{1/2}, \tag{3.10}$$

which is the desired expression for the Regge poles of (1.1) valid for $E\sim 0$ and $q(0)<1$. An expression equivalent to (3.10) and more useful for some purposes is

$$\lambda_n(E)\approx\lambda_n(0)-\left(\frac{q(0)p(0)}{N(0)\lambda_n(0)}\right)M\sin[\pi q(0)](r_0E/4)^{q(0)}\times\exp[-i\pi q(0)]. \tag{3.11}$$

Since we are taking $\mathrm{Re}\lambda>0$, it follows that $\mathrm{Re}q$, $\mathrm{Re}p$, and $N(0)$ are also positive. Consequently, we see from (3.7) that $M>0$. Since $q(0)<1$, (3.11) implies that

(1) If $E<0$, then $\lambda_n(E)$ is real and $\lambda_n(E)<\lambda_n(0)$.

(2) If $E>0$, then $\lambda_n(E)$ has a positive imaginary part. When $0<q(0)<\frac{1}{2}$, $\mathrm{Re}\lambda_n(E)\leq\lambda_n(0)$, while if $\frac{1}{2}<q(0)<1$, $\mathrm{Re}\lambda_n(E)>\lambda_n(0)$. These results agree with those predicted in I.

A similar calculation may be performed in the case $q(0)>1$. For example, if $E<0$, we find

$$\lambda_n(E)\approx\lambda_n(0)-\frac{1}{2\lambda_n(0)}(r_0|E|/4)\left(\frac{q(0)(\rho^2-p^2(0))}{(q^2(0)-1)}\right). \tag{3.12}$$

Again, $\lambda_n(E)<\lambda_n(0)$, as expected.

We note that Eq. (3.10) implies that $\lambda_n(E)$ may have branch points at values of E such that $N(E)=|V_0|^{1/2}\pm|V_2|^{1/2}$, at which $\lambda_n(E)=0$. The values of E at which these branch points are located are given approximately, by,

$$(r_0|E|/4)^{q(0)}=\frac{[N(0)-(|V_0|^{1/2}\pm|V_2|^{1/2})]}{M\sin[\pi q(0)]}, \tag{3.13}$$

with $\arg E=\exp(i\pi)$. That is, to this approximation E is real and negative. If the right-hand side of (3.13) is sufficiently small these values of E will correspond to the approximate locations of actual branch points of $\lambda_n(E)$.

When $\nu\to-\frac{1}{2}$ we find that

$$\lim Rs_\nu(k)=1,\quad \nu\to-\tfrac{1}{2}, \tag{3.14a}$$

$$\lim Y_\nu(k)=-1,\quad \nu\to-\tfrac{1}{2}, \tag{3.14b}$$

for all k. In particular, when $E\sim 0$, we see that (3.10) is not valid when $q(0)\sim 0$. This case was examined in detail in I. One finds directly from (3.1) that $\lambda_n(E)$ is given by

$$\mathrm{Re}(\lambda_n^2(E)-V_2)^{1/2}\approx\frac{2n\pi(\pi-\gamma)}{|\ln|E||^2}-\frac{2n^2\pi^2Y_{00}^2}{|\ln|E||^3}, \tag{3.15a}$$

$$\mathrm{Im}(\lambda_n^2(E)-V_2)^{1/2}\approx\frac{2n\pi}{|\ln|E||}, \tag{3.15b}$$

where $n=\pm1,\ \pm2,\cdots$, $E=|E|\exp(i\gamma)$ with $|E|\sim 0$ and in the present example

$$Y_{00}=\left.\frac{\partial Y_\nu(k)}{\partial\nu}\right|_{\substack{k=0\\ q=0}}=\ln(r_0/4)+4\psi(1)+\psi(\tfrac{1}{2}(1+\bar p+\rho))+\psi(\tfrac{1}{2}(1+\bar p-\rho)), \tag{3.16}$$

where $\psi(z)$ is the logarithmic derivative of the gamma function and $\bar p=(V_2-V_0)^{1/2}$ while ρ is given by (2.2).

Evidently, an infinite number of Regge poles approach the points $\lambda=\pm V_2^{1/2}$ as $E\to 0$ along any direction in the complex energy plane.

Lastly, we consider briefly the case when $V_2>V_0>0$ and $V_0^{1/2}<\lambda<V_2^{1/2}$. Here q becomes pure imaginary and (3.2) does not approach a definite limit as $E\to 0$. Following the discussion given in Sec. 6 of I, we note that in this case $Y_{iq}(0)=\exp[iy(|q|,0)]$ and therefore the Regge poles in $V_0^{1/2}<\lambda<V_2^{1/2}$ are given by

$$(V_2-\lambda_n^2(E))^{1/2}\approx\frac{2n\pi}{|\ln|E||}+\frac{2n\pi Y_{00}}{|\ln|E||^2}+\cdots,\quad n=\pm1,\ \pm2\cdots, \tag{3.17}$$

with Y_{00} defined in (3.16). Thus, an infinite number of poles approach the point $V_2^{1/2}$ along the real axis as $E\to 0^-$.

4. CONCLUSION

We have obtained the exact solution of the radial Schrödinger equation and the exact S matrix for arbitrary λ and k for the potential $V(r)$ defined in (1.1). We find that the S matrix is analytic in the whole k plane with a kinematic branch point at $k=0$ which is characterized by the Floquet parameter $\nu(\lambda,k)$ associated with the Schrödinger equation. Further, S is a meromorphic function of λ in the λ plane cut from $-V_0^{1/2}$ to $V_0^{1/2}$.

We obtained an expression for the Regge poles $\lambda_n(E)$ in the right-hand plane and studied their behavior at low energy. We find that our results are in agreement with those predicted in I.

Lastly, we verified that $\lambda_n(E)$ has branch points in the E plane and gave an approximate expression for their

possible location at low energy. The branch points are of the square root type and do not appear in the S matrix.

APPENDIX A

The recurrence relation (2.9) may be solved by using the method of continued fractions.[2] If η is sufficiently small, the coefficients $Ds^{\nu}_{\pm m}(\eta)$ may be obtained in terms of a series of powers of η. We find the results[3]

$$Ds^{\nu}_{1}(\eta) = -\left(\frac{Ks^{\nu}_{1}}{Ls^{\nu}_{1}}\right)\eta + O(\eta^3), \tag{A1}$$

$$Ds^{\nu}_{-1}(\eta) = -\left(\frac{Ms^{\nu}_{-1}}{Ls^{\nu}_{-1}}\right)\eta + O(\eta^3), \tag{A2}$$

and, in general,

$$Ds^{\nu}_{\pm m}(\eta) \approx \eta^m. \tag{A3}$$

The initial condition (2.13) on ν is found as follows. Setting $\eta = 0$ in (2.9), we conclude that we must have $Ds^{\nu}_{0}(0) = 1$ and $Ds^{\nu}_{\pm m}(0) = 0$ for $m \neq 0$ and

$$\lambda s_{\nu}(\eta) = \left(\nu - \tfrac{1}{2}(p+\rho)\right)_m \left(\nu + 1 + \tfrac{1}{2}(p+\rho)\right)_m. \tag{A4}$$

Using this result and (2.12), we see that (2.13) follows.

In order to obtain the next term in the expansion of ν in powers of η we substitute (A1), (A.2) in (2.9) (with $m = 0$), thereby obtaining (A4) with the following additional terms on its right-hand side:

$$\left(\frac{Ks^{\nu}_{0}Ms^{\nu}_{-1}}{Ls^{\nu}_{-1}} + \frac{Ms^{\nu}_{0}Ks^{\nu}_{1}}{Ls^{\nu}_{1}}\right)\eta^2 + O(\eta^4). \tag{A5}$$

This formula yields ν to order η^2. The above procedure may be repeated to any desired order in η.

Using the above results, we readily find the following expansion for the function $Rs_{\nu}(k)$ defined in (2.24)–(2.26):

$$Rs_{\nu}(\eta) = 1 + (2\eta)\left(\frac{q(p^2-\rho^2)}{(q^2-1)^2}\right) + O(\eta^2), \tag{A6}$$

from which it is obvious that at $E = 0$ we have $Rs_{\nu}(0) = 1$.

APPENDIX B

Here we outline a derivation of the S matrix for a potential $V(r)$ which is a superposition of (1.1) and an arbitrary Yukawa potential $U(r)$ of finite mass m_0. We use the method of variation of parameters with the unperturbed linearly independent solutions $Ps_{\nu}^{(3)}(r)$, defined in (2.5) and $Ps_{\nu}^{(4)}(r)$, which is given by[3]

$$Ps_{\nu}^{(4)}(r) = r^{1/2+\rho}(r^2 + r_0)^{(1+\rho)/2} \times \sum_{m=-\infty}^{+\infty} Ds_m{}^{\nu} Ps_{\nu,m}^{(4)}(r), \tag{B1}$$

where

$$Ps^{(4)}_{\nu,m}(r) = (-1)^{-m-\nu-1+(p-\rho)/2}\,\frac{\left(\nu+1-\frac{1}{2}(p+\rho)\right)_m}{\left(\nu+1+\frac{1}{2}(p+\rho)\right)_m} \times (-r^2/r_0)^{-\rho}\,{}_2F_1(A, B; C; -r^2/r_0), \tag{B2}$$

with A, B, C given by (2.7). Here ${}_2F_1(A, B; C; z)$ is the hypergeometric function and the coefficients $Ds_m{}^{\nu}$ and the Floquet parameter ν are the same as in (2.5) and (2.26).

Setting $V(r) = (1.1) + U(r)$, we solve the Schrödinger Eq. (2.1) by the method of variation of parameters and find that the S matrix is given by an expression identical to (2.22) with the function $Y_{\nu}(k)$ replaced by $\bar{Y}_{\nu}(k)$, where

$$\bar{Y}_{\nu}(k) = Y_{\nu}(k)\left(\frac{T_{\nu}(k)}{T_{-\nu-1}(k)}\right), \tag{B3}$$

with $Y_{\nu}(k)$ as defined in (2.23) and $T_{\nu}(k)$ given by

$$T_{\nu}(k) = \frac{\Gamma(1+p)}{\Gamma(1-p)}\left(W(3,4) - \int_0^{\infty} Ps_{\nu}{}^{(4)}(r')U(r')\psi(r')\,dr'\right) + \frac{\Gamma\left(\nu+1+\frac{1}{2}(p-\rho)\right)\Gamma\left(\nu+1+\frac{1}{2}(p+\rho)\right)}{\Gamma\left(\nu+1-\frac{1}{2}(p-\rho)\right)\Gamma\left(\nu+1-\frac{1}{2}(p+\rho)\right)} \times \int_0^{\infty} Ps_{\nu}{}^{(3)}(r')U(r')\psi(r')\,dr', \tag{B4}$$

where $W(3, 4)$ is the Wronskian of $Ps_{\nu}{}^{(3)}(r)$ and $Ps_{\nu}{}^{(4)}(r)$ which may be easily computed at $r = 0$. The functions $\psi(r')$ in (B4) are given by appropriate iteration series, which are certainly convergent for small enough k. The cumbersome nature of the functions we are dealing with precludes a more extensive discussion of the above expressions. However, we are principally interested in a few properties of the S matrix and $\bar{Y}_{\nu}(k)$ which have been used in I, II. Thus, we readily verify from (B4) that the results (2.27), (2.28), and (2.29) hold for $\bar{Y}_{\nu}(k)$ and the S matrix. Similarly, we also verify that the result (3.14b) holds for $\bar{Y}_{\nu}(k)$.

[1] R. O. Mastalir, J. Math. Phys. 16, 743, 749 (1974) preceding papers, hereafter referred to as I and II, respectively.
[2] *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1955), Vol. 3, Chaps. 15, 16.
[3] R. O. Mastalir, *Theory of Confluent Heun Functions* (to be published).
[4] Our notation for the Floquet parameter here follows the conventional one in the theory of spheroidal functions, wherein linearly independent Floquet solutions are labelled y_{ν} and $y_{-\nu-1}$. The parameter ν in Papers I, II corresponds to $2\nu+1$ here, as well as in Ref. 3, as may be seen by inspection of Eq. (2.13).

Double coset analysis for symmetry adapting Nth rank tensors of $U(n)$ to its unitary subgroups

John J. Sullivan

Physics Department, University of New Orleans, New Orleans, Louisiana 70122
(Received 1 July 1974)

Representations of the unitary group $U(n)$ symmetry adapted to the subgroup sequences $U(n) \supset \begin{matrix} \otimes U(n_j) \searrow \\ \otimes U(_in) \nearrow \end{matrix} \otimes U(_in_j)$ are considered using double coset decomposition. The matrix elements of the double coset representatives are related to identical coefficients developed in an analogous manner for the symmetric group [J. J. Sullivan, J. Math. Phys. **14**, 387 (1973)].

I. INTRODUCTION

The relationship between the unitary and symmetric groups implicit in the Shur—Weyl[1] construction of tensor representations has provided a powerful tool for analyzing the Racah algebra of the unitary group. Aside from the direct relevance these groups have for elementary particle, nuclear, and atomic physics, a complete understanding of their algebras facilitates study of their (continuous or finite) subgroups.

In recent work[2] (hereafter referred to as I) we have used double coset techniques to establish the orthogonality and completeness relations of the symmetric group as conditions also holding for the recoupling coefficients of the unitary group. The double coset representatives (hereafter DCR) of the decomposition of $S_{_1N} \otimes S_{_2N} \backslash S_N / S_{N_1} \otimes S_{N_2}$ are in one to one correspondance with double coset symbols

$$\begin{bmatrix} N & N_j \\ {}_iN & {}_iN_j \end{bmatrix} \equiv \begin{bmatrix} N & N_1 & N_2 \\ {}_1N & {}_1N_1^0 - K & {}_1N_2^0 + K \\ {}_2N & {}_2N_1^0 + K & {}_2N_2^0 - K \end{bmatrix}$$

which indicate the action of the DCR on the set N_j is to fix ${}_iN_j$ elements within the set ${}_iN$ (which amounts to the transposition of K ordered elements if ${}_iN_j^0 \equiv |\, {}_iN \cap N_j|$). Because of Shur's lemma the double coset matrix elements (DCME) possess certain diagonal features and can be indicated by a symbol

$$\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix},$$

where ${}_i\lambda_j$ is a partition of ${}_iN_j$ identifying an irreducible representation (irrep) of $S_{_iN_j}$. The DCME is identified as a recoupling coefficient in $U(n)$ by means of the correspondence between outer product coupling in S_N and Kronecker product coupling (Clebsch—Gordan reduction) in $U(n)$. The orthogonality, character, and competeness conditions in S_N provide nontrivial relations satisfied by the recoupling coefficients of $U(n)$.

The use of projection operators belonging to S_N to couple general Nth rank tensor products does not explicitly depend on the dimensionality of the tensors being coupled. Use of projection techniques in I led to further results that implied general structural relations between the coupling coefficients of unitary groups of different dimensions and tensors of different rank.

In this paper we exploit the duality between the rank of a tensor and the dimension of the underlying space to show the same coefficients introduced in I are the DCME of DCR with double coset symbols

$$\begin{bmatrix} n & n_j \\ {}_in & {}_in_j \end{bmatrix} \equiv \begin{bmatrix} n & n_1 & n_2 \\ {}_1n & {}_1n_1^0 - K & {}_1n_2^0 + K \\ {}_2n & {}_2n_1^0 + K & {}_2n_2^0 - K \end{bmatrix}$$

for the decomposition $U({}_1n) \otimes U({}_2n) \backslash U(n) / U(n_1) \otimes U(n_2)$. The subgroup dimensions specify the generalized branching scheme[3] for symmetry adapting the $U(n)$ basis states. The double coset development of I considers finite groups. This is extended to the continuous unitary group in Sec. II. It is also shown that the DCME of the permutation subset of DCR are just those matrix elements needed for generating a general matrix element in $U(n)$ by coupling presumably known matrix elements of the subgroups. Section III establishes the identification of these DCME with the coefficients introduced in I. Section IV contrasts the results developed here with those developed in I.

II. THE DOUBLE COSET REPRESENTATIVE $U({}_1n) \otimes U({}_2n) \backslash Un / U(n_1) \otimes U(n_2)$

For conciseness the initial results of this section are presented in a statement-proof form. Following two preliminary lemmas, it is proved that the DCR is an n_1-parameter (for purposes of argument it is assumed $n_2 \geq {}_2n \geq {}_1n \geq n_1$) unitary matrix that can be put in a form appropriate to $SO(2)^{n_1}$. It is then shown one needs to know only the matrix elements of a permutational subset of DCR.

Lemma II: Any square matrix Y formed as the ordered AA^+ that is positive because A can be considered as a vector mapping of a space equipped with a scalar product such that

$$(\underline{y}, \underline{y}) \equiv (\underline{Ax}, \underline{Ax}) \geq 0 \quad \text{for all } x.$$

Lemma II: Any square matrix y formed as the ordered product of factor matrices A_i (not necessarily square) is equivalent by a similarity transformation to all matrices formed by cyclic permulation of the order of the factor matrices. i.e., $Y \equiv P_iA_i \sim Y_\pi \equiv P_iA_{\pi i}$, π a cyclic permutation. If Y and Y_π have different dimensions, the equivalence hold for the lower dimension matrix extended to the higher dimension by the requisite array of zeroes. The equivalence holds because $\mathrm{tr}(Y^n) = \mathrm{tr}(Y_\pi^n)$ for $n =$ any integral power, as the trace is invariant under cyclic permutation of the order of factors. Thus the

characteristic equations of the set of matrices Y_τ are identical and their equivalence follows.[4]

Theorem: Any n dimensional unitary matrix

$$U \equiv \begin{pmatrix} {}_1A_1 & {}_1A_2 \\ {}_2A_1 & {}_2A_2 \end{pmatrix}$$

can be brought to the following form:

$$\begin{pmatrix} {}_1U\,{}_1A_1\,U_1 & {}_1U\,{}_1A_2\,U_2 \\ {}_2U\,{}_2A_1\,U_1 & {}_2U\,{}_2A_2\,U_2 \end{pmatrix} = \begin{pmatrix} d & 0 & \tau \\ 0 & E & 0 \\ -\tau^* & 0 & d^* \end{pmatrix}, \tag{1}$$

where ${}_1U \in U({}_1n)$, ${}_2U \in U({}_2n)$, $U_1 \in U(n_1)$, $U_2 \in U(n_2)$, d and τ are n_1 dimensional square matrices such that $|d_i|^2 + |\tau_i|^2 = 1$, and E is the unit matrix of dimension $n - 2n_1$. The diagonal elements of d may be considered real and positive while the diagonal elements of τ may be taken as real or imaginary [i.e., the right-hand side of Eq. (1) has n_1 independent parameters].

Proof: The unitarity condition requires

$${}_1A_1\,{}_1A_1^\dagger + {}_1A_2\,{}_1A_2^\dagger = E_{1n}, \tag{2a}$$

$${}_2A_1\,{}_2A_1^\dagger + {}_2A_2\,{}_2A_2^\dagger = E_{2n}, \tag{2b}$$

$${}_1A_1^\dagger\,{}_1A_1 + {}_2A_1^\dagger\,{}_2A_1 = E_{n_1}, \tag{2c}$$

$${}_1A_2^\dagger\,{}_1A_2 + {}_2A_2^\dagger\,{}_2A_2 = E_{n_2}, \tag{2d}$$

$${}_1A_1\,{}_2A_1^\dagger + {}_1A_2\,{}_2A_2^\dagger = O_{1n2n}, \tag{2e}$$

$${}_1A_1^\dagger\,{}_1A_2 + {}_2A_1^\dagger\,{}_2A_2 = O_{n_1n_2}. \tag{2f}$$

By Lemma I there exist unitary transformations ${}_1U$, ${}_2U$, $U_1^\dagger$, and $U_2^\dagger$ that diagonalize the left-hand side of (2a), (2b), (2c), and (2d) respectively. By Lemma II the diagonal form of these equations must be

$$(d^2 \dot{+} O_{1n-n_1}) + (\tau^2 \dot{+} E_{1n-n_1}) = E_{2n}, \tag{2a'}$$

$$(\tau^2 \dot{+} O_{2n-n_1}) + (d^2 \dot{+} E_{2n-n_1}) = E_{2n}, \tag{2b'}$$

$$d^2 + \tau^2 = E_{n_1}, \tag{2c'}$$

$$(\tau^2 \dot{+} O_{2n-n_1} \dot{+} E_{1n-n_1}) + (d^2 \dot{+} E_{2n-n_1} \dot{+} O_{n_2-2n}) = E_{n_2}, \tag{2d'}$$

where we note ${}_1n - n_1 = n_2 - {}_2n$.

To satisfy these equations and the trasformed equations of (2e) and (2f), one must take

$$\begin{pmatrix} {}_1U\,{}_1A_1\,U_1 & {}_1U\,{}_1A_2\,U_2 \\ {}_2U\,{}_2A_1\,U_1 & {}_2U\,{}_2A_2\,U_2 \end{pmatrix} = \begin{matrix} \\ n_1 \\ {}_1n - n_1 \\ {}_2n - n_1 \\ n_1 \end{matrix} \begin{matrix} \begin{matrix} n_1 & n_2 - {}_2n & {}_2n - n_1 & n_1 \end{matrix} \\ \begin{pmatrix} d & 0 & 0 & \tau \\ 0 & E & 0 & 0 \\ 0 & 0 & E & 0 \\ -\tau^* & 0 & 0 & d^* \end{pmatrix} \end{matrix},$$

where the dimensions of the blocks are as indicated (all diagonal blocks are square matrices) and d may be considered positive and real. QED

The above form for the DCR can be displayed in the usual form of exponentiation of the infinitesimal Lie algebra. If e_{jk}, $1 \leq j,\ k \leq n$, are the n^2 matrix basis elements (one in the jkth position, zeroes elsewhere) we take the basis of the infinitesimal Lie algebra to be the anti-Hermitian matrices

$$H_j \equiv ie_{jj}, \quad R_{jk} \equiv e_{jk} - e_{kj}, \quad \text{and} \quad I_{jk} \equiv i(e_{jk} + e_{kj}), \quad j < k.$$

The basis matrices squared give $x_{jk}^2 = -E_{(j)(k)} \dot{+} O_{n-2}$ where $E_{(j)(k)}$ is the two-dimensional unit matrix with one in the jth and kth positions. The one-parameter subgroups are thus

$$\exp(\beta X_{jk}) = (\cos\beta\ E_{(j)(k)} + \sin\beta\ X_{jk}) \dot{+} E_{n-2}.$$

The DCR then can be taken as a product of n_1 mutually commuting one parameter factors

$$\overset{n_1}{\underset{j=1}{\otimes}} \exp(\beta_j I_{j,n-n_1+j}) = \exp\left(\sum_{j=1}^{n_1} \beta_j I_{j,n-n_1+j}\right). \tag{3}$$

The choice of the R or I matrices and the particular ordering j, $n - n_1 + j$ is unimportant as long as each element of the set n_1 is coupled to a distinct element of the set ${}_2n$. For $n_2 \geq 2$ each factor of the DCR is equivalent by a permutation transformation (a transposition) to a similar element contained in $U(n_2)$ whose matrix is presumed known. For $n_2 \geq 2$ one can take n_1 mutually commuting transpositions as, e.g.,

$$(j, n - 2n_j + j)\exp(\beta_j I_{j,n-n_1+j})(j, n - 2n_1 + j) + j) = \exp(\beta_j I_{n-2n_1+j,n-n_1+j}).$$

Thus the fundamental coupling matrices that must be determined for a given irrep of $U(n)$ are those corresponding to the symmetric group DCR in the decomposition $S_{1n} \otimes S_{2n} \backslash S_n / S_{n_1} \otimes S_{n_2}$. Because elements belonging to the group $U({}_2n - n_1) \otimes U({}_1n - n_1) \otimes U(1)^{n_1}$ commute with all the DCR, the number of independent group parameters is

$${}_1n^2 + {}_2n^2 + n_1^2 + n_2^2 + n_1 - ({}_2n - n_1)^2 - ({}_1n - n_1)^2 - n_1 = n^2$$

as it should be.

The development indicated here is essentially a generalized Euler angle parametrization of the group. Just as the D.C. decomposition of S_N reduces to Yamanouchi's result[5] for ${}_1N = 1 = N_1$, the procedure given here reduces to Wigner's development of $SU(2)$[6] and Holland's[7] development of $SU(3)$ where in both cases $n_1 = 1 = {}_1n$. For convenience the $SU(2)$ development is given in the Appendix, and the reader is referred to Holland's paper for the $U(1) \otimes SU(2) \backslash SU(3) / U(1) \otimes SU(2)$ decomposition. To aid in identifying the permutation elements, we note for $U(n) \supset S_n$ under the imbedding $\{1\} \dot{+} = (n) + (n-1, 1)$ a transpose can be expressed as $(jk) = \exp[-\pi/2(H_j + H_k)]\exp(\pi/2)I_{jk}$.

III. TENSOR COUPLING IN THE UNITARY GROUP

In this section we show the matrix elements of the DCR for $S_{1n} \otimes S_{2n} \backslash S_n / S_{n_1} \otimes S_{n_2}$ in an Nth rank tensor irrep of $U(n)$ are identical to the matrix elements of the corresponding DCR for $S_{1N} \otimes S_{2N} \backslash S_N / S_{N_1} \otimes S_{N_2}$. The argument utilizes projection operators in S_N and the generalized branching relations for $U(n)/U(n_1) \otimes U(n_2)$ and is a particular application of Eqs. (4.8), (4.9), (4.10) of I for the case $n_j \cap n_k = \delta_{jk} n_j$. As those relations are rather involved, we will give a complete development here. An Nth rank tensor of $U(n)$ can be projected from the pro-

duct of an N_1th rank tensor of $U(n_1)$ and an N_2th rank tensor of $U(n_2)$ where

$$N_1+N_2=N,$$

$$n_1+n_2=n \text{ by}$$

$$\left\langle \begin{matrix} & m & \\ N & \tau & n_1+n_2 \\ \tau_1 & & \tau_2 \\ M_1 & & M_2 \end{matrix} \right\rangle = \frac{(\tau\,|\,m;\tau_1 m_1,\tau_2 m_2)}{\eta} \times \left\langle \begin{matrix} & m_1 & \\ N_1 & \tau_1 & n_1 \\ & M_1 & \end{matrix} \right\rangle \left\langle \begin{matrix} & m_2 & \\ N_2 & \tau_2 & n_2 \\ & M_2 & \end{matrix} \right\rangle .$$

The upper labels specify the transformation properties under action by the group S_N and the lower labels specify the transformation properties under action by the group $U(n)\supset U(n_1)\otimes U(n_2)$. By using the D.C. development of the projection operator the normalization constant is easily evaluated as

$$\eta=\left(\frac{N_1!N_2!\,|\,\tau\,|}{N!\,|\,\tau_1\,|\,|\,\tau_2\,|}\right)^{1/2},$$

where $|\,\tau|$ means the dimensions of the irrep of the symmetric group. Let $U(k)\in S_n\subset U(n)$ be that particular operation that takes k ordered elements from the sets n_1 and n_2 and fixes them in the sets ${}_1n$ and ${}_2n$ so that it has D.C. symbol

$$\begin{bmatrix} n & n_1 & n_2 \\ {}_1n & {}_1n_1^0-k & {}_1n_2^0+k \\ {}_2n & {}_2n_1^0+k & {}_2n_2^0-k \end{bmatrix}.$$

Assuming $n_2\geq {}_2n\geq {}_1n\geq n_1$, we would have ${}_1n_1^0=n_1$, ${}_2n_1^0=0$, $n_2^0={}_1n=n_1$, ${}_2n_2^0={}_2n$, and $0\leq k\leq n_1$.

Consider the matrix element

$$\begin{bmatrix} \tau & & U(k) \\ {}_1\tau & {}_2\tau & \tau_1 \quad \tau_2 \\ {}_1\tau_1\ {}_1\tau_2\ {}_2\tau_1\ {}_2\tau_2 & {}_1\tau_1'\ {}_2\tau_1'\ {}_1\tau_2'\ {}_2\tau_2' & \\ {}_1M_1\ {}_1M_2\ {}_2M_1\ {}_2M_2 & {}_1M_1'\ {}_2M_1'\ {}_1M_2'\ {}_2M_2' & \end{bmatrix}$$

$$\equiv \left\langle \begin{matrix} & m & \\ N & \tau & {}_1n+{}_2n \\ {}_1\tau & & {}_2\tau \\ {}_1\tau_1\ {}_1\tau_2 & & {}_2\tau_1\ {}_2\tau_2 \\ {}_1M_1\ {}_1M_2 & & {}_2M_1\ {}_2M_2 \end{matrix} \right\rangle^{*} U(k) \left\langle \begin{matrix} & m & \\ N & \tau & n_1+n_2 \\ & \tau_1 \quad \tau_2 & \\ {}_1\tau_1'\ {}_2\tau_1' & & {}_1\tau_2'\ {}_2\tau_2' \\ {}_1M_1'\ {}_2M_1' & & {}_1M_2'\ {}_2M_2' \end{matrix} \right\rangle, \quad (4)$$

where the additional specification of the basis with respect to $U(n)$ corresponds to the action of $U(k)$ on the tensor and therefore is indexed as in the D.C. symbol. By considering both tensors as projected from product tensors the right-hand side becomes

$$\left(\frac{{}_1N!{}_2N!N_1!N_2!}{|\,{}_1\tau|\,|\,{}_2\tau|\,|\,\tau_1|\,\tau_2|}\right)^{1/2} \sum_{q,\,i\lambda_j} \left\langle \begin{matrix} {}_1m_1\ {}_1m_2 \\ {}_1\lambda_1\ {}_1\lambda_2 \\ {}_1N\ {}_1\tau\ {}_1n \\ {}_1\tau_1 \quad {}_1\tau_2 \\ {}_1M_1\ {}_1M_2 \end{matrix} \right\rangle^{*} \left\langle \begin{matrix} {}_2m_1\ {}_2m_2 \\ {}_2\lambda_1\ {}_2\lambda_2 \\ {}_2N\ {}_2\tau\ {}_2n \\ {}_2\tau_1 \quad {}_2\tau_2 \\ {}_2M_1\ {}_2M_2 \end{matrix} \right\rangle^{*}$$

$$\times \underline{qU(k)} \left\langle \begin{matrix} {}_1m_1\ {}_2m_1 \\ {}_1\lambda_1\ {}_2\lambda_1 \\ N_1\ \tau_1\ n_1 \\ {}_1\tau_1'\ {}_2\tau_1' \\ {}_1M_1'\ {}_2M_1' \end{matrix} \right\rangle \left\langle \begin{matrix} {}_1m_2\ {}_2m_2 \\ {}_1\lambda_2\ {}_2\lambda_2 \\ N_2\ \tau_2\ n_2 \\ {}_1\tau_2'\ {}_2\tau_2' \\ {}_1M_2'\ {}_2M_2' \end{matrix} \right\rangle$$

$$\times \begin{bmatrix} \tau & \tau_1 & \tau_2 \\ {}_1\tau & {}_1\lambda_1\ {}_1\lambda_2 & |\,{}_1\lambda_1\,|\,|\,{}_1\lambda_2\,|\,|\,{}_2\lambda_1\,|\,|\,{}_2\lambda_2\,| \\ {}_2\tau & {}_2\lambda_1\ {}_2\lambda_2 & {}_1N_1!\,{}_1N_2!\,{}_2N_1!\,{}_2N_2! \end{bmatrix}. \quad (5)$$

Each subtensor is further expanded in a Clebsch–Gordan series appropriate to the action of q on the tensors and their respective dimensions. E.g.,

$$\left\langle \begin{matrix} {}_1m_1\ {}_2m_1 \\ {}_1\lambda_1\ {}_2\lambda_1 \\ N_1 \quad \tau_1 \quad n_1 \\ {}_1\tau_1'\ {}_2\tau_1' \\ {}_1M_1'\ {}_2M_1' \end{matrix} \right\rangle = \left\langle \begin{matrix} {}_1m_1 \\ {}_1N_1\ {}_1\lambda_1\ {}_1n_1 \\ {}_1\mu_1'\ {}_2\mu_1' \\ {}_1P_1'\ {}_2P_1' \end{matrix} \right\rangle \left\langle \begin{matrix} {}_2m_1 \\ {}_2N_1\ {}_2\lambda_1\ {}_2n_1 \\ {}_1\nu_1'\ {}_2\nu_1' \\ {}_1Q_1'\ {}_2Q_1' \end{matrix} \right\rangle$$

$$\times \left(\begin{matrix} {}_1\lambda_1 & {}_2\lambda_1 & \tau_1 \\ {}_1\mu_1'\ {}_2\mu_1' & {}_1\mu_1'\ {}_2\mu_1' & {}_1\tau_1'\ {}_2\tau_1' \\ {}_1P_1'\ {}_2P_1' & {}_1Q_1'\ {}_2Q_1' & {}_1M_1'\ {}_2M_1' \end{matrix} \right)_{n_1}. \quad (6)$$

The final tensor contraction can be carried out in the form

$$\left\langle \begin{matrix} {}_1m_1 \\ {}_1N_1\ {}_1\lambda_1\ {}_1n_1-k,{}_1n_2+k_1 \\ {}_1\mu_1 \quad {}_1\mu_2 \\ {}_1P_1 \quad {}_1P_2 \end{matrix} \right\rangle^{*} \left\langle \begin{matrix} {}_1m_2 \\ {}_1N_2\ {}_1\lambda_2\ {}_1n_1-k,{}_1n_2+k_1 \\ {}_1\nu_1 \quad {}_1\nu_2 \\ {}_1Q_1 \quad {}_1Q_2 \end{matrix} \right\rangle^{*}$$

$$\times \left\langle \begin{matrix} {}_2m_1 \\ {}_2N_1\ {}_2\lambda_1\ {}_2n_1+k_2,{}_2n_2-k \\ {}_2\mu_1 \quad {}_2\mu_2 \\ {}_2P_1 \quad {}_2P_2 \end{matrix} \right\rangle^{*} \left\langle \begin{matrix} {}_2m_2 \\ {}_2N_2\ {}_2\lambda_2\ {}_2n_1+k_2,{}_2n_2-k \\ {}_2\nu_1 \quad {}_2\nu_2 \\ {}_2Q_1 \quad {}_2Q_2 \end{matrix} \right\rangle^{*}$$

$$\times qU(k) \left\langle \begin{matrix} {}_1m_1 \\ {}_1N_1\ {}_1\lambda_1\ {}_1n_1-k,{}_2n_1+k_1 \\ {}_1\mu_1'\ {}_2\mu_1' \\ {}_1P_1'\ {}_2P_1' \end{matrix} \right\rangle$$

$$\times\left\langle\begin{matrix} {}_2m_1 \\ {}_2N_1\ {}_2\lambda_1\ {}_1n_1-k,\ {}_2n_1+k_1 \\ {}_1\nu_1'\ \ {}_2\nu_1' \\ {}_1Q_1'\ \ {}_2Q_1' \end{matrix}\right\rangle\left\langle\begin{matrix} {}_1m_2 \\ {}_1N_2\ {}_1\lambda_2\ {}_1n_2+k_2,\ {}_2n_2-k \\ {}_1\mu_2'\ \ {}_2\mu_2' \\ {}_1P_2'\ \ {}_2P_2' \end{matrix}\right\rangle$$

$$\times\left\langle\begin{matrix} {}_2m_2 \\ {}_2N_2\ {}_2\lambda_2\ {}_1n_2+k_2,\ {}_2n_2-k \\ {}_1\nu_2'\ \ {}_2\nu_2' \\ {}_1Q_2'\ \ {}_2Q_2' \end{matrix}\right\rangle, \tag{7}$$

where the k_1 and k_2 subscripts indicate the initial sets to which they belong. The action of $U(k)$ is to interchange $k_1 \leftrightarrow k_2$ on the left while q interchanges ${}_2N_1 \leftrightarrow {}_1N_2$ also on the left. The dimensional overlap requires

$${}_1\mu_2=0={}_2\mu_1'={}_1\nu_1={}_2\mu_2'={}_1\nu_1'={}_2\mu_2={}_2\nu_1={}_1\nu_2',$$

$${}_1\mu_1={}_1\lambda_1={}_1\mu_1',\quad {}_2\nu_1'={}_2\lambda_1={}_2\mu_1,\quad {}_1\nu_2={}_1\lambda_2={}_1\mu_2',$$

$${}_2\nu_2={}_2\lambda_2={}_2\nu_2',\quad {}_1P_1={}_1P_1',\quad {}_2Q_1'={}_2P_1,\quad {}_1Q_2={}_1P_2',\quad \text{and}$$

$${}_2Q_2={}_2Q_2'.$$

The Clebsch–Gordan coefficients in turn require

$${}_i\lambda_j={}_i\tau_j={}_i\tau_j' \quad \text{and} \quad {}_iP_j={}_iQ_j={}_iM_j={}_iM_j'.$$

Upon contraction of tensors the left-hand side becomes

$$\delta_{i}\tau_{j\,i}\tau_{j'}\delta_{i}M_{j\,i}M_{j'}\left(\frac{{}_1N!\,{}_2N!\,N_1!\,N_2!}{|{}_1\tau|\,|{}_2\tau|\,|\tau_1|\,|\tau_2|}\right)^{1/2}$$

$$\times\frac{|{}_1\tau_1|\,|{}_1\tau_2|\,|{}_2\tau_1|\,|{}_2\tau_2|}{{}_1N_1!\,{}_1N_2!\,{}_2N_1!\,{}_2N_2!}\begin{bmatrix}\tau & \tau_1 & \tau_2\\ {}_1\tau & {}_1\tau_1 & {}_1\tau_2\\ {}_2\tau & {}_2\tau_1 & {}_2\tau_2\end{bmatrix}$$

$$\times\left(\begin{matrix} {}_1\tau_1\ \ {}_1\tau_2 \\ {}_1M_1\ 0\ 0\ {}_1M_2 \end{matrix}\middle|\begin{matrix} {}_1\tau \\ {}_1\tau_1\ \ {}_1\tau_2 \\ {}_1M_1\ \ {}_1M_2 \end{matrix}\right)_{1^n}^{*}\left(\begin{matrix} {}_2\tau_1\ \ {}_2\tau_2 \\ {}_2M_1\ 0\ 0\ {}_2M_2 \end{matrix}\middle|\begin{matrix} {}_2\tau \\ {}_2\tau_1\ \ {}_2\tau_2 \\ {}_2M_1\ \ {}_2M_2 \end{matrix}\right)_{2^n}^{*}$$

$$\times\left(\begin{matrix} {}_1\tau_1\ \ {}_2\tau_1 \\ {}_1M_1\ 0\ 0\ {}_2M_1 \end{matrix}\middle|\begin{matrix} \tau_1 \\ {}_1\tau_1\ \ {}_2\tau_1 \\ {}_1M_1\ \ {}_2M_1 \end{matrix}\right)_{n_1}\left(\begin{matrix} {}_1\tau_2\ \ {}_2\tau_2 \\ {}_1M_2\ 0\ 0\ {}_2M_2 \end{matrix}\middle|\begin{matrix} \tau_2 \\ {}_1\tau_2\ \ {}_2\tau_2 \\ {}_1M_2\ \ {}_2M_2 \end{matrix}\right)_{n_2}. \tag{8}$$

The Clebsch–Gordan coefficients can be evaluated, again by projection techniques, as

$$\left(\begin{matrix} {}_1\tau_1\ \ {}_2\tau_1 \\ {}_1M_1\ 0\ 0\ {}_2M_1 \end{matrix}\middle|\begin{matrix} \tau_1 \\ {}_1\tau_1\ \ {}_2\tau_1 \\ {}_1M_1\ \ {}_2M_1 \end{matrix}\right)_{n_1}=\left\langle\begin{matrix} {}_1m_1 \\ {}_1N_1\ {}_1\tau_1\ n_1 \\ {}_1M_1\ 0 \end{matrix}\right\rangle^{+}$$

$$\times\left\langle\begin{matrix} {}_2m_1 \\ {}_2N_1\ {}_2\tau_1\ n_1 \\ 0\ \ {}_2M_1 \end{matrix}\right\rangle\frac{(\tau_1|{}_1\tau_1 m_1\,{}_2\tau_1\,{}_2m_1;{}_1\tau_1\,{}_1m_1\,{}_2\tau_1\,{}_2m_1)}{n}$$

$$\times\left\langle\begin{matrix} {}_1m_1 \\ {}_1n\ {}_1\tau_1\ n_1 \\ {}_1M_1\ 0 \end{matrix}\right\rangle\left\langle\begin{matrix} {}_2m_1 \\ {}_2N_1\ {}_2\tau_1\ n_1 \\ 0\ \ {}_2M_1 \end{matrix}\right\rangle=\eta=\frac{{}_1N_1!\,{}_2N_1!\,|\tau_1|}{N_1!\,|{}_1\tau_1|\,|{}_2\tau_1|}^{1/2}. \tag{9}$$

So the result follows:

$$\begin{bmatrix}\tau & & U(k) & \\ {}_1\tau & {}_2\tau & \tau_1 & \tau_2\\ {}_1\tau_1\ {}_1\tau_2 & {}_2\tau_1\ {}_2\tau_2 & {}_1\tau_1'\ {}_2\tau_1' & {}_1\tau_2'\ {}_2\tau_2'\\ {}_1M_1\ {}_1M_2 & {}_2M_1\ {}_2M_2 & {}_1M_1'\ {}_2M_1' & {}_1M_2'\ {}_2M_2'\end{bmatrix}$$

$$=\delta_{i}\tau_{j'\,i}\tau_{j\,}\delta_{i}M_{j\,i}M_{j'}\begin{bmatrix}\tau & \tau_1 & \tau_2\\ {}_1\tau & {}_1\tau_1 & {}_1\tau_2\\ {}_2\tau & {}_2\tau_1 & {}_2\tau_2\end{bmatrix}. \tag{10}$$

IV. DISCUSSION

Because of the various groups involved we recapitulate the results of this paper and of I as to the identifications established for the recoupling coefficients. I.e.,

$$\left\langle\begin{matrix} {}_1m_1\ {}_1m_2\ {}_2m_1\ {}_2m_2 \\ {}_1\lambda_1\ \ {}_1\lambda_2\ \ {}_2\lambda_1\ \ {}_2\lambda_2 \\ {}_1\lambda \qquad {}_2\lambda \\ N \quad \lambda \quad n \\ {}_1\tau \qquad {}_2\tau \\ {}_1\tau_1\ {}_1\tau_2\ {}_2\tau_1\ {}_2\tau_2 \\ {}_1M_1\ {}_1M_2\ {}_2M_1\ {}_2M_2 \end{matrix}\right\rangle^{+} q_L U(k) \left\langle\begin{matrix} {}_1m_1\ {}_2m_1\ {}_1m_2\ {}_2m_2 \\ {}_1\lambda_1\ \ {}_2\lambda_1\ \ {}_1\lambda_2\ \ {}_2\lambda_2 \\ \lambda_1 \qquad \lambda_2 \\ N \quad \lambda \quad n \\ \tau_1 \qquad \tau_2 \\ {}_1\tau_1\ {}_2\tau_1\ {}_1\tau_2\ {}_2\tau_2 \\ {}_1M_1\ {}_2M_1\ {}_1M_2\ {}_2M_2 \end{matrix}\right\rangle$$

$$=\begin{bmatrix}\lambda & \lambda_1 & \lambda_2\\ {}_1\lambda & {}_1\lambda_1 & {}_1\lambda_2\\ {}_2\lambda & {}_2\lambda_1 & {}_2\lambda_2\end{bmatrix}\begin{bmatrix}\tau & \tau_1 & \tau_2\\ {}_1\tau & {}_1\tau_1 & {}_1\tau_2\\ {}_2\tau & {}_2\tau_1 & {}_2\tau_2\end{bmatrix}, \tag{11}$$

where the recoupling coefficients are compatible with the D.C. symbols

$$\begin{bmatrix}N & N_1 & N_2\\ {}_1N & {}_1N_1^0-L & {}_1N_2^0+L\\ {}_2N & {}_2N_1^0+L & {}_2N_2^0-L\end{bmatrix}\quad\text{and}\quad\begin{bmatrix}n & n_1 & n_2\\ {}_1n & {}_1n_1^0-k & {}_1n_2^0+k\\ {}_2n & {}_2n_1^0+k & {}_2n_2^0-k\end{bmatrix}$$

respectively. Note the D.C. symbol of S_N does not restrict the lower pattern nor does the D.C. symbol of $U(n)$ restrict the upper pattern. In I it is noted the recoupling coefficient can be regarded as the matrix element of q_L in the mixed basis or as the unitary (recoupling) transformation between q acting on the bases expressed according to the right sequence and the bases expressed according to the left sequence of the upper patterns. Completely analogous considerations hold for $U(k)$ and the lower patterns.

The coefficients

$$\begin{bmatrix}\lambda & \lambda_j\\ {}_i\lambda & {}_i\lambda_j\end{bmatrix}$$

are tensor recoupling coefficients of $S_N \otimes U(n)$ with respect to either the S_N group properties (upper pattern) or the $U(n)$ group properties (lower pattern). Alternately they are matrix elements in an irrep of S_N expressed in

a particular (mixed) bases or they are matrix elements in an irrep of $U(n)$ expressed in particular (mixed) bases, whereas in I the orthogonality and completeness relations of group representation theory are directly applied, one must be cautious about their interpretation here. The coefficients are matrix elements of only those permutation elements $\pi \in S_n \subset U(n)$, while the representation is irreducible with respect to $U(n)$. Application of the orthogonality and completeness conditions in $U(n)$ requires the appropriate invariant density and a procedure as in Holland's paper must be followed. In the special case of $N=n$ with restriction to the weight space $W=(1^n)$ an irrep of $U(n)$ is an irrep of S_n[8] and the orthogonality and completeness conditions give results identical to those of I. By using both the structure of the upper and lower tensor labels we hope to present in a future communication an efficient procedure for actually constructing the DCME by coupling totally symmetric tensors in the individual weights.

APPENDIX: DOUBLE COSET DEVELOPMENT OF $U(1)\backslash SU(2)/U(1)$

$SU(2)$ is obtained by exponentiation of the three-parameter infinitesimal Lie algebra with defining basis matrices

$$X_1 \equiv \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad X_2 \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad X_3 \equiv \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

and structure constants

$$[X_i, X_j] = 2\epsilon_{ijk} X_k.$$

The defining representation is given by

$$\begin{pmatrix} x_0 + ix_1 & x_2 + ix_3 \\ -x_2 + ix_3 & x_0 - ix_1 \end{pmatrix} \text{ with } x_0^2 + x_1^2 + x_2^2 + x_3^2 = 1.$$

The group parameter space is in one-to-one correspondence with the points of the unit sphere in four dimensions. The usual coordinates are

$$x_0 = \cos A = \cos\theta_1 = \cos\phi_1 \cos\phi_2,$$
$$x_1 = (\alpha_1/A)\sin A = \sin\theta_1 \cos\theta_2 = \cos\phi_1 \sin\phi_2,$$
$$x_2 = (\alpha_2/A)\sin A = \sin\theta_1 \sin\theta_2 \cos\theta_3 = \sin\phi_1 \cos\phi_3,$$
$$x_3 = (\alpha_3/A)\sin A = \sin\theta_1 \sin\theta_2 \sin\theta_3 = \sin\phi_1 \sin\phi_3,$$
$$A^2 \equiv \alpha_1^2 + \alpha_2^2 + \alpha_3^2.$$

The first set corresponds to $\exp(\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3)$, the second set to spherical coordinates in 4-space, and the last to the D.C. decomposition

$$\exp(\alpha_1 x_1)\exp(\beta x_2)\exp(\alpha_1' x_1)$$

with $\alpha_1 + \alpha_1' \equiv \phi_2$ and $\alpha_1 - \alpha_1' \equiv \phi_3$,

which is seen to be identical with the Euler angle description. The invariant group density is given respectively as

$$\frac{dx_1 dx_2 dx_3}{x_0} = \frac{\sin^2 A}{A^2} d\alpha_1 d\alpha_2 d\alpha_3$$
$$= \sin^2\theta_1 \sin^2\theta_2 \, d\theta_1 d\theta_2 d\theta_3 = \cos\phi_1 \sin\phi_1 \, d\phi_1 d\phi_2 d\phi_3.$$

The matrices of $SU(2)$ are easily displayed using the totally symmetric projection operator of S_N as

$$\begin{bmatrix} j = N/2 & U(\alpha_j) \\ M' & M \end{bmatrix} \equiv \left\langle \begin{matrix} 1 \\ N \quad N \quad 2 \\ N/2 + M' \quad N/2 - M' \end{matrix} \right\rangle^*$$
$$\times U(\alpha_j) \left\langle \begin{matrix} 1 \\ N \quad N \quad 2 \\ N/2 + M \quad N/2 - M \end{matrix} \right\rangle$$
$$= \sum_{q_i} \langle N/2 + M', +1 \rangle^* \langle N/2 - M', -1 \rangle^*$$
$$\times q_L U(\alpha_j) \langle N/2 + M, +1 \rangle \langle N/2 - M, -1 \rangle$$
$$\times \left[\binom{N}{N/2 + M} \binom{N}{N/2 + M'} \right]^{-1/2} N!,$$

where q_L has D.C. symbol

$$\begin{bmatrix} N & N/2 + M & N/2 - M \\ N/2 + M' & N/2 + M - L & M' - M + L \\ N/2 - M' & L & N/2 - M' - L \end{bmatrix}$$

assuming $M' \geq M$.

Expansion of the tensors by the trivial Clebsch–Gordan series of $U(1)$ in accordance with the action of q_L and contraction of the resulting tensors gives

$$\begin{bmatrix} j = N/2 & U(\alpha_j) \\ M' & M \end{bmatrix}$$
$$= \sum_L \frac{[(N/2 + M)!(N/2 - M)!(N/2 + M')!(N/2 - M')!]^{1/2}}{(N/2 + M - L)!(M' - M + L)!L!(N/2 - M' - L)!}$$
$$\times (x_0 + ix_1)^{N/2 + M - L} (x_2 + ix_3)^{M' - M + L}$$
$$\times (-x_2 + ix_3)^L (x_0 - ix_1)^{N/2 - M' - L},$$

which is a standard form for the matrix element (viz. Eq. 9-76, p. 355, Hamermesh[9]).

Orthogonality and completeness give the relations

$$2(2j+1) \int_0^{\pi/2} \begin{bmatrix} j & \phi_1 \\ M' & M \end{bmatrix} \begin{bmatrix} j' & \phi_1 \\ M' & M \end{bmatrix} \cos\phi_1 \sin\phi_1 \, d\phi_1 = \delta^{jj'}$$

and

$$\frac{2}{\pi} \sum_j \sin(2j+1)\theta_1 \sin(2j+1)\theta_1' = \delta(\theta_1 - \theta_1')$$

(using spherical coordinates θ_1, θ_2, θ_3).

[1] H. Weyl, *Classical Groups* (Princeton U.P., Princeton, N.J., 1946).
[2] J.J. Sullivan, J. Math. Phys. **14**, 387 (1973).
[3] C. Itzykson and M. Nauenberg, Rev. Mod. Phys. **38**, 95 (1966); C.R. Hagen and A.J. MacFarlane, J. Math. Phys. **6**, 1366 (1965); J. Mickelsson, J. Math. Phys. **11**, 2803 (1970); R.T. Sharp, J. Math. Phys. **13**, 183 (1972).
[4] D.E. Littlewood, *The Theory of Group Characters* (Oxford Press at Clarendon, Oxford, 1958), viz. Secs. 1.5, 10.1, and 10.2.
[5] J.J. Sullivan, Phys. Rev. A **5**, 29 (1972), viz. p. 36.
[6] E.P. Wigner, *On the Matrices Which Reduce the Kronecker Products of Representations of S.R. Groups* (Sect. II. 12), reproduced in L.C. Biedenharn and H. Van Dam, *Quantum Theory of Angular Momentum* (Academic, New York, 1965).
[7] D.F. Holland, J. Math. Phys. **10**, 531 (1969).
[8] M. Moshinsky, J. Math. Phys. **7**, 691 (1966).
[9] M. Hamermesh, *Group Theory* (Addison-Wesley, Reading, Mass., 1962).

Second order error in variational calculation of matrix elements

Edward Gerjuoy*

Physics Department, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
(Received 24 June 1974)

The second order error $\delta F^{(2)}$, made by employing the Schwartz–Dalgarno–Delves variational principle for the diagonal matrix element $\phi^\dagger W\phi$ of an arbitrary Hermitian operator W, is examined in the case that ϕ is the bound ground state eigenfunction of some given Hamiltonian H. This variational principle characteristically involves not only a trial estimate ϕ_t of ϕ, but also a trial estimate $L_t(\phi_t)$ of a well-defined but generally not exactly known auxiliary function $L(\phi)$. It has previously been shown that, for certain special choices of a trial Hamiltonian H_t, the trial $L_t(\phi_t)$ can be found from a minimum principle. The present work finds that for these same special H_t it is possible to express $\delta F^{(2)}$ in comparatively simple closed form, depending only on known quantities, so that $\delta F^{(2)}$ should be calculable when the system described by H is not too complicated. However, these results for $\delta F^{(2)}$ are obtained on the assumption that $L_t(\phi_t)$ is known essentially exactly for any given ϕ_t; the practical utility of the formulas derived still must be tested, therefore. If $L_t(\phi_t)$ can be determined to this necessary accuracy, one expects that combining the computed $\delta F^{(2)}$ with the usual variational estimate of $\phi^\dagger W\phi$ will be a significant improvement over the usual variational estimate alone. Under the same circumstances, when W is a positive definite operator, the expression for $\delta F^{(2)}$ can provide nonrigorous but nonetheless potentially useful second order (variational) upper and lower bounds on the exact $\phi^\dagger W\phi$.

1. INTRODUCTION

We shall be concerned with the diagonal matrix element

$$W_{11} = \phi_1{}^\dagger W\phi_1 \equiv (\phi_1, W\phi_1) \tag{1.1}$$

of an arbitrary known linear Hermitian operator W, where ϕ_1, satisfying

$$(H - E_1)\,\phi_1 = 0, \tag{1.2}$$

is the normalized bound ground state eigenfunction of a given Hamiltonian H. To avoid unduly complicating our discussion, we assume here and henceforth that E_1 is nondegenerate; to simplify our notation we shall drop the subscripts on ϕ_1 and E_1 (i.e., $\phi_1 \equiv \phi$, $E_1 \equiv E$), and shall use

$$\lambda = -W_{11} \equiv -\phi^\dagger W\phi. \tag{1.3}$$

In general, neither ϕ nor E is exactly known. In this circumstance, a well-known variational principle[1–5]—useable for arbitrary off-diagonal or diagonal matrix elements of W—may provide the most practical means of estimating W_{11}. A very straightforward derivation of this so-called Schwartz—Dalgarno—Delves variational principle has been given by Gerjuoy, Rau and Spruch,[6] and applications to various W have been performed recently by Krieger and Sahni.[7]

The variational principle for W_{11} is

$$F \equiv \langle W_{11}\rangle_{\rm var} = \phi_t{}^\dagger W\phi_t + L_t{}^\dagger[(H - E_t)\,\phi_t] + [(H - E_t)\,\phi_t]^\dagger L_t \tag{1.4}$$

where ϕ_t (assumedly normalized) and E_t are trial estimates of the exact ϕ, E, respectively, and where L_t is a trial estimate of an exact "auxiliary" function L satisfying the inhomogeneous equation

$$(H - E)\,L = -W\phi - \lambda\phi \tag{1.5}$$

together with the specification [undetermined by (1.3)]

$$\phi^\dagger L = 0. \tag{1.6}$$

Equation (1.5) suggests that L_t be determined from equations of the form

$$(H_t - E_t)\,L_t = q_t(\phi_t) \equiv q_t \tag{1.7}$$

where H_t and q_t are appropriately chosen functionals of ϕ_t; the desired property of (1.7) is that as $\phi_t \to \phi$, the solution L_t should $\to L$. Generally, the "trial" Hamiltonian H_t cannot[8] be the original H, but there is a wide class of H_t consistent with the desired property; the choice of q_t is determined once H_t is chosen. If $H_t \to H$ as $\phi_t \to \phi$, then it surely is the case that

$$q_t = -W\phi_t - \lambda_t\phi_t \tag{1.8a}$$

where

$$\lambda_t = -\phi_t{}^\dagger W\phi_t; \tag{1.8b}$$

however, it is not necessary[8] that $H_t \to H$ as $\phi_t \to \phi$. In fact, Gerjuoy *et al.*[8] have found a particular choice of H_t which does not approach H as $\phi_t \to \phi$, but which permits L_t to be estimated from a minimum principle, i.e., which implies that the functional

$$M(L_{tt}) = L_{tt}{}^\dagger(H_t - E_t)\,L_{tt} - L_{tt}{}^\dagger q_t - q_t{}^\dagger L_{tt} \tag{1.9}$$

attains its minimum value $M(L_t)$ when (for given ϕ_t) the quantity L_{tt} equals the L_t satisfying (1.7). An alternative choice for H_t, which does approach H as $\phi_t \to \phi$, but which retains the desired minimum property of the functional (1.9), also has been reported.[9]

The importance of the minimum principle (1.9) is that it provides a vehicle for accurate computation of a reasonable L_t for any given ϕ_t. In the present paper we obtain the interesting result that in the two known cases[8,9] for which H_t yields the minimum principle (1.9), use in (1.4) of the associated exact L_t minimizing (1.9) leads to a rather simple closed form calculable expression for the second order error (to be defined precisely below) made by the Schwartz—Dalgarno—Delves variational estimate of the matrix element W_{11}. The present result is noteworthy because simple calculable expressions for second order errors made by variational estimates are uncommon. Moreover, as will be further amplified below, such expressions for the second order variational error can be the basis for nonrigorous but nonetheless potentially useful second order bounds

bracketing the exact value of W_{11}. These nonrigorous second order bounds should be compared with the rigorous second order bounds (involving, as might be expected, more complicated expressions than ours) derived and discussed by Blau, Rau, and Spruch.[10] We stress that although both types[8,9] of H_t yielding the minimum principle (1.9) can be constructed in the case that the desired matrix element is

$$W_{nn} = \phi_n{}^\dagger W \phi_n, \tag{1.10}$$

(with ϕ_n the bound nth excited state eigenfunction), the results of this paper apply only to the ground state case $n=1$. We have not attempted to extend our results to excited state $n>1$ matrix elements (1.10), in part because it is obvious from our derivation that in the case $n>1$ a closed form expression for the second order error, if obtainable at all, will not be nearly as simple in form as when $n=1$. In the event the actual ground state is degenerate under some symmetry operator R, it can be seen that our results apply provided ϕ_t, L, and L_t have the same symmetry as ϕ under the operation R, a proviso which imposes some restrictions on W. For instance, if the ground state has total angular momentum $J=1$, and if ϕ_1 in (1.1) now denotes the $M=0$ sublevel, then ϕ_t, L, and L_t should belong to $J_z=0$; in general, to ensure (1.5) and (1.7) permit solutions L and L_t having this desired symmetry, W must commute with the operator J_z.

2. THE SECOND ORDER ERROR

The errors $\delta\phi$ and δE are defined by

$$\delta\phi = \phi_t - \phi, \tag{2.1a}$$

$$\delta E = E_t - E. \tag{2.1b}$$

Correspondingly, we define

$$\delta L = L_t - L, \tag{2.2a}$$

$$\delta F = \langle W_{11}\rangle_{\text{var}} - W_{11}. \tag{2.2b}$$

The quantity δF is the error made in estimating W_{11} from the variational principle (1.4). Evidently $\delta F=0$ when $\phi_t=\phi$ and $E_t=E$, i.e., the zeroth order error in δF vanishes. Similarly, because (1.4) has been constructed[6] to be a variational principle, the first order error (the collection of terms proportional to $\delta\phi$, to $\delta\phi^\dagger$, to δL, etc.) in δF also vanishes, as is verified below. Thus the leading terms in δF are of second order (terms proportional to $\delta\phi^\dagger\delta\phi$, to $\delta\phi^\dagger\delta L$, to $\delta L^\dagger\delta\phi$, etc.). The collection of these second order terms, excluding terms of third order and higher, is the second order error $\delta F^{(2)}$ made by using (1.4) with given $\delta\phi$, δE and δL from (2.1) and (2.2).

In the form (1.4) for $\langle W_{11}\rangle_{\text{var}}$, it is implicit[6] that

$$\phi_t{}^\dagger\phi_t = 1, \tag{2.3a}$$

$$E_t = \phi_t{}^\dagger H \phi_t. \tag{2.3b}$$

Since the exact ϕ is normalized, Eq. (2.3a) yields

$$\phi^\dagger\delta\phi + (\delta\phi)^\dagger\phi + \delta\phi^\dagger\delta\phi = 0. \tag{2.4a}$$

Similarly, from Eqs. (2.3b) and (2.4)

$$\begin{aligned}\delta E &= \phi^\dagger H\delta\phi + \delta\phi^\dagger H\phi + \delta\phi^\dagger H\delta\phi\\ &= E[\phi^\dagger\delta\phi + (\delta\phi^\dagger)\phi] + \delta\phi^\dagger H\delta\phi\\ &= \delta\phi^\dagger(H-E)\,\delta\phi\end{aligned} \tag{2.4b}$$

implying that δE is of second order.

From (1.4) and (2.2b) we now see that the first and second order terms in δF are

$$\begin{aligned}\delta F^{(1)} + \delta F^{(2)} = {}& \phi^\dagger W\delta\phi + \delta\phi^\dagger W\phi + \delta\phi^\dagger W\delta\phi\\ &+ L^\dagger[(H-E)\,\delta\phi] + \delta L^\dagger[(H-E)\,\phi]\\ &+ \delta L^\dagger[(H-E)\,\delta\phi] - (\delta E)\,L^\dagger\phi\\ &+ [(H-E)\,\delta\phi]^\dagger L + [(H-E)\,\phi]^\dagger\delta L\\ &+ [(H-E)\,\delta\phi]^\dagger\,\delta L - (\delta E)\,\phi^\dagger L.\end{aligned} \tag{2.5}$$

In (2.5), terms containing $(H-E)\,\phi$ vanish by (1.2); terms proportional to δE vanish by (1.6). Also, because E does not lie in the continuum, the solution L to (1.5) can be supposed quadratically integrable for reasonably well behaved W; the same supposition already was implicit in (1.6). Therefore, in (2.5) we also have

$$\begin{aligned}&L^\dagger[(H-E)\,\delta\phi] = [(H-E)\,L]^\dagger\delta\phi,\\ &[(H-E)\,\delta\phi]^\dagger L = \delta\phi^\dagger[(H-E)\,L].\end{aligned} \tag{2.6}$$

As a matter of fact, the relations (2.6) are fundamental to the derivation[6] of the variational principle. Henceforth, manipulations such as (2.6), based on the hermiticity of H in the space of quadratically integrable functions, will be performed without comment. Employing (1.5) on the right sides of (2.6) and recalling (2.4a), we find that all first order terms in (2.5) cancel [as they must, if (1.4) indeed is a variational principle], leaving us [after introducing λ from (1.3)] with

$$\begin{aligned}\delta F^{(2)} = {}& \delta\phi^\dagger W\delta\phi + \delta L^\dagger[(H-E)\,\delta\phi] + [(H-E)\,\delta\phi]^\dagger\delta L\\ &+ \lambda\delta\phi^\dagger\delta\phi.\end{aligned} \tag{2.7}$$

Equation (2.7)—which also has been obtained by Aranoff and Percus[5]—is the general expression for the second order error made by using (1.4); to make further progress, it is necessary to further delineate δL, i.e., to delineate L_t. Actually, it is easily verified that if the condition

$$\phi_t{}^\dagger L_t = 0 \tag{2.8}$$

is obeyed by L_t, then Eq. (2.7) is an exact expression for the total error δF, i.e., with (2.8) the error δF of (2.2b) is precisely the purely second order expression on the right side of (2.7). However, we soon shall be performing manipulations which involve dropping third order and higher order contributions to (2.7), so that whether or not (2.7) as it stands exactly equals δF is of little practical consequence.

3. CHOICES FOR TRIAL HAMILTONIAN

One H_t yielding the minimum principle (1.9) is[8]

$$H_t = H_{\text{mod},t} = H - HP_tH/E_t \tag{3.1}$$

where the projection operator

$$P_t = \phi_t\phi_t{}^\dagger \tag{3.2a}$$

can be regarded as an estimate of the unknown projection operator

$$P = \phi\phi^\dagger. \tag{3.2b}$$

Although as $\phi_t \to \phi$ this $H_t \to H - EP$, which is $\neq H$, nevertheless the associated L_t obeys[8]

$$(H_{\mathrm{mod},t} - E_t) L_t = - W\phi_t - \lambda_t \phi_t, \tag{3.3}$$

i.e., obeys Eq. (1.7) with q_t given by (1.8). From (2.3b), (3.1), and (3.2a)

$$\phi_t{}^\dagger H_{\mathrm{mod},t} = H_{\mathrm{mod},t}\phi_t = 0. \tag{3.4}$$

Therefore, multiplying (3.3) by $\phi_t{}^\dagger$ on the left, and recalling (1.8b), we see that (3.3) implies (2.8).

Define

$$\delta H = H_{\mathrm{mod},t} - H, \tag{3.5a}$$

$$\delta\lambda = \lambda_t - \lambda = - (\phi^\dagger W\delta\phi + \delta\phi^\dagger W\phi + \delta\phi^\dagger W\delta\phi). \tag{3.5b}$$

Then Equation (3.3) becomes

$$(H + \delta H - E - \delta E)(L + \delta L) = - W(\phi + \delta\phi) - (\lambda + \delta\lambda)(\phi + \delta\phi)$$

which, making use of (1.5), takes the form

$$(H - E)\,\delta L = - (\delta H - \delta E)\,L - (\delta H - \delta E)\,\delta L - W\delta\phi - \lambda\delta\phi - (\delta\lambda)\,\phi - \delta\lambda\delta\phi. \tag{3.6}$$

Equation (3.6), which is exact, can be used to replace $(H - E)\,\delta L$ in the terms

$$\delta L^\dagger[(H - E)\,\delta\phi] = [(H - E)\,\delta L]^\dagger\delta\phi, \qquad [(H - E)\,\delta\phi]^\dagger\delta L = \delta\phi^\dagger[(H - E)\,\delta L] \tag{3.7}$$

appearing in (2.7). When this replacement is made, the resultant expression for $\delta F^{(2)}$ obviously will be the correct second order error even if all terms of second and higher order are dropped on the right side of (3.6). Actually, the right side of (3.6) contains terms nominally of zero order, because we know $H_{\mathrm{mod},t}$ does not approach H as $\phi_t \to \phi$. Specifically,

$$\begin{aligned}\delta H &= - \frac{HP_tH}{E_t} = - \frac{H(\phi + \delta\phi)(\phi + \delta\phi)^\dagger H}{E + \delta E} \\ &= - \frac{H(\phi\phi^\dagger + (\delta\phi)\,\phi^\dagger + \phi\delta\phi^\dagger)\,H}{E} \\ &= - E\phi\phi^\dagger - (H\delta\phi)\,\phi^\dagger - \phi\delta\phi^\dagger H\end{aligned} \tag{3.8}$$

to terms of second order. The nominally zero order contribution $E\phi\phi^\dagger L$ to $(\delta H)\,L$ vanishes, however, in view of (1.6), so that the right side of (3.6) indeed is of first order. For our present purposes, therefore, namely reformulating the second order expression (2.7), we can simplify (3.6) to

$$(H - E)\,\delta L = \phi\delta\phi^\dagger HL + E\phi\phi^\dagger\delta L - W\delta\phi - \lambda\delta\phi - (\delta\lambda)\,\phi \tag{3.9}$$

where we have included the first order contribution $E\phi\phi^\dagger\delta L$ from the nominally second order term $\delta H\delta L$ in (3.6).

Using (3.9) and (3.7) in (2.7), and remembering that λ and $\delta\lambda$ are purely real, we obtain after some algebra

$$\begin{aligned}\delta F^{(2)} = &- \delta\phi^\dagger W\delta\phi - \lambda\delta\phi^\dagger\delta\phi - (\delta\lambda)[\phi^\dagger\delta\phi + (\delta\phi)^\dagger\phi] \\ &+ (\delta\phi^\dagger HL)(\delta\phi^\dagger\phi) + (L^\dagger H\delta\phi)(\phi^\dagger\delta\phi) \\ &+ E(\phi^\dagger\delta L)(\delta\phi^\dagger\phi) + E(\delta L^\dagger\phi)(\phi^\dagger\delta\phi)\end{aligned} \tag{3.10}$$

to terms of third order, a phrase we should not have to repeat. From (1.6) and (2.8)

$$\phi^\dagger\delta L + (\delta\phi)^\dagger L + \delta\phi^\dagger\delta L = 0 \tag{3.11a}$$

whose adjoint is

$$\delta L^\dagger\phi + L^\dagger\delta\phi + \delta L^\dagger\delta\phi = 0. \tag{3.11b}$$

Equations (3.11) permit us to replace $\phi^\dagger\delta L$ and $\delta L^\dagger\phi$ in (3.10) by $-\delta\phi^\dagger L$ and $-L^\dagger\delta\phi$, respectively. Because of (2.4a), the $\delta\lambda$ terms in (3.10) can be dropped. Hence (3.10) simplifies to

$$\begin{aligned}\delta F^{(2)} = &- \delta\phi^\dagger W\delta\phi - \lambda\delta\phi^\dagger\delta\phi + [\delta\phi^\dagger(H - E)\,L](\delta\phi^\dagger\phi) \\ &+ [L^\dagger(H - E)\,\delta\phi](\phi^\dagger\delta\phi).\end{aligned} \tag{3.12}$$

We will return to (3.12) after considering the alternative choice of H_t yielding the minimum principle (1.9), namely[9]

$$\begin{aligned}H_t = \hat{H}_{\mathrm{mod},t} &= P_tHP_t + (1 - P_t)\,H(1 - P_t) \\ &= H - \phi_t\phi_t{}^\dagger H - H\phi_t\phi_t{}^\dagger + 2E_t\phi_t\phi_t{}^\dagger.\end{aligned} \tag{3.13}$$

Thus we now have, two terms of second order,

$$\begin{aligned}\delta H = \hat{H}_{\mathrm{mod},t} - H &= - (\delta\phi)\,\phi^\dagger H - \phi\delta\phi^\dagger H - (H\delta\phi)\,\phi^\dagger \\ &\quad - (H\phi)\,\delta\phi^\dagger + 2E(\phi\delta\phi^\dagger + \delta\phi\phi^\dagger) \\ &= - \phi\delta\phi^\dagger H - H\delta\phi\phi^\dagger + E(\phi\delta\phi^\dagger + \delta\phi\phi^\dagger) \\ &= - (H - E)\,\delta\phi\phi^\dagger - \phi\delta\phi^\dagger(H - E)\end{aligned} \tag{3.14}$$

which is of first order, reflecting the fact that $H_{\mathrm{mod},t} \to H$ as $\phi_t \to \phi$. Consequently, the equation for the present L_t—which is not identical with the L_t satisfying Eq. (3.3)—surely is

$$(\hat{H}_{\mathrm{mod},t} - E_t)\,L_t = - W\phi_t - \lambda_t\phi_t. \tag{3.15}$$

From (3.13),

$$\phi_t{}^\dagger\hat{H}_{\mathrm{mod},t} = E_t\phi_t{}^\dagger \tag{3.16}$$

Therefore, recalling (1.8b), we see that both sides of (3.15) vanish identically after multiplying by $\phi_t{}^\dagger$ on the left. It follows that L_t is incompletely determined by Eq. (3.15), just as L is incompletely determined by (1.5); it is necessary to specify $\phi_t{}^\dagger L_t$, and we shall adopt the specification (2.8). The facts that with Eq. (3.15) the condition (2.8) must be *imposed* whereas (2.8) is a *consequence* of (3.3) reflect the facts that (3.3) is constructed[8] to have no bound state eigenvalues, whereas $\hat{H}_{\mathrm{mod},t}$ has the eigenvalue E_t and eigenfunction ϕ_t.

We now return to Eq. (3.6), which—because the right sides of (3.15) and (3.3) are identical—remains valid for the present $\hat{H}_{\mathrm{mod},t}$ trial Hamiltonian. Now (3.14) and (1.6) imply

$$(\delta H)\,L = - \phi\delta\phi^\dagger(H - E)\,L. \tag{3.17}$$

Thus we now have

$$(H - E)\,\delta L = \phi\delta\phi^\dagger(H - E)\,L - W\delta\phi - \lambda\delta\phi - (\delta\lambda)\,\phi \tag{3.18}$$

instead of (3.9). Using(3.18) in (3.7), and substituting in (2.7), we find that the resultant expression for $\delta F^{(2)}$ is precisely our former (3.12). In other words, whether L_t from (3.3) or L_t from (3.15) is used in the variational principle (1.4), the second order error made is the same and is given by (3.12) in terms of $\delta\phi$ and the exact L. Moreover, Eq. (1.5) permits us to eliminate $(H - E)\,L$ from (3.12), thereby yielding

$$\delta F^{(2)} = -\delta\phi^\dagger W\delta\phi - \lambda\delta\phi^\dagger\delta\phi - (\delta\phi^\dagger W\phi)(\delta\phi^\dagger\phi) - (\phi^\dagger W\delta\phi)(\phi^\dagger\delta\phi) - \lambda[(\delta\phi^\dagger\phi)^2 + (\phi^\dagger\delta\phi)^2] \quad (3.19)$$

which depends explicitly only on ϕ and $\delta\phi$; explicit dependences on L and δL have disappeared.

4. ERROR AS A FUNCTION OF TRIAL EIGENFUNCTION

As it stands, Eq. (3.19) is not a useable formula for $\delta F^{(2)}$, because it involves the unknown quantities ϕ and $\delta\phi$; in order to actually compute $\delta F^{(2)}$, we must reexpress (3.19) so that it depends only on the known trial function ϕ_t. This we can do as follows.

Suppose $\delta F^{(2)}$ can be rewritten in the form

$$\delta F^{(2)} = \delta\phi^\dagger S\delta\phi \quad (4.1)$$

where S is an operator to be determined. Suppose further that there exists an operator N such that

$$(H-E)\,N(H-E) = S. \quad (4.2)$$

In these events, we would have

$$\begin{aligned}\delta F^{(2)} &= \delta\phi^\dagger(H-E)\,N(H-E)\,\delta\phi \\ &= [(H-E)\,\delta\phi]^\dagger N[(H-E)\,\delta\phi] \\ &= [(H-E)\,\phi_t]^\dagger N[(H-E)\,\phi_t] \end{aligned} \quad (4.3)$$

by virtue of (1.2) and the definition (2.1a) of $\delta\phi$. Since the right side of (4.3) is already of second order, in (4.3) it is permissible to replace E by E_t and N by some first order estimate N_t. Thus we would obtain the formula

$$\delta F^{(2)} = [(H-E_t)\,\phi_t]^\dagger N_t[(H-E_t)\,\phi_t] \quad (4.4)$$

from which the second order error should be calculable.

We now address the problems of finding first S and then N. To obtain (3.19) in the form (4.1), each term in (3.19) must contain one $\delta\phi^\dagger$ (on the left) and one $\delta\phi$ (on the right). We can recast (3.19) in this desired form by judiciously taking advantage of (2.4a), which permits replacement of $\phi^\dagger\delta\phi$ by $-\delta\phi^\dagger\phi$ and vice versa. In this fashion we obtain

$$\delta F^{(2)} = -\delta\phi^\dagger W\delta\phi - \lambda\delta\phi^\dagger\delta\phi + (\delta\phi^\dagger W\phi)(\phi^\dagger\delta\phi) + (\delta\phi^\dagger\phi)(\phi^\dagger W\delta\phi) + 2\lambda(\delta\phi^\dagger\phi)(\phi^\dagger\delta\phi). \quad (4.5)$$

Equation (4.5) is in the form (4.1) with

$$S = -W - \lambda\mathbf{1} + (W\phi)\,\phi^\dagger + \phi(W\phi)^\dagger + 2\lambda\phi\phi^\dagger. \quad (4.6)$$

We now observe, recalling the definition (1.5) for λ, that

$$\phi^\dagger S = S\phi = 0. \quad (4.7)$$

Indeed, in terms of the projection operator P defined by (3.2b),

$$S = -(P-\mathbf{1})(W+\lambda\mathbf{1})(P-\mathbf{1}). \quad (4.8)$$

Consequently, Eq. (4.2) is solvable for N even though in the full space of quadratically integrable functions the operator $H-\lambda$ does not have an inverse when λ equals the eigenvalue E of H. It is convenient to introduce the function $\hat{G}$—which has been termed[8] a Green's function in the generalized sense—satisfying

$$(H-E)\,\hat{G} = P-\mathbf{1}. \quad (4.9)$$

Then Eqs. (4.8) and (4.9) imply Eq. (4.2) is satisfied by the operator

$$N = -\hat{G}[W+\lambda\mathbf{1}]\,\hat{G}. \quad (4.10)$$

However, Eq. (4.9) does not determine the projection of $\hat{G}$ on ϕ, just as (1.5) did not determine the projection of L on ϕ. Correspondingly, Eq. (4.2) does not determine $\phi^\dagger N$ or $N\phi$. For completeness, therefore, we will specify

$$\phi^\dagger\hat{G} = 0. \quad (4.11)$$

Therefore, since

$$P-\mathbf{1} = -\sum_{i\neq 1}\phi_i\phi_i^\dagger \quad (4.12)$$

summed over all excited states of H,

$$\hat{G} = -\sum_{i\neq 1}\frac{\phi_i\phi_i^\dagger}{E_i-E} \quad (4.13)$$

and the counterpart to (4.11) is

$$\hat{G}\phi = 0. \quad (4.14)$$

With Eqs. (4.11) and (4.14) the operator N defined by Eq. (4.10) is completely specified. In fact,

$$\phi^\dagger N = N\phi = 0. \quad (4.15)$$

Evidently, a reasonable trial N_t in (4.4) is

$$N_t = -\hat{G}_t[W+\lambda_t\mathbf{1}]\,\hat{G}_t \quad (4.16)$$

where $\hat{G}_t$ is any reasonable trial estimate of $\hat{G}$. One possibility is to let $\hat{G}_t$ be the solution to

$$(\hat{H}_{\mathrm{mod},t}-E_t)\,\hat{G}_t = P_t-\mathbf{1} \quad (4.17a)$$

subject to

$$\phi_t^\dagger\hat{G}_t = \hat{G}_t\phi_t = 0. \quad (4.17b)$$

Defining $\hat{G}_t$ via Eqs. (4.17) has the advantage that $\hat{G}_t$—like L_t satisfying (3.15)—then can be estimated from a minimum principle of the form (1.9); moreover, to obtain a reasonable N_t (4.16) for use in estimating the second order error $\delta F^{(2)}$, it is not necessary to have a highly accurate $\hat{G}_t$, as the derivation of (4.4) has made plain. An alternative possibility for $\hat{G}_t$, based on (4.13), is

$$\hat{G}_t = -\sum_{i\neq 1}\frac{\phi_{it}\phi_{it}^\dagger}{E_{it}-E_t}, \quad (4.18)$$

where the set ϕ_{it} and associated E_{it} are a set of trial eigenfunctions and eigenvalues estimating the exact eigenfunctions ϕ_i and eigenvalues E_i of H, with of course ϕ_{1t} and E_{1t} equal to our previous ϕ_t and E_t, respectively.

This completes our assigned task of expressing the second order error $\delta F^{(2)}$ in terms of known quantities. We stress that although the possibility of finding the simple closed formula (4.4) for $\delta F^{(2)}$ is of undoubted theoretical interest, the practical utility of these results remains to be established. Whether $\hat{G}_t$ is defined via (4.17) or (4.18), calculating $\delta F^{(2)}$ from (4.4) and (4.16) will not be a trivial matter, especially in many-particle problems where matrix elements quadratic in H always are very awkward to compute. Nevertheless the expression (4.4) should be calculable in few-particle systems (e.g., in the case that H is the Hamiltonian

of the He atom), and certainly is calculable in the case of a single particle bound by a potential.

An even more serious impediment to practical application of (4.4) is the fact that the foregoing results have assumed Eq. (1.7) for L_t has been solved essentially exactly for the given ϕ_t; in practice, the required accuracy in L_t may be difficult to achieve. It is worth remarking, however, that if the L_t used in (1.4) is the effectively exact solution of (1.7), the quantity

$$\langle W_{11}\rangle_{\text{supv}} = \langle W_{11}\rangle_{\text{var}} - \delta F^{(2)} \tag{4.19}$$

obtained from (1.4), (2.2b), and (4.4) should differ from the exact W_{11} by at most third order, i.e., should be a supervariational estimate of W_{11}. In actual calculations, ϕ_t probably will be determined from the Rayleigh–Ritz calculation yielding E_t via (2.3b), and one then expects that as the number of arbitrary parameters in ϕ_t is increased the estimate of W_{11} from (4.19) will converge distinctly more rapidly than does the original variational estimate (1.4).

When W is a positive definite operator, Eq. (4.4) yields simple upper and lower bounds on $\delta F^{(2)}$. Introducing the notation

$$\Psi_t = \hat{G}_t(H - E_t)\,\phi_t, \tag{4.20}$$

and recognizing that $\hat{G}_t$ from (4.17) or (4.18) obeys

$$\hat{G}_t{}^\dagger = \hat{G}_t$$

[a relation implicit in (4.17b)], Eqs. (4.16 and (4.4) yield

$$\delta F^{(2)} = -\,\Psi_t{}^\dagger[W + \lambda_t 1]\,\Psi_t. \tag{4.21}$$

Since λ_t from (1.8b) is a negative number when W is positive definite, Eq. (4.21) immediately implies

$$-\,\Psi_t{}^\dagger W \Psi_t < \delta F^{(2)} < (\phi_t{}^\dagger W \phi_t)(\Psi_t{}^\dagger \Psi_t). \tag{4.22}$$

Or, using (4.19),

$$\{\langle W_{11}\rangle_{\text{var}} - (\phi_t{}^\dagger W \phi_t)(\Psi_t{}^\dagger \Psi_t)\} < \langle W_{11}\rangle_{\text{supv}} < \{\langle W_{11}\rangle_{\text{var}} + \Psi_t{}^\dagger W \Psi_t\} \tag{4.23}$$

We emphasize that although (4.23) (like all formulas in this paper) assumes $L_t(\phi_t)$ has solved (1.7) exactly, the above inequality does not yield rigorous bounds on the exact W_{11}, because $\langle W_{11}\rangle_{\text{supv}}$ differs from the exact W_{11} by third and higher order terms. Nevertheless, if the L_t used in (1.4) really is the effectively exact solution of (1.7), then Eq. (4.23) should provide quite reliable variational (i.e., second order) bounds on the exact W_{11} whenever $\langle W_{11}\rangle_{\text{supv}}$ has converged close to its final (presumably the exact $\phi^\dagger W \phi$) limit; the reason for this assertion is that in these circumstances the second order terms involving Ψ_t in (4.23) should be much larger in absolute value than the residual third order error in $\langle W_{11}\rangle_{\text{supv}}$.

Before closing, a brief discussion of the errors introduced by using trial L_t which do not solve (1.7) exactly may be worthwhile. Suppose that for given ϕ_t the quantity L_{tt} is our approximation to the exact L_t solving (1.7), and define

$$\Delta L = L_{tt} - L_t. \tag{4.24}$$

Then if L_{tt} rather than L_t is used to compute $\langle W_{11}\rangle_{\text{var}}$ from (1.4), our computed estimate of $\delta F^{(2)}$ will be in error by an amount

$$\Delta F^{(2)} = \Delta L^\dagger[(H - E)\,\delta\phi] + [(H - E)\,\delta\phi]^\dagger \Delta L, \tag{4.25a}$$

recognizing that in (1.4)

$$L_{tt} = L + \delta L + \Delta L. \tag{4.25b}$$

But our result (4.4) for $\delta F^{(2)}$ is of order $\delta\phi^\dagger \delta\phi$, recalling (3.19) and (4.1). It follows that the actually obtained second order error—in the value of $\langle W_{11}\rangle_{\text{var}}$ computed using the actual L_{tt} in (1.4)—will continue to be represented by (4.4), provided only that the right side of (4.25a) is of higher order than $\delta\phi^\dagger \delta\phi$, i.e., provided only that ΔL is of higher order than $\delta\phi$ for the particular ϕ_t chosen. The error in $\langle W_{11}\rangle_{\text{supv}}$ from (4.19), computed using L_{tt} rather than L_t in (1.4), will not be of third order unless ΔL can be regarded as being of order $(\delta\phi)^2$. Because the right side of (4.3) already is of second order, any reasonable N_t—namely, one differing from N by first order—keeps the error in the computed $\langle W_{11}\rangle_{\text{supv}}$ at third order. The mere fact that—for any given ϕ_t—Ψ_t in (4.23) depends via (4.20) on a quantity $\hat{G}_t$ we have some freedom to choose [recall Eq. (4.16–(4.18)] implies (4.23) cannot yield rigorous bounds.

*Work was supported in part by the Advanced Research Project Agency under Contract DA-31-124-ARO-D-440, and by the National Aeronautics and Space Administration under Contract No. No6-39-011-035.

[1]C. Schwartz, Ann. Phys. (N.Y.) **2**, 156 (1959); **2**, 170 (1959).
[2]A. Dalgarno and A. L. Stewart, Proc. R. Soc. Lond. A **257**, 534 (1960); J. C. Y. Chen and A. Dalgarno, Proc. Phys. Soc. Lond. **85**, 399 (1965).
[3]L. M. Delves, Nucl. Phys. **45**, 313 (1963); L. M. Delves, Proc. Phys. Soc. Lond. **92**, 55 (1967).
[4]J. O. Hirschfelder, W. B. Brown, and S. T. Epstein, Adv. Quantum Chem. **1**, 255 (1964).
[5]S. Aranoff and J. Percus, Phys. Rev. **166**, 1255 (1968).
[6]E. Gerjuoy, A. R. P. Rau, and L. Spruch, Phys. Rev. A **8**, 662 (1973).
[7]J. B. Krieger and V. Sahni, Phys. Rev. A **3**, 919, 928 (1972); V. Sahni and J. B. Krieger, Phys. Rev. A **8**, 65 (1973).
[8]E. Gerjuoy, A. R. P. Rau, L. Rosenberg, and L. Spruch, Phys. Rev. A **9**, 108 (1974).
[9]E. Gerjuoy, L. Rosenberg, and L. Spruch, J. Math. Phys. **16**, 455 (1975).
[10]R. Blau, A. R. P. Rau, and L. Spruch, Phys. Rev. A **8**, 119, 131. (1973).

A note on the unified Dirac–von Neumann formulation of quantum mechanics

D. Tjøstheim

NTNF/NORSAR, P.O. Box 51, N-2007 Kjeller, Norway
(Received 29 October 1974)

It is demonstrated that the mathematical model of a rigged Hilbert space is ideally suited for obtaining a unified Dirac–von Neumann formulation of quantum mechanics. It is shown that the eigenbras of an observable A can be interpreted as weak derivatives of certain functionals associated with the resolution of identity E_u, $u \in (-\infty, \infty)$, associated with A.

1. FORMULATION OF THE PROBLEM

In a paper by Marlow[1] an attempt was made to unify the Dirac[2] and von Neumann[3] formulations of quantum mechanics using the mathematical model of a direct integral of Hilbert spaces. Unfortunately, this work suffered from some inconveniences as was pointed out by Antoine.[4] Recently it has become increasingly popular[4,5,6] to use a rigged Hilbert space as mathematical model for obtaining a rigorous interpretation of the Dirac formalism. The purpose of this note is to demonstrate that a rigged Hilbert space also appears to be ideally suited for formulating a unified Dirac—von Neumann formalism in the spirit of Marlow.

We consider (as does Marlow) a single observable (self-adjoint operator) A in the Hilbert space H of physical states. The spectral decomposition[3] $A = \int u\, dE_u$, where E_u, $u \in (-\infty, \infty)$, is the resolution of identity associated with A, was obtained by von Neumann and forms the basis for his formulation of quantum mechanics.

The concept of a rigged Hilbert space was introduced by Gel'fand. It consists of a triplet $\Phi \subset H \subset \Phi'$ (where H is identified with H') where Φ is a dense subspace of the Hilbert space H and where Φ is equipped with a topology that makes it a nuclear countable Hilbert space. Furthermore, the topology of Φ is finer than the one induced on Φ by the inner product in H. The space Φ' is the space of continuous linear functionals on Φ. The problem of constructing a "canonical" space Φ for a given physical system is not yet solved in complete generality. In this note we will content ourselves by assuming that there exists a dense subspace Φ of H such that $\Phi \subset D(A)$ is stable under A, such that $\Phi \subset H \subset \Phi'$ is a rigged Hilbert space and A is continuous in the topology of Φ. [$D(A)$ is used to denote the domain of definition of A.]

It is known[4] that a rigorous formulation of the Dirac formalism results if the eigenbras of the observable A are identified with those generalized eigenvectors of A which correspond to the points of the Hilbert space spectrum of A. The problem is to find a connection between these generalized eigenvectors and the von Neumann spectral decomposition $A = \int u\, dE_u$.

2. WEAK DERIVATIVES OF FUNCTIONALS

Let[7] $H \longrightarrow \int_\Lambda H(u)\, d\mu(u)$ be a realization of H as a direct integral of Hilbert spaces induced by the operator A. The set $\Lambda \subset R^1$ is the spectrum of A, and $\dim H(u) = d(u)$, $u \in \Lambda$, is the spectral multiplicity of A at the point u. We denote by $e_i(u)$, $i = 1, 2, \ldots, d(u)$, an orthonormal basis in $H(u)$. Since the measure μ is finite,[7] the vector fields e_i': $u \to e_i(u)$, $i = 1, 2, \ldots, e_i(u) = 0$ for $i > d(u)$, are contained in $\int_\Lambda H(u)\, d\mu(u)$. Denote by e_i the corresponding elements of H. Then

$$(e_i, e_i)_H = \int_\Lambda (e_i(u), e_i(u))_u\, d\mu(u) \leq \mu(\Lambda),$$

where $(\cdot, \cdot)_H$ and $(\cdot, \cdot)_u$ are the inner products in H and $H(u)$, respectively. Using the elements e_i, a smooth transition between the Dirac and von Neumann spectral decompositions of A can be obtained.

Consider an arbitrary element ϕ in Φ and let $\phi \longrightarrow \phi(u)$ be the realization of ϕ induced by the realization $H \longrightarrow \int_\Lambda H(u)\, d\mu(u)$. Then

$$(E(\Delta)\, e_i, \phi) = \int_\Delta (e_i(u), \phi(u))_u\, d\mu(u),$$

where we have used the fact that E_u, $u \in \Lambda$, constitutes a resolution of identity. ($\Delta \subset R^1$ is a Borel set.) Denote by μ_i the complex measure defined by $\mu_i(\Delta) = (E(\Delta)\, e_i, \phi)$. Using the Schwarz inequality it is not difficult to show that μ_i is absolutely continuous with respect to the finite positive measure μ_{e_i} defined by $\mu_{e_i}(\Delta) = (E(\Delta)\, e_i, e_i)$. Since the measure μ can be defined[7] as

$$\mu(\Delta) = \sum_{i=1}^{N} a_i\, \mu_{e_i}(\Delta),$$

where $\sum_{i=1}^{N} a_i < \infty$, $a_i > 0$, and where $N = \sup_{u \in \Lambda} d(u)$ may possibly be ∞, it follows that μ_i is absolutely continuous with respect to μ. From the Radon—Nikodym theorem for complex measures[8] it follows that the function $h_i^\phi(u) = (e_i(u), \phi(u))_u$ can be identified with the Radon—Nikodym derivative $d\mu_i/d\mu$.

Considered as functions of ϕ, $h_i^u(\phi) = h_i^\phi(u)$, $i = 1, 2, \ldots, d(u)$, are elements of Φ' and, in fact, they constitute[7] a complete set of generalized eigenvectors of A. What remains, therefore, is to establish a relation between $h_i^u(\phi)$ and E_u.

Consider the linear functional $f_i^u(\phi) = (E_u\, e_i, \phi)$. Then $f_i^u \in \Phi'$ and it can be shown that the *weak derivative*[7] $g_i^u(\phi) = df_i^u(\phi)/d\mu(u)$ of f_i^u with respect to μ exists and is well defined as a continuous linear functional on Φ. From the definition of μ_i and the fact that

$$\frac{d\mu_i}{d\mu}(u) = (e_i(u), \phi(u))_u = h_i^u(\phi),$$

it follows that g_i^u and h_i^u can be identified. If we use the Dirac bra notation $\langle ui|$ for the generalized eigenvector

h_i^u, we have that

$$\langle ui \mid \phi \rangle = g_i^u(\phi) = \frac{d(E_u e_i, \phi)}{d\mu(u)}$$

or (with a slight abuse of notation)

$$\langle ui \mid = \frac{dE_u e_i}{d\mu}$$

and this relation represents the connection between the Dirac and von Neumann spectral decompositions of A.

ACKNOWLEDGMENT

I am grateful to professor S. Tjøtta, Department of Applied Mathematics, University of Bergen, for suggesting the topic of this investigation and for several encouraging discussions.

[1]A.R. Marlow, J. Math. Phys. **6**, 919 (1965).
[2]P.A.M. Dirac, *The Principles of Quantum Mechanics* (Clarendon, Oxford, 1958), 4th ed.
[3]J. von Neumann, *Mathematical Foundation of Quantum Mechanics* (Princeton U.P. Princeton, New Jersey, 1955).
[4]J.P. Antoine, J. Math. Phys. **10**, 53, 2276 (1969).
[5]J.E. Roberts, J. Math. Phys. **7**, 1097 (1966); Commun. Math. Phys. **3**, 98 (1966).
[6]O. Melsheimer, J. Math. Phys. **15**, 902, 917 (1974).
[7]I.M. Gel'fand, G.E. Shilov, and N.I. Vilenkin, *Generalized Functions* (Academic, New York, 1964), Vols. III-IV.
[8]W. Rudin, *Real and Complex Analysis* (McGraw-Hill, New York, 1966).

Temporally inhomogeneous scattering theory for modified wave operators

Joseph H. Hendrickson

Department of Mathematical Sciences, State University of New York, Binghamton, New York 13901
(Received 4 October 1974)

A theorem of Alsholm and Kato, which gives existence of modified wave operators for a large class of long range potentials, is extended to include time dependent potentials. It is then shown that these temporally inhomogeneous modified wave operators $W_{D\pm}(S)$ vary continuously, in some sense, on the potentials. This result is new for both time dependent and time independent potentials. In addition, part of the nonuniqueness problem of modified wave operators is resolved by noting that the modified wave operators are asymptotically unique.

1. INTRODUCTION

In nonrelativistic scattering theory a particle at time $t\in\mathbb{R}$ is represented by $u(t,\cdot)\in L^2(\mathbb{R}^n)$. The Hamiltonian $H(t)$ of the particle is, for each $t\in\mathbb{R}$, a self-adjoint operator on $L^2(\mathbb{R}^n)$ and determines the motion of the particle according to the Schrödinger equation:

$$\frac{\partial}{\partial t}u(t,x)=-iH(t)u(t,x).$$

Kato[1] has given conditions on $H(t)$ under which the Schrödinger equation can be solved in the sense of finding a family of unitary *evolution operators* $\{U(t,s):t,s\in\mathbb{R}\}$ satisfying $u(t,x)=U(t,s)u(s,x)$. The Hamiltonian for a free particle is $H_0=-\Delta/2$. Potential scattering concerns itself with Hamiltonians of the form $H(t)=H_0+V(t,x)$, where $V(t,\cdot)\in L^2_{1oc}(\mathbb{R}^n)$. Goldstein and Monlezun[2] have reformulated Kato's conditions in the case of potential scattering:

(AI) Assume $V(t,x)=\sum_{j=0}^m V^j(t,x)$, where $V^j(t,x)$ is real valued and in $L^{p_j}(\mathbb{R}^n)$ with $2\leq p_j<\infty$ and $p_j>n/2$ for $j=1,\ldots,m$ and with $p_0=\infty$. Assume that as a function of t, $V^j:\mathbb{R}\to L^{p_j}(\mathbb{R}^n)$ is piecewise strongly continuously differentiable.

Condition AI also implies that $\mathcal{D}\equiv\mathcal{D}(H_0)=\mathcal{D}(H(t))=W^{2,2}(\mathbb{R}^n)$, the Sobolev space of order 2, for all $t\in\mathbb{R}$.

The standard wave operators are defined as

$$W_\pm(s)=s\text{-}\lim_{t\to\pm\infty}U(s,t)U_0(t,s),$$

where $U_0(t,s)=\exp[-i(t-s)H_0]$ is the evolution operator for H_0. This definition was originally proposed by Jauch[3] and extended to time dependent Hamiltonians by Monlezun.[4] The existence of these strong limits is an expression of the fact that the motion described by $U(t,s)$ is asymptotically free. If $f_\pm(0,\cdot)$ are the free particles that asymptotically approximate $u(0,x)$, then $u(s,x)=W_\pm(s)f_\pm(s,x)$. For time independent, short range potentials, i.e., $V(x)=O(|x|^{-1-\epsilon})$ for $\epsilon>0$, this convergence is well known. (See Jauch.[3]) However, Dollard[5,6] showed that for the Coulomb potential $1/|x|$ convergence fails, indicating that such "long range" potentials have a residual effect at large distances. Dollard was able to force convergence by the addition of an ad hoc "anomolous term" to the free evolution operator. This was not totally intuitively satisfactory and others (Amrein, Martin, and Misra[7]; Lavine[8]; Thomas[9]) redefined the wave operators in terms of momentum observables and were able to show convergence. These results are made reasonable by the following examples of classical scattering in one dimension.

First, consider the short range potential $V(x)=-1/x^2$. Solving $\ddot{x}(\pm)=-V'(x)$, Newton's second law, one easily sees that the motion is asymptotically free (straight line) motion:

$$x(t)\doteq\pm\sqrt{2c_1}\,t\pm\sqrt{2c_1}\;c_2\quad\text{for large } t,$$

where c_1, c_2 are arbitrary constants. In the long range case $V(x)=-1/|x|$, motion remains asymptotically unfree:

$$x(t)\doteq\pm\sqrt{2c_1}\;t\pm\sqrt{2c_1}\;c_2+(1/c_1)\log(2\sqrt{x}).$$

However, in agreement with the results mentioned above, the momentum even in the long range case is asymptotically free (constant):

$$\dot{x}(t)=\pm(2x^{-1}+2c_1)^{1/2}\doteq\sqrt{2c_1}.$$

For details see the author's dissertation.[10]

This indicates that the asymptotic dynamics, while not free, do conserve momentum; i.e., their Hamilton does not depend explicitly on x and is, therefore, of the form $H_0+P(t,p)$, where $p=-i\Delta_x$. If $P(t,p)$ were set equal to $V(t,pt)$, this would agree with Dollard's anomolous term. For a more intuitive motivation, see Alsholm,[11] Hendrickson,[10] Herbst.[12] To show convergence with this definition, it is necessary to place growth conditions on $V(t,x)$ in each variable. The following conditions are modeled after those of Alsholm and Kato[13]:

(AII) Assume $V(t,x)=V_1(t,x)+V_2(t,x)+V_L(t,x)$ and

(a) there exist positive constants c, ϵ, β, γ, and M such that

$$1\geq\beta>\tfrac{1}{2}\quad\text{and}\quad\gamma>(1-\beta)^2\beta^{-1}$$

and such that the following hold:

(b) $|V_2(t,x)|\leq c(1+|x|)^{-1-\epsilon}$.

(c) $D_t^{\alpha_1}D_x^{\alpha_2}V_L(t,x)\in L^1_{1oc}(\mathbb{R}^{n+1})$ for $|\alpha_1|=0,1$ and $\alpha_2=0,1,2,3$. The derivatives are taken as distributions.

(d) $|D_x^\alpha V_L(t,x)| \le \begin{cases} c(1+|x|)^{-1-\beta}, & |\alpha|=1, \\ c(1+|x|)^{-2-\gamma}, & |\alpha|=2,\ 3. \end{cases}$

(e) $|D_t D_x^\alpha V_L(t,x)|$
$$\le \begin{cases} c(1+|t|)^{-1}(l+|x|)^{-1-\beta}, & |\alpha|=1 \\ c(1+|t|)^{-1}(l+|x|)^{-2-\gamma}, & |\alpha|=2,\ 3. \end{cases}$$

(f) $V_1(t,\cdot) \in L^2(\mathbb{R}^n)$ for all $|t| > t_0 > 0$ for some constant t_0 and $\|V_1(t,\cdot)\|_2 \le M$ for all $|t| > t_0$.

Unnecessary growth conditions on the essentially short range potentials V_1 and V_2 are avoided by using only V_L in the definition below of the anomolous term.

If $F \in L^2(\mathbb{R}^n)$, its Fourier transform and inverse transform are denoted $\hat{F}$ and $\check{F}$ respectively, where

$$\hat{F}(\rho) = \text{l.i.m.}\,(1/2\pi)^{n/2} \int_{\mathbb{R}^n} \exp(-ix\cdot p) F(x)\,dx.$$

$F(p)$ can be considered as an operator in $L^2(\mathbb{R}^n)$ defined by

$$F(p)u(x) = [F(p)\hat{u}(p)]^{\check{}}.$$

In particular, $F(p) = p$ is the operator $-i\nabla_x$. In this context, we define the Dollard anomolous term generalized to time dependent potentials and the associated asymptotic or "semifree" evolution operators.

Definition: Let $X_s^t(p) = \int_s^t V_L(\tau, p\tau)\,d\tau$. To conform with the notation of Alsholm and Kato, we abbreviate $X_0^t(p) = X_t(p)$.

Definition: Let

$$U_0'(t,s) = \exp(-i\int_s^t H_0 + V_L(\tau, p\tau)\,d\tau)$$
$$= \exp[-i(t-s)H_{0_e} - iX_s^t(p)]$$

be the evolution operator for $H_0 + V_L(t, pt)$.

The following theorem generalizes that of Alsholm and Kato[13] to the case of time dependent potentials.

Theorem 1: Let $n \ge 3$. Assume AI and AII. Then the temporally inhomogeneous modified wave operators

$$W_{D\pm}(s) = \text{s-}\lim_{t\to\pm\infty} U(s,t)U_0'(t,s)$$

exist for all $s \in \mathbb{R}$. In particular, if $u \in C_0^\infty(\mathbb{R}^n\backslash\{0\})^{\check{}}$, i.e., $\hat{u}$ is infinitely differentiable with compact support missing the origin, then there are positive constants c_u and ν, which depend only on u, M, C, ϵ, β, and γ such that, for $|t| > t_0$,

$$\|W_{D\pm}(s)u - U(s,t)U_0'(t,s)u\| \le c_u t^{-\nu}.$$

2. PROOF OF THEOREM 1

Throughout this paper, u shall always refer to an element of the dense set $C_0^\infty(\mathbb{R}_n\backslash\{0\})^{\check{}}$ with $K = \text{supp}\,\hat{u}$. We shall often use without comment the fact that convergence of a sequence of uniformly bounded operators on this dense set implies strong convergence. Let $W(t) = U(0,t)U_0'(t,0)u$ and $\phi(t) = \|(d/dt)W(t)\|$. We first reduce Theorem 1 to the problem of bounding $\phi(t)$ by $c_u t^{-1-\nu}$. By assuming this bound, the case of $W_{D\pm}(0)$ follows from the Cook–Kuroda method:

$$\|W(t_2) - W(t_1)\| \le \left\|\int_{t_1}^{t_2} \frac{d}{dt} W(t)\,dt\right\|$$
$$= \frac{c_u}{\nu} t^{-\nu}\Big|_{t_1}^{t_2} \to 0 \quad \text{as } t \to \pm\infty.$$

For the general case we use the following lemma, which follows directly from the definition of $W_{D\pm}(s)$.

Lemma 1: If $W_{D\pm}(t)$ exists for some $t \in \mathbb{R}$, then $W_{D\pm}(s)$ exists for every $s \in \mathbb{R}$ and

$$W_{D\pm}(s) = U(s,t)W_{D\pm}(t)U_0'(t,s).$$

Thus

$$\|W_{D\pm}(s)u - U(s,t)U_0'(t,s)u\|$$
$$= \|[W_{D\pm}(0) - U(0,t)U_0'(t,0)]U_0'(0,s)u\| \le C_w t^{-1-\nu},$$

where $C_w = U_0'(0,s)u \in C_0^\infty(\mathbb{R}^n\ \{0\})^{\check{}}$.

So, turning our attention to $\phi(t)$, we see

$$\phi(t) = \left\|\frac{d}{dt} U(0,t)U_0'(t,0)u\right\|$$
$$= \|[V(t,x) - V_L(t,pt)]U_0'(t,0)u\|$$
$$\le \|V_1(t,x)U_0'(t,0)u\|$$
$$+ \|V_2(t,x)U_0'(t,0)u\|$$
$$+ \|[V_L(t,x) - V_L(t,pt)]U_0'(t,0)u\|$$
$$\equiv \phi_1(t) + \phi_2(t) + \phi_3(t).$$

The terms $\phi_2(t)$ and $\phi_3(t)$ correspond to what Alsholm and Kato call $\phi_S(t)$ and $\phi_L(t)$. Although the terms are somewhat different, the bounds are arrived at by arguments similar enough to make repetition unnecessary. One must merely note upon what the constants c_u and ν depend. In bounding $\phi_1(t)$ we use the following identity from Alsholm[11]:

$$\exp(it|p|^2/2)F(x)\exp(-it|p|^2/2) = \exp(-i|x|^2/2t)F(tp)$$
$$\times \exp(i|x|^2/2t).$$

$$\phi_1(t) = \|V_1(t,x)\exp(-itH_0)\exp(-iX_t)u\|_2$$
$$= \|V_1(t,pt)\exp(i|x|^2/2t)\exp(-iX_t)u\|_2$$
$$\le \|V_1(t,pt)\|_2 \|\exp(-iX_t)u\|_\infty$$
$$\le t^{-n/2}\|V_1(t_i)\|_2 \|\exp(-iX_t)\hat{u}\|_1$$
$$\le t^{-n/2} M \|\hat{u}\|_1.$$

We note that the only need for restricting $n \ge 3$ was to insure $n/2 > 1$ at this point and thus allow singular, Coulomb-like potentials. For detailed proofs of the bounds for $\phi_2(t)$ and $\phi_3(t)$ and for examples of time dependent potentials to which Theorem 1 applies, see the author's dissertation.[10]

3. ASYMTOTIC UNIQUENESS OF WAVE OPERATORS

The decomposition of V is not unique since V_L is allowed to contain as little or as much of the short range part of V as satisfies AII. However, the nonuniqueness this introduces into the definition of the wave operator vanishes in the limit.

Proposition: Assume $V = V_1 + V_2 + V_L = V_1' + V_2' + V_L'$ satisfies AI and AII with respect to each decomposition. If $W_{D\pm}(s)$ and $W'_{D\pm}(s)$ are the respective wave operators of Theorem 1, then

$$\text{s-}\lim_{s\to\pm\infty} W_{D\pm}(s) - W'_{D\pm}(s) = 0.$$

Proof:

$$\lim_{s\to\pm\infty} \| W_{D\pm}(s)u - W'_{D\pm}(s)u\|_2$$

$$= \lim_{s\to\pm\infty}\lim_{t\to\pm\infty} \| U(s,t)U_0(t,s)\exp(-i\textstyle\int_s^t V_L(\tau,p\tau)\,d\tau)u$$

$$- U(s,t)U_0(t,s)\exp(-i\textstyle\int_s^t V_L'(\tau,p\tau)d\tau)u\|_2$$

$$= \lim_{s\to\pm\infty}\lim_{t\to\pm\infty} \| u - \exp(-i\textstyle\int_s^t V_L' - V_L(\tau,p\tau)d\tau)u\|_2$$

$$= \lim \lim \| [1 - \exp(-i\textstyle\int_s^t V_L' - V_L(\tau,p\tau)\,d\tau)]\hat{u}\|_2$$

$$= \lim_{s\to\pm\infty}\lim_{t\to\pm\infty} \| \sup_{p\in k} \| \textstyle\int_s^t V_L' - V_L(\tau,p\tau)\,d\tau\|_\infty \|u\|_2 \to 0$$

as $s, t \to \pm\infty$ since $V_L' - V_L = V_1 - V_1' + V_2 - V_2' =$ an L^2 function + a short range function. ∎

4. APPROXIMATION THEOREM

In Theorem 1, it was noted that the rate of convergence of $W_{D\pm}(s)u$ which was established depended only on the bounding constants of the potential, i.e., on M, c, ϵ, β, and γ, rather than on the potential directly. Thus, if a collection of potentials can be bounded uniformly by such constants, then their respective wave operators will converge uniformly. This observation is the basis of the following result.

Theorem 2: Let V, V_L, $V_m: \mathbb{R}\times\mathbb{R}^n \to \mathbb{R}$, $m = 1, 2, 3, \cdots$, be such that

(BI) The evolution operators $\{U(t,s)\}$ for $H(t) = H_0 + V(t,\cdot)$ exist.

(BII) $V_m = V_{1,m} + V_{2,m} + V_{L,m}$ satisfy AI and AII with the given decompositions for $m = 1, 2, 3, \cdots$.

(BIII) There exist positive constants M, ϵ, β, γ and c such that

(i) $\gamma > (1-\beta)^2\beta^{-1}$,

(ii) $\epsilon_m \to \epsilon$, $\beta_m \to \beta$, $\gamma_m \to \gamma$, $c_m \to c$, $M_m \to M$, where ϵ_m, β_m, γ_m, c_m, and M_m are the bounding constants of AII associated with V_m.

(BIV) For every t, there exists a p_t such that $n \le p_t \le \infty$ and $\| V(t,\cdot) - V_m(t,\cdot)\|_{p_t} \to 0$ as $m \to \infty$.

(BV) For all $p \in \mathbb{R}^n$, $t \to V_L(t,pt)$ is in $L^1_{loc}(\mathbb{R})$ and for all compact $k \subseteq \mathbb{R}^n\backslash\{0\}$, $\sup_{p\in k} | \int_s^t V_L(\tau,p\tau) - V_{L,m}(\tau,p\tau)\,d\tau| \to 0$ as $s, t \to \pm\infty$.

Let $W_{D\pm,m}(s)$ be the wave operators for V_m and let

$$\bar{W}_{D\pm}(s) = \text{s-}\lim_{t\to\pm\infty} U(s,t)U_0(t,s)\exp(-i\textstyle\int_s^t V_L(\tau,p\tau)\,d\tau).$$

Then $\bar{W}_{D\pm}(s)$ exists and equals $\text{s-}\lim_{m\to\infty} W_{D\pm,m}(s)$.

Theorem 2 will be proved by a series of lemmas. Let $\{U_m(t,s)\}$ be the evolution operators for $H_m(t) = H_0 + V_m(t,\cdot)$. We use the following notation where $u \in C_0^\infty(\mathbb{R}^n\backslash\{0\})^\vee$:

$$X_s^t(p) = \int_s^t V_L(\tau,p\tau)\,d\tau,$$

$$X_{s,m}^t(p) = \int_s^t V_{L,m}(\tau,p\tau)\,d\tau,$$

$$W(t) = U(s,t)U_0(t,s)\exp(-iX_s^t)u,$$

$$W_m(t) = U_m(s,t)U_0(t,s)\exp(-iX_{s,m}^t)u,$$

$$W = \lim_{t\to\pm\infty} W(t),$$

$$W_m = \lim_{t\to\pm\infty} W_m(t).$$

Lemma 2.1: $U(t,s) = \text{s-}\lim_{m\to\infty} U_m(t,s)$.

Proof: By Goldstein,[14] it suffices to show that $[iH(t) - \xi]^{-1} - [iH_m(t) - \xi]^{-1} \to 0$ for all $\xi > 0$ and $t \in \mathbb{R}$. Note that $[iH_m(t) - \xi]^{-1}$ is uniformly bounded by $1/\xi$.

$$\| [iH(t) - \xi]^{-1}u - [iH_m(t) - \xi]^{-1}u\|_2$$

$$= \| [iH_m(t) - \xi]^{-1}[V_m(t,\cdot) - V(t,\cdot)][iH(t) - \xi]^{-1}u\|_2$$

$$\le \xi^{-1}\| V_m(t,\cdot) - V(t,\cdot)\|_{p_t} \| [iH(t) - \xi]^{-1}u\|_r,$$

where $1/r + 1/p_t = \frac{1}{2}$. Since $\| V_m(t,\cdot) - V(t,\cdot)\|_{p_t} \to 0$ and $n \le p_t \le \infty$ by assumption, it suffices to show that $\| [iH(t) - \xi]^{-1}u\|_r < \infty$ for $2 \le r \le 2n/(n-2)$. But $v \equiv [iH(t) - \xi]^{-1}u \in \mathcal{D} \equiv W^{2,2}$. Thus $\|v\|_2 < \infty$. Also $D^\alpha v \in L^2(\mathbb{R}^n)$ for all $|\alpha| = 1$, which implies $\|v\|_{2n/(n-2)} < \infty$ by Sobolev's inequality. (See Friedman.[15])

Lemma 2.2: $\text{s-}\lim_{m\to\infty} \exp(-iX_{s,m}^t) = \exp(-iX_s^t)$.

Proof:

$$\| \exp(-iX_{s,m}^t)u - \exp(-iX_s^t)u\|_2$$

$$\le \|u\|_2 \sup_{p\in K} \left| \exp(-iX_{s,m}^t)(p) - \exp(-iX_s^t)(p)\right|$$

$$\le \|u\|_2 \sup_{p\in k} \left| \textstyle\int_s^t V_{L,m}(\tau,p\tau) - V_L(\tau,p\tau)\,d\tau\right| \to 0$$

by assumption.

Lemma 2.3: For each $t \in \mathbb{R}$, $\lim_{m\to\infty} W_m(t) = W(t)$.

Proof:

$$\| W(t) - W_m(t)\|$$

$$= \| [U(s,t)\exp(-iX_s^t) - U_m(s,t)\exp(-iX_{s,m}^t)]U_0(t,s)u\|$$

$$\le \| [U(s,t) - U_m(s,t)]\exp(-iX_s^t)U_0(t,s)u\|$$

$$+ \| U_m(s,t)[\exp(-iX_s^t) - \exp(-iX_{s,m}^t)]U_0(t,s)u\| \to 0$$

by Lemmas 2.1 and 2.2.

Lemma 2.4: $\{W_m\}$ is a Cauchy sequence in m.

Proof: By BIII, we can assume that the bounds ϵ_m, β_m, γ_m, C_m, and M_m can be replaced by uniform bounds. Thus, by Theorem 1, there exists $c_u > 0$, $v > 0$ such that $\sup_m \| W_m - W_m(t)\| \le c_u t^{-v} \equiv a(t) \to 0$ as $t \to \pm\infty$. Let $\epsilon_1 > 0$. For some fixed t_1 so large that $a(t_1) < \epsilon_1$, choose $N > 0$ such that m, $\bar{m} > N$ implies $\| W_m(t_1) - W_{\bar{m}}(t_1)\| < \epsilon_1$. Then

$$\| W_m - W_{\bar{m}}\|$$

$$\le \| W_m - W_m(t_1)\| + \| W_m(t_1) - W_{\bar{m}}(t_1)\| + \| W_{\bar{m}}(t_1) - W_{\bar{m}}\|$$

$$\le 3\epsilon_1.$$

Lemma 2.5: The limits $W = \lim_{t\to\pm\infty} W(t)$ exist.

Proof: We show $\{W(t)\}$ is Cauchy as $t \to \infty$. Let $\epsilon_1 > 0$ and choose T so large that $t > T$ implies $a(t) < \epsilon_1$. Let $t, \bar{t} > T$. Choose m, $\bar{m}$ so large that

$$\|W(t) - W_m(t)\| + \|W(\bar{t}) - W_{\bar{m}}(\bar{t})\| + \|W_m - W_{\bar{m}}\| < \epsilon_1.$$

Then

$$\begin{aligned}\|W(t) - W(\bar{t})\| &\leq \|W(t) - W_m(t)\| + \|W_m(t) - W_m\| + \|W_m - W_{\bar{m}}\| \\ &\quad + \|W_{\bar{m}} - W_{\bar{m}}(\bar{t})\| + \|W_{\bar{m}}(\bar{t}) - W(\bar{t})\| \leq 3\epsilon_1.\end{aligned}$$

Lemma 2.6: $W = \lim_{m\to\infty} W_m$.

Proof: Let $\epsilon_1 > 0$. Choose $|t|$ so large that $\|W - W(t)\| + a(t) < \epsilon_1$. Choose $N > 0$ such that $m > N$ implies $\|W(t) - W_m(t)\| < \epsilon_1$. Then, for all $m > N$,

$$\begin{aligned}\|W - W_m\| &\leq \|W - W(t)\| + \|W(t) - W_m(t)\| + \|W_m(t) - W_m\| \\ &< 2\epsilon_1. \blacksquare\end{aligned}$$

ACKNOWLEDGMENTS

The author would like to thank the referee for pointing out the related results of Kato[16] on continuous variation of the wave operators on the potential and the results of Dollard[17] on adiabatic switching. Sincere thanks are also extended to Dr. Jerome A. Goldstein for his guidance in writing the dissertation upon which this paper is based.

[1]T. Kato, J. Math. Soc. Japan **5**, 208 (1953).
[2]J.A. Goldstein and C.J. Monlezun, "Temporally Inhomogeneous Scattering Theory II: Approximation Theory and Second Order Equations," in preparation.
[3]J.M. Jauch, Helv. Phys. Acta. **31**, 553 (1969).
[4]C.J. Monlezun, "Temporally Inhomogeneous Scattering Theory," J. Math. Anal. Appl., to appear.
[5]J.D. Dollard, J. Math. Phys. **5**, 729 (1964).
[6]J.D. Dollard, Rocky Mt. J. Math. **1**, 5 (1971).
[7]W. Amrein, Ph.A. Martin, and B. Misra, Helv. Phys. Acta. **43**, 313 (1970).
[8]R. Lavine, J. Func. Anal. **5**, 368 (1970).
[9]L.E. Thomas, J. Func. Anal. **15**, 364 (1974).
[10]J.H. Hendrickson, Ph.D. dissertation, Tulane University (1974).
[11]P. Alsholm, Ph.D. dissertation, University of California, Berkeley (1972).
[12]I.W. Herbst, Comm. Math. Phys. **35**, 193 (1974).
[13]P. Alsholm and T. Kato, "Scattering with Long Range Potentials," in *Proceedings of the Symposium on Pure Mathematics of the American Mathematical Society* (Am. Math. Soc., Providence, R.I., 1971), Vol. XXIII, pp. 393–99.
[14]J.A. Goldstein, J. Math. Soc. Japan **24**, 558 (1972).
[15]A. Friedman, *Partial Differential Equations* (Holt, Rinehart, and Winston, New York, 1969).
[16]T. Kato, *Perturbation Theory for Linear Operators* (Springer, New York, 1966), p. 551.
[17]J.P. Dollard, J. Math. Phys. **7**, 802 (1966).

Studies in the Kerr–Newman metric

S. K. Bose

Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
(Received 30 October 1974)

The Kerr–Newman metric is analyzed according to the null tetrad formalism. The components of the Weyl and the Ricci tensors are calculated and these tensors are then projected on a suitable null-tetrad basis. The spin coefficients of Newman and Penrose are also calculated. These results are applied to obtain the equations of gravitational and neutrino perturbations in the Kerr–Newman metric.

I. INTRODUCTION

In this note we shall work out some standard properties of the Kerr—Newman metric.[1] First the components of the Riemann, the Ricci, and the Weyl conformal tensors are calculated. Next the Weyl and the Ricci tensors are analyzed according to the null-tetrad formalism due to Newman and Penrose.[2] A tetrad basis is chosen such that its two real null vectors are the repeated principal null vectors of the Weyl tensor. The twelve spin coefficients defined by Newman and Penrose[3] are also calculated. These results are summarized in the next Sec. II. It should be noted that not all results of Sec. II are new. In particular, the expressions for the tetrad projections of the Maxwell tensor and hence also of the Ricci tensor (with a different choice of tetrad basis than in this paper) have already been given in the paper of Newman *et al.*[1] But the rest of the material in Sec. II is new. Finally, these results are applied to study the equations governing the neutrino and the gravitational perturbations in the Kerr—Newman geometry. Our calculation here closely parallels the work of Teukolsky[3] who has given an elegant derivation of the equations governing perturbations in an uncharged Kerr metric. It is found that the neutrino equation for the present case is a simple generalization of the corresponding equation of Teukolsky, but the equation for gravitational perturbation is considerably more involved. In fact, a decoupled equation does not result for the latter in contrast to the situation in uncharged Kerr metric.[3]

II. ANALYSIS OF THE KERR-NEWMAN METRIC IN TERMS OF NULL-TETRAD FORMALISM

The components of the Riemann, the Ricci, and the Weyl conformal tensors for the Kerr—Newman metric are listed in the Appendix. From these expressions we can calculate the tetrad projections of these tensors once a choice of the tetrad is made. We shall consider a tetrad $\{l^\mu, n^\mu, m^\mu, m^{*\mu}\}$ of null vectors satisfying the usual conditions

$$l_\mu n^\mu = -m_\mu m^{*\mu} = 1, \quad l_\mu m^\mu = n_\mu m^\mu = 0. \tag{1}$$

Then

$$g^{\mu\nu} = l^\mu n^\nu + n^\mu l^\nu - m^\mu m^{*\nu} - m^{*\mu} m^\nu. \tag{2}$$

The real vectors l^μ and n^μ will be chosen to be the double principal null vectors of the Weyl tensor. In the null coordinate (see Appendix) the explicit form of the tetrad is then[4]

$$l^\mu = \delta^\mu_1, \quad n^\mu = \frac{r^2+a^2}{\Sigma}\delta^\mu_0 - \frac{\Delta}{2\Sigma}\delta^\mu_1 + \frac{a}{\Sigma}\delta^\mu_3,$$
$$m^\mu = \frac{1}{\sqrt{2}\,(r+ia\cos\theta)}\left\{ia\sin\theta\,\delta^\mu_0 + \delta^\mu_2 + \frac{i}{\sin\theta}\delta^\mu_3\right\}. \tag{3}$$

In the above, $\Sigma = r^2 + a^2\cos^2\theta$ and $\Delta = r^2 + a^2 + e^2 - 2mr$. $m^{*\mu}$ is the complex conjugate of m^μ. Using the above tetrad (3) the projections of the various tensors (given in the Appendix) can be calculated by straightforward calculations. The result of this exercise for the Weyl tensor is

$$\Psi_0 \equiv -C_{\mu\nu\lambda\sigma} l^\mu m^\nu l^\lambda m^\sigma = 0, \quad \Psi_1 \equiv -C_{\mu\nu\lambda\sigma} l^\mu n^\nu l^\lambda m^\sigma = 0, \tag{4}$$
$$\Psi_3 \equiv -C_{\mu\nu\lambda\sigma} m^{*\mu} n^\nu l^\lambda n^\sigma = 0, \quad \Psi_4 \equiv -C_{\mu\nu\lambda\sigma} m^{*\mu} n^\nu m^{*\lambda} n^\sigma = 0,$$

$$\Psi_2 \equiv -C_{\mu\nu\lambda\sigma} m^{*\mu} n^\nu l^\lambda m^\sigma = -\frac{1}{(r-ia\cos\theta)^3(r+ia\cos\theta)}\left[m(r+ia\cos\theta) - e^2\right]. \tag{5}$$

Thus the null vectors l^μ and n^μ given by Eq. (3) are along the repeated principal null direction of the Weyl tensor. The tetrad components of the Ricci tensor are similarly calculated:

$$\Phi_{00} \equiv -\tfrac{1}{2}R_{\mu\nu} l^\mu l^\nu = 0, \quad \Phi_{01} \equiv -\tfrac{1}{2}R_{\mu\nu} l^\mu m^\nu \equiv \Phi^*_{10} = 0,$$
$$\Phi_{02} \equiv -\tfrac{1}{2}R_{\mu\nu} m^\mu m^\nu \equiv \Phi^*_{20} = 0, \quad \Phi_{22} \equiv -\tfrac{1}{2}R_{\mu\nu} n^\mu n^\nu = 0, \tag{6}$$
$$\Phi_{12} \equiv -\tfrac{1}{2}R_{\mu\nu} n^\mu m^\nu \equiv \Phi^*_{21} = 0, \quad \Phi_{11} \equiv -\tfrac{1}{4}R_{\mu\nu}(l^\mu n^\nu + m^\mu m^{*\nu}) = \frac{e^2}{2\Sigma^2}.$$

Finally, the tetrad components of the electromagnetic field tensor $F_{\mu\nu}$ are the following:

$$\Phi_0 \equiv F_{\mu\nu} l^\mu m^\nu = 0, \quad \Phi_2 \equiv F_{\mu\nu} m^{*\mu} n^\nu = 0,$$
$$\Phi_1 \equiv \tfrac{1}{2}F_{\mu\nu}(l^\mu n^\nu + m^{*\mu} m^\nu) = \frac{e}{2}\,\frac{1}{(r-ia\cos\theta)^2}. \tag{7}$$

Thus l^μ and n^μ are also the principal null vectors of the Maxwell tensor.

Newman and Penrose have defined twelve spin coefficients. These are next calculated using the tetrad of Eq. (3) with the following result:

$$\kappa \equiv l_{\mu;\nu} m^\mu l^\nu = 0, \quad \nu \equiv -n_{\mu;\nu} m^{*\mu} n^\nu = 0,$$
$$\sigma \equiv l_{\mu;\nu} m^\mu m^\nu = 0, \quad \lambda \equiv -n_{\mu;\nu} m^{*\mu} m^{*\nu} = 0,$$

$$\epsilon \equiv \tfrac{1}{2}(l_{\mu;\nu}n^\mu l^\nu - m_{\mu;\nu}m^{*\mu}l^\nu) = 0,$$

$$\rho \equiv l_{\mu;\nu}m^\mu m^{*\nu} = -1/(r - ia\cos\theta),$$

$$\tau \equiv l_{\mu;\nu}m^\mu n^\nu = -\frac{ia\sin\theta}{\sqrt{2}\,\Sigma}, \quad \pi \equiv -n_{\mu;\nu}m^{*\mu}l^\nu$$

$$= \frac{ia\sin\theta}{\sqrt{2}\,(r - ia\cos\theta)^2},$$

$$\beta \equiv \tfrac{1}{2}(l_{\mu;\nu}n^\mu m^\nu - m_{\mu;\nu}m^{*\mu}m^\nu) = \frac{\cot\theta}{2\sqrt{2}(r + ia\cos\theta)}, \tag{8}$$

$$\alpha \equiv \tfrac{1}{2}(l_{\mu;\nu}n^\mu m^{*\nu} - m_{\mu;\nu}m^{*\mu}m^{*\nu}) = \pi - \beta^*,$$

$$\mu \equiv -n_{\mu;\nu}m^{*\mu}m^\nu = -\Delta/2\Sigma(r - ia\cos\theta),$$

$$\gamma \equiv \tfrac{1}{2}(l_{\mu;\nu}n^\mu n^\nu - m_{\mu;\nu}m^{*\mu}n^\nu) = \mu + (r - m)/2\Sigma.$$

It is noted that the effect of charge e is present in only two spin coefficients μ and γ and that too through the function Δ. The rest of the spin coefficients are identical with those for uncharged Kerr metric. The vanishing of the coefficients κ, σ, λ and ν is a special instance of a theorem due to Goldberg and Sachs[5] proved originally for algebraically specialized vacuum metrics. The vanishing of ϵ is due to the choice of tetrad Eq. (3).[6] In the remainder of this paper we shall apply the results of this section in order to study the equations for neutrino and gravitational perturbations.

III. EQUATIONS GOVERNING PERTURBATIONS AROUND THE KERR-NEWMAN METRIC

We shall consider equations governing the neutrino test fields and the gravitational perturbations (linearized theory) in a manner closely following the treatment of Teukolsky.[3] A key role in these discussions is played by the following commutation relation

$$[D - (p+1)\epsilon + \epsilon^* + q\rho - \rho^*](\delta - p\beta + q\tau) - [\delta - (p+1)\beta - \alpha^* + \pi^* + q\tau](D - p\epsilon + q\rho) = 0, \tag{9}$$

where p and q are any two constants, $D = l^\mu \partial/\partial x^\mu$ and $\delta = m^\mu \partial/\partial x^\mu$. Equation (9) was derived by Teukolsky[3] for any type-D vacuum metric. Here we note that Eq. (9) is valid also in the present case. This is because the relevant Newman–Penrose equations, from which Eq. (9) is derived, are the same in the present case as with vacuum-type D metrics due to the fact that none of them involves the quantity Φ_{11} which is the only non-vanishing component of the Ricci tensor as we have seen in the preceding section. To facilitate comparison with the work of Teukolsky,[3] the final form of the perturbation equations to be derived below will be written out in the Boyer–Lindquist coordinate. In this coordinate the Kerr–Newmann metric has the form[7]:

$$d\tau^2 = \left(1 - \frac{2mr - e^2}{\Sigma}\right)dt^2 - \frac{\Sigma}{\Delta}dr^2 - \Sigma\,d\theta^2 + \frac{2a\sin^2\theta}{\Sigma}(2mr - e^2)\,dt\,d\phi - \sin^2\theta\left[r^2 + a^2 + \frac{a^2\sin^2\theta}{\Sigma}(2mr - e^2)\right]d\phi^2 \tag{10}$$

and the connection of the above with the null coordinate is

$$dt = du + \frac{r^2 + a^2}{\Delta}dr, \quad d\phi = d\hat{\phi} + \frac{a}{\Delta}dr, \quad r = r, \quad \theta = \theta. \tag{11}$$

The tetrad of Eq. (3) when written in the Boyer–Lindquist coordinate has $[t, r, \theta, \phi]$ components

$$l^\mu = \left[\frac{r^2 + a^2}{\Delta}, 1, 0, \frac{a}{\Delta}\right], \quad n^\mu = [r^2 + a^2, -\Delta, 0, a]/2\Sigma,$$
$$m^\mu = [ia\sin\theta, 0, 1, i/\sin\theta]/[\sqrt{2}(r + ia\cos\theta)]. \tag{12}$$

The spin coefficients and the tetrad projections of the various tensors of interest are, of course, the same in both these coordinates. We can now begin to consider perturbation equations. The equation for the neutrino is the simplest and will be treated first.

A. The neutrino equation

The sourceless neutrino equation in the notation of Ref. 3 is

$$(\delta^* - \alpha + \pi)\chi_0 = (D - \rho + \epsilon)\chi_1, \tag{13}$$

$$(\Delta + \mu - \gamma)\chi_0 = (\delta + \beta - \tau)\chi_1, \tag{14}$$

when χ_0 and χ_1 are the projections of the two component spinors on suitable dyad legs.[8] Treat the neutrino as a test field. Decoupled equation for χ_0 then follows from (13), (14), and Eq. (9) with $p = -1$, $q = -1$:

$$[(D + \epsilon^* - \rho - \rho^*)(\Delta - \gamma + \mu) - (\delta - \alpha^* - \tau + \pi^*) \times (\delta^* - \alpha + \pi)]\chi_0 = 0. \tag{15}$$

The equation for χ_1 follows from above under the interchange $l \leftrightarrow n$, $m \leftrightarrow m^*$. These equation when written out in the Boyer–Lindquist coordinate become

$$\left(\frac{(r^2 + a^2)^2}{\Delta} - a^2\sin^2\theta\right)\frac{\partial^2\Psi}{\partial t^2} + \frac{2a}{\Delta}(2mr - e^2)\frac{\partial^2\Psi}{\partial t\,\partial\phi} + \left(\frac{a^2}{\Delta} - \frac{1}{\sin^2\theta}\right)\frac{\partial^2\Psi}{\partial\phi^2}$$
$$- \Delta^{-s}\frac{\partial}{\partial r}\,\Delta^{s+1}\frac{\partial\Psi}{\partial r} - \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)$$
$$- 2s\left(\frac{a(r - m)}{\Delta} + \frac{i\cos\theta}{\sin^2\theta}\right)\frac{\partial\Psi}{\partial\phi} \tag{16}$$
$$- 2s\left(\frac{m(r^2 - a^2) - e^2r}{\Delta} - r - ia\cos\theta\right)\frac{\partial\Psi}{\partial t}$$
$$+ (s^2\cot^2\theta - s)\Psi = 0.$$

In the above, $s = 1/2$ when $\Psi = \chi_0$ and $s = -1/2$ when $\Psi = \rho^{-1}\chi_1$. The quantity Δ in Eq. (16) stands for $\Delta = r^2 + a^2 + e^2 - 2mr$. Thus, Eq. (16) is a simple generalization of the neutrino equation due to Teukolsky.[3] From the work of Ref. 3 we may further conclude that Eq. (16) is separable in the Boyer–Lindquist coordinate.

B. Equation of gravitational perturbation

The desired equations follow at once from the relevant Newman-Penrose equation, the Bianchi identi-

ties,[9] and the knowledge of the unperturbed metric in Sec. II.

$$(\delta^* - 4\alpha + \pi)\Psi_0^B - (D - 4\rho - 2\epsilon)\Psi_1^B - 3\kappa^B\Psi_2 = (\delta + \pi^* - 2\alpha^* - 2\beta)\Phi_{00}^B - (D - 2\epsilon - 2\rho^*)\Phi_{01}^B - 2\kappa^B\Phi_{11}, \tag{17}$$

$$(\Delta - 4\gamma + \mu)\Psi_0^B - (\delta - 4\tau - 2\beta)\Psi_1^B - 3\sigma^B\Psi_2 = (\delta + 2\pi^* - 2\beta)\Phi_{01}^B - (D - 2\epsilon + 2\epsilon^* - \rho^*)\Phi_{02}^B + 2\sigma^B\Phi_{11}, \tag{18}$$

$$(D - \rho - \rho^* - 3\epsilon + \epsilon^*)\sigma^B - (\delta - \tau + \pi^* - \alpha^* - 3\beta)\kappa^B - \Psi_0^B = 0. \tag{19}$$

In the above we have followed the standard practice of denoting a perturbed quantity with a superscript B. Quantities without a superscript denote their unperturbed values. Using Eq. (19), the commutation relation (9) with $p=2$, $q=-4$, and the equations for unperturbed Weyl tensor,

$$D\Psi_2 = \rho(3\Psi_2 + 2\Phi_{11}), \quad \delta\Psi_2 = \tau(3\Psi_2 - 2\Phi_{11}), \tag{20}$$

it is possible to eliminate Ψ_1^B from (17) and (18). The resulting equation for Ψ_0^B is

$$[(\delta - 3\beta - \alpha^* + \pi^* - 4\tau)(\delta^* - 4\alpha + \pi) - (D - 3\epsilon + \epsilon^* - 4\rho - \rho^*) \times (\Delta - 4\gamma + \mu) + 3\Psi_2 + 2\Phi_{11}]\Psi_0^B = T - 4\Phi_{11}[(\delta - 3\beta - \alpha^*)\kappa^B + (\rho + \rho^*)\sigma^B] \tag{21}$$

with

$$T = (\delta - 3\beta - \alpha^* + \pi^* - 4\tau)[(\delta + \pi^* - 2\alpha^* - 2\beta)\Phi_{00}^B - (D - 2\epsilon - 2\rho^*)\Phi_{01}^B] - (D - 3\epsilon + \epsilon^* - 4\rho - \rho^*) \times [(\delta + 2\pi^* - 2\beta)\Phi_{01}^B - (D - 2\epsilon + 2\epsilon^* - \rho^*)\Phi_{02}^B]. \tag{22}$$

The presence of terms involving perturbations in the spin coefficients κ^B and σ^B make Eq. (32) so much more difficult than in the case of uncharged Kerr metric,[3] where these terms are absent. In fact, the difficulty persists even in the limiting case of zero rotation of the source (Reissner–Nordström limit). It is possible to simplify things a bit further. We have the freedom to subject Eq. (21) to infinitesimal tetrad rotations. By a suitable choice of the latter we can make $\kappa^B = 0$. When written out in Boyer–Lindquist coordinate, the resulting Eq. (21) now becomes

$$\left(\frac{(r^2+a^2)^2}{\Delta} - a^2\sin^2\theta\right)\frac{\partial^2\Psi_0^B}{\partial t^2} + \frac{2a(2mr-e^2)}{\Delta}\frac{\partial^2\Psi_0^B}{\partial t\,\partial\phi} + \left(\frac{a^2}{\Delta} - \frac{1}{\sin^2\theta}\right)\frac{\partial^2\Psi_0^B}{\partial\phi^2} - \frac{1}{\Delta^2}\frac{\partial}{\partial r}\left(\Delta^3\frac{\partial\Psi_0^B}{\partial r}\right) - \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi_0^B}{\partial\theta}\right) - 4\left(\frac{a(r-m)}{\Delta} + \frac{i\cos\theta}{\sin^2\theta}\right)\frac{\partial\Psi_0^B}{\partial\phi} - 4\left(\frac{m(r^2-a^2)-e^2r}{\Delta} - r - ia\cos\theta\right) \times \frac{\partial\Psi_0^B}{\partial t} + \left(4\cot^2\theta - 2 - \frac{2e^2}{\Sigma}\right)\Psi_0^B = -2\Sigma\,T - \frac{8e^2r}{\Sigma^2}\sigma^B. \tag{23}$$

Similarly, with $\kappa^B = 0$ Eq. (19) becomes

$$\left(\frac{r^2+a^2}{\Delta}\frac{\partial}{\partial t} + \frac{\partial}{\partial r} + \frac{a}{\Delta}\frac{\partial}{\partial\phi} + \frac{2r}{\Sigma}\right)\sigma^B - \Psi_0^B = 0. \tag{24}$$

Equations (23) and (24) are the equations for gravitational perturbation. A similar set of equations can be obtained for Ψ_4^B from Eq. (21) via the interchange $l \leftrightarrow n$, $m \leftrightarrow m^*$. Let us now consider the source term T which occurs in Eq. (23). The general expression for T is given by Eq. (22). If, however, we restrict ourselves to electrovac perturbations, then $\Phi_{00}^B = \Phi_{02}^B = 0$ and $\Phi_{01}^B = 2\Phi_1^*\Phi_0^B$ and the expression for T undergoes appropriate simplification. It is not surprising that for electrovac perturbations Ψ_0^B is coupled to perturbed Maxwell tensor Φ_0^B. It also seems possible to consider a further restrictive class of perturbations, namely, those with $\Phi_0^B = 0$, i.e., $T = 0$. These are purely gravitational perturbations unaccompanied by electromagnetic perturbations. On the other hand, an examination of the Maxwell's equations for the present problem reveals that it is impossible to consider perturbations in the electromagnetic field without, at the same time, allowing metric perturbations. This is because the Maxwell's equations couple the unperturbed electromagnetic tensor Φ_1 with first-order perturbations in the spin coefficients ρ^B, τ^B, π^B, and μ^B as well as with perturbations in the Newman–Penrose operators D^B, Δ^B, and δ^B. These arise from perturbations in the tetrad system and hence are connected with metric perturbations. Without further restrictions the Maxwell's equations for the present problem are thus rather involved, which is the reason why they are not considered further in this paper.

ACKNOWLEDGMENTS

The author thanks Professors W.D. McGlinn and W.R. Johnson for conversations and encouragement. He is also much indebted to Dr. M.Y. Wang and Mr. C.H. Lee for checking some of these calculations.

APPENDIX

In the null coordinate the Kerr–Newman metric is[1]

$$d\tau^2 = g_{\mu\nu}\,dx^\mu\,dx^\nu = \left(1 - \frac{2mr-e^2}{\Sigma}\right)du^2 + 2\,du\,dr + \frac{2a\sin^2\theta}{\Sigma}(2mr-e^2)\,du\,d\hat{\phi} - 2a\sin^2\theta\,dr\,d\hat{\phi} - \Sigma\,d\theta^2 - \sin^2\theta \times \left(r^2 + a^2 + \frac{a^2\sin^2\theta}{\Sigma}(2mr-e^2)\right)d\hat{\phi}^2. \tag{A1}$$

We follow the notation $x^0 = u$, $x^1 = r$, $x^2 = \vartheta$, $x^3 = \hat{\phi}$. The components of the Riemann tensor can be calculated from (A1) after a straightforward but extremely lengthy calculation. The details of this calculation will not be reported here, but will be supplied to the interested reader upon request. Here only the final result will be quoted. Define the Riemann tensor as

$$V_{\rho;\nu;\mu} - V_{\rho;\mu;\nu} = R_{\mu\nu\rho\sigma}V^\sigma \tag{A2}$$

for any vector V. The components $R_{\mu\nu\rho\sigma}$ calculated from (A1) are then the following:

$$R_{0112} = R_{0203} = R_{0323} = R_{1212} = R_{1231} = 0,$$

$$R_{0101}=\frac{1}{\Sigma^3}[2mr(r^2-3a^2\cos^2\theta)-e^2(3r^2-a^2\cos^2\theta)],$$

$$R_{0102}=\frac{3a^2\sin 2\theta}{2\Sigma^3}[m\Sigma-2r(2mr-e^2)],$$

$$R_{0103}=\frac{a\sin^2\theta}{\Sigma^3}[mr\Sigma+(2mr-e^2)(a^2\cos^2\theta-r^2)],$$

$$R_{0113}=a\sin^2\theta R_{0101},\quad R_{0123}=\frac{2(r^2+a^2)+a^2\sin^2\theta}{3a}R_{0102},$$

$$R_{0212}=\frac{\Sigma}{a\sin^2\theta}R_{0103},\quad R_{0213}=\frac{r^2+a^2+2a^2\sin^2\theta}{3a}R_{0102},$$

$$\begin{aligned}R_{0202}=\frac{1}{\Sigma^3}\{&(2mr-e^2)^2(r^2-a^2\cos^2\theta)-(2mr-e^2)[mr\Sigma\\&+r^4+2r^2a^2\sin^2\theta-a^4\cos^4\theta-4a^4\sin^2\theta\cos^2\theta]\\&+mr\Sigma(r^2+a^2)\}\end{aligned}$$

$$\begin{aligned}R_{0223}=\frac{a\sin^2\theta}{\Sigma^3}\{&(2mr-e^2)^2(r^2-a^2\cos^2\theta)-(2mr-e^2)\\&\times[mr\Sigma+2(r^2+a^2)(r^2-2a^2\cos^2\theta)]\\&+mr\Sigma(r^2+a^2)\},\end{aligned}\tag{A3}$$

$$R_{0303}=\frac{\Delta}{a}R_{0103},\quad R_{0312}=-\frac{\Sigma}{3a}R_{0102},$$

$$R_{0313}=\frac{r^2+a^2}{a}R_{0103},\quad R_{1223}=\Sigma R_{0103},$$

$$R_{1313}=a\sin^2\theta R_{0113},\quad R_{2331}=-\sin^2\theta(r^2+a^2)R_{0102},$$

$$\begin{aligned}R_{2323}=&\frac{a^2\sin^4\theta}{\Sigma^3}(2mr-e^2)^2(r^2-a^2\cos^2\theta)\\&+\frac{a^2\sin^4\theta}{\Sigma^2}mr(r^2+a^2)\\&-(2mr-e^2)\frac{\sin^2\theta}{\Sigma^3}\{(r^2+a^2)[(r^2+a^2)\\&\times(r^2-4a^2\cos^2\theta)+a^2(r^2+a^2\cos^4\theta)]\\&+mra^2\sin^2\theta\Sigma\}.\end{aligned}$$

In the above $\Sigma=r^2+a^2\cos^2\theta$ and $\Delta=r^2+a^2+e^2-2mr$. From the Riemann tensor we compute the components of the Ricci tensor

$$\begin{aligned}&R_{\mu\nu}(=g^{\lambda\kappa}R_{\lambda\mu\nu\kappa}),\\&R_{11}=R_{12}=R_{02}=R_{23}=0,\\&R_{01}=-e^2/\Sigma^2,\quad R_{13}=-a\sin^2\theta R_{01},\quad R_{22}=-e^2/\Sigma,\\&R_{00}=-\frac{e^2}{\Sigma^3}[\Delta+a^2\sin^2\theta],\quad R_{03}=-a\sin^2\theta R_{00}+\frac{ae^2\sin^2\theta}{\Sigma^2}\\&R_{33}=-a\sin^2\theta R_{03}-\frac{(r^2+a^2)e^2\sin^2\theta}{\Sigma^2}.\end{aligned}\tag{A4}$$

From the components of the Riemann and the Ricci tensors, we calculate the Weyl tensor:

$$\begin{aligned}C_{\mu\nu\lambda\sigma}=&R_{\mu\nu\lambda\sigma}+\tfrac{1}{2}(g_{\mu\lambda}R_{\nu\sigma}-g_{\mu\sigma}R_{\nu\lambda}+g_{\nu\sigma}R_{\mu\lambda}-g_{\nu\lambda}R_{\mu\sigma}\\&+\tfrac{1}{6}R(g_{\mu\sigma}g_{\nu\lambda}-g_{\mu\lambda}g_{\nu\sigma}),\end{aligned}\tag{A5}$$

$$\begin{aligned}&C_{0112}=C_{0203}=C_{0323}=C_{1212}=C_{1231}=0,\\&C_{0101}=R_{0101}+e^2/\Sigma^2,\quad C_{0102}=R_{0102},\quad C_{0103}=R_{0103},\\&C_{0113}=R_{0113}+\frac{ae^2\sin^2\theta}{\Sigma^2},\quad C_{0123}=R_{0123},\quad C_{0212}=R_{0212},\\&C_{0213}=R_{0213},\quad C_{0202}=R_{0202}+a^2e^2\sin^2\theta/\Sigma^2,\\&C_{0223}=R_{0223}+\frac{ae^2(r^2+a^2)\sin^2\theta}{\Sigma^2},\quad C_{0303}=R_{0303},\\&C_{0312}=R_{0312},\quad C_{0313}=R_{0313},\quad C_{1223}=R_{1223},\\&C_{1313}=R_{1313}+a^2e^2\sin^4\theta/\Sigma^2,\quad C_{2331}=R_{2331},\\&C_{2323}=R_{2323}+e^2(r^2+a^2)^2\sin^2\theta/\Sigma^2.\end{aligned}\tag{A6}$$

It needs hardly to be remarked that not all of the 21 components of $C_{\mu\nu\lambda\sigma}$ are linearly independent, but only 10 are. Also, the Ricci tensors of (A4) satisfy the constraint $R\equiv R^\lambda_\lambda=0$, as they must. Similarly, components of the Riemann tensor (A3) satisfy the required identity $R_{0123}+R_{0312}+R_{0231}=0$. From the above expressions for the Weyl and the Ricci tensors, we can calculate their tetrad projections. When this is done with the tetrad of Eq. (3) of text, we get the results quoted in Sec. II. We conclude this section with one final remark. We have not quoted the components of the Maxwell tensor. These may be calculated from the formula

$$F_{\mu\nu}=\Phi_1(n_\mu l_\nu-n_\nu l_\mu+m_\mu m^*_\nu-m_\nu m^*_\mu)+\text{c.c.}\tag{A7}$$

when c.c. denotes complex conjugate of the preceding term and expressions for Φ_1 and the vectors l, n, m are given in Sec. II. The components of $F_{\mu\nu}$ so calculated then agree with expressions given in standard references.[10]

[1]E.T. Newman, E. Couch, K. Chinapared, A. Exton, A. Prakash, and R. Torrence, J. Math. Phys. **6**, 918 (1965).
[2]E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).
[3]S.A. Teukolsky, Astrophys. J. **185**, 635 (1973); also, Phys. Rev. Lett. **29**, 1114 (1972).
[4]The tetrad of Eq. (3) is related to that in Ref. 1 via a rotation.
[5]J. Goldberg and R. Sachs, Acta Phys. Polon. **22**, Suppl. 13 (1962).
[6]W. Kinnersley, J. Math. Phys. **10**, 1195 (1969).
[7]R.H. Boyer and R.W. Lindquist, J. Math. Phys. **8**, 265 (1967); B. Carter, Phys. Rev. **174**, 1559 (1968).
[8]The operator Δ which occurs in Eqs. (14), (15), (18), and (21) (and *only* in these equations) stands for the Newman–Penrose operator $n^\mu\,\partial/\partial x^\mu$. Throughout the rest of this paper the symbol Δ denotes the quantity $r^2+a^2+e^2-2mr$, and no occasion should arise to confuse between the two.
[9]See F.A.E. Pirani, *Lectures on General Relativity*, Brandeis Summer Institute in Theoretical Physics (Prentice-Hall, Englewood Cliffs, N.J., 1964).
[10]C.W. Misner, K.S. Thorne, and J.A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973), p. 878. Also, B. Carter, Ref. 7.

Mathematical aspects of kinetic model equations for binary gas mixtures

David E. Greene

Department of Mathematics, Air Force Institute of Technology, Wright-Patterson Air Force Base, Ohio
(Received 8 April 1974)

A system of integrodifferential equations, which has a structure similar to the Boltzmann equations for a binary gas mixture and which qualitatively describes wave propagation, is investigated. The Oppenheim model is used and a linear initial-value problem is considered. The initial-value problem is shown to be well set mathematically with certain specifications on the initial distribution functions. Justification is made for the use of Fourier–Laplace transforms. A discussion is made of the dispersion relation and its analytic continuation. The roots $\sigma(k)$ of the dispersion relation are shown to lie in three distinct regions of the σ plane: the hydrodynamic region, the semihydrodynamic region, and the rarefied region. It is established that the roots $\sigma(k)$ are bounded by $-1+\delta < \mathrm{Re}\sigma \leq 0$ under the assumption of plane-wave solutions which implies that the system is stable and that plane waves cease to exist if $\mathrm{Re}\sigma \leq -1+\delta$.

1. INTRODUCTION

While many issues of the Boltzmann equation remain unresolved, very substantial progress has been made in the study of kinetic model equations for a simple gas—a gas composed of like molecules. These model equations are integrodifferential equations which qualitatively represent the Boltzmann equation.

In this investigation the theory for simple gas kinetic models (particularly the work of Sirovich and Thurber[1]) is extended to kinetic models for gas mixtures. This study reveals significant physical and mathematical features which result from the interaction of the component gases as described by the kinetic models.

The Oppenheim model[2] was selected as the focus of this study because this model (1) generates the conservation equations, (2) satisfies an H-theorem, and (3) has a relatively simple form. This model is representative of other kinetic models and the theory developed, in principle, applies to other models as well.

2. A KINETIC MODEL FOR BINARY GAS MIXTURES

The Oppenheim model

$$\frac{df_1}{dt}=\frac{\partial f_1}{\partial t}+\xi\cdot\frac{\partial f_1}{\partial x}+\frac{X_1}{m_1}\cdot\frac{\partial f_1}{\partial \xi}=\nu_{11}(f_1^0-f_1)+\nu_{12}(f_1^{12}-f_1),$$

$$\frac{df_2}{dt}=\frac{\partial f_2}{\partial t}+\xi'\cdot\frac{\partial f_2}{\partial x}+\frac{X_2}{m_2}\cdot\frac{\partial f_2}{\partial \xi'}=\nu_{12}(f_2^{12}-f_2)+\nu_{22}(f_2^0-f_2) \tag{2.1}$$

is a system of coupled integrodifferential equations for the distribution functions of the component gases. The molecular velocities, masses and external forces for each gas are, respectively, ξ and ξ', m_1 and m_2, and X_1 and X_2. The terms ν_{ij} are the collision frequencies of the molecules; ν_{11} and ν_{22} are the self-collision frequencies and ν_{12} is the cross-collision frequency. The moments and collision terms are defined by

$$\begin{aligned}
&R_i=K/m_i,\\
&n_i=\int f_i\,d\xi,\\
&n_iu_i=\int \xi f_i\,d\xi,\\
&\rho_{12}=m_1n_1+m_2n_2,\\
&\rho_{12}u_{12}=m_1n_1u_1+m_2n_2u_2,\\
&3n_iR_iT_i=\int(\xi-u_i)^2 f_i\,d\xi,\\
&3n_iR_i\bar{T}_i=\int(\xi-u_{12})^2 f_i\,d\xi,\\
&n_{12}=n_1+n_2,\\
&n_{12}T_{12}=n_1\bar{T}_1+n_2\bar{T}_2,
\end{aligned} \tag{2.2}$$

$$f_i^0=\frac{n_i}{(2\pi R_iT_i)^{3/2}}\exp[-(\xi-u_i)^2/2R_iT_i],$$

$$f_i^{12}=\frac{n_i}{(2\pi R_iT_{12})^{3/2}}\exp[-(\xi-u_{12})^2/2R_iT_{12}].$$

In the following analysis the external forces X_i are assumed to be zero.

The system is in equilibrium only if f_1 and f_2 are absolute Maxwellian distributions (this assertion is a consequence of the H-theorem for the model[3]), and we may linearize the model about these distributions. In (2.1) we let

$$\begin{aligned}
&f_i=f^{0i}+g_i,\\
&n_i=n_i^0+\hat{n}_i,\\
&u_i=u_i^0+\hat{u}_i,\\
&T_i=T_i^0+\hat{T}_i,
\end{aligned} \tag{2.3}$$

where f^{0i} are the absolute Maxwellian distributions; the notation ^{0} refers to the equilibrium state; and g_i, $\hat{n}_i$, $\hat{u}_i$, and $\hat{T}_i$ are small perturbations. We assume that $u_1^0=u_2^0=0$, $T_1^0=T_2^0=T^0$ and retain the lowest order perturbation terms. The following dimensionless variables are introduced

$$\begin{aligned}
&\tilde{t}=(\nu_{11}+\nu_{12})t,\\
&\tilde{x}=(\nu_{11}+\nu_{12})x/(R_1T_1^0)^{1/2},\\
&\tilde{u}_i=\hat{u}_i/(R_1T_1^0)^{1/2},\\
&\tilde{n}_i=\hat{n}_i/n_i^0,\\
&\tilde{T}_i=\hat{T}_i/T_i^0,\\
&\tilde{\xi}=\xi/(R_1T_1^0)^{1/2},\\
&\hat{\xi}=\xi'/(R_2T_2^0)^{1/2},
\end{aligned} \tag{2.4}$$

$$\tilde{g}_1 = \frac{(2\pi R_1 T_1^0)^{3/2}}{n_1^0} \exp(\xi^2/2) g_1,$$

$$\tilde{g}_2 = \frac{(2\pi R_2 T_2^0)^{3/2}}{n_2^0} \exp(\hat{\xi}^2/2) g_2.$$

Retaining the same notation for the dimensionless variables as was used for the dimensional variables, we obtain the linear form of the Oppenheim model:

$$\frac{\partial g_1}{\partial t} + \xi \cdot \frac{\partial g_1}{\partial x} + g_1 = n_1 + a_1 \xi \cdot u_1 + a_2 (\tfrac{1}{2}\xi^2 - \tfrac{3}{2}) T_1 + a_3 \xi \cdot u_2 + a_4 (\tfrac{1}{2}\xi^2 - \tfrac{3}{2}) T_2, \tag{2.5}$$

$$\frac{\partial g_2}{\partial t} + \frac{\hat{\xi}}{r} \cdot \frac{\partial g_2}{\partial x} + \mu g_2 = \hat{a}_1 \hat{\xi} \cdot u_1 r + \hat{a}_2 (\tfrac{1}{2}\hat{\xi}^2 - \tfrac{3}{2}) T_1 + \mu n_2 + \hat{a}_3 \hat{\xi} \cdot u_2 r + \hat{a}_4 (\tfrac{1}{2}\hat{\xi}^2 - \tfrac{3}{2}) T_2,$$

which may be written

$$\frac{\partial g_1}{\partial t} + \xi \cdot \frac{\partial g_1}{\partial x} + g_1 = \sum_{n=0}^{N} b_n \phi_n(\xi),$$

$$\frac{\partial g_2}{\partial t} + \frac{\hat{\xi}}{r} \cdot \frac{\partial g_2}{\partial x} + \mu g_2 = \sum_{n=0}^{N} \hat{b}_n \phi_n(\hat{\xi}). \tag{2.6}$$

The terms in (2.6) are defined by

$$r = (m_2/m_1)^{1/2},$$
$$\nu = \nu_{11} + \nu_{12},$$
$$\mu = (\nu_{22} + \nu_{12})/\nu; \tag{2.7}$$

$$b_0 = n_1,$$
$$b_1 = a_1 u_1 + a_3 u_2,$$
$$b_2 = \tfrac{3}{2}(a_2 T_1 + a_4 T_2); \tag{2.8}$$

$$\hat{b}_0 = \mu n_2,$$
$$\hat{b}_1 = r(\hat{a}_1 u_1 + \hat{a}_3 u_2),$$
$$\hat{b}_2 = \tfrac{3}{2}(\hat{a}_2 T_1 + \hat{a}_4 T_2); \tag{2.9}$$

$$a_1 = \frac{\nu_{11}}{\nu} + \frac{\nu_{12}}{\nu} M_1,$$
$$a_2 = \frac{\nu_{11}}{\nu} + \frac{\nu_{12}}{\nu} N_1,$$
$$a_3 = (\nu_{12}/\nu) M_2,$$
$$a_4 = (\nu_{12}/\nu) N_2; \tag{2.10}$$

$$\hat{a}_1 = (\nu_{12}/\nu) M_1,$$
$$\hat{a}_2 = (\nu_{12}/\nu) N_1,$$
$$\hat{a}_3 = \frac{\nu_{22}}{\nu} + \frac{\nu_{12}}{\nu} M_2,$$
$$\hat{a}_4 = \frac{\nu_{22}}{\nu} + \frac{\nu_{12}}{\nu} N_2; \tag{2.11}$$

$$N_1 = n_1^0/(n_1^0 + n_2^0),$$
$$N_2 = n_2^0/(n_1^0 + n_2^0),$$
$$M_1 = m_1 n_1^0/(m_1 n_1^0 + m_2 n_2^0),$$
$$M_2 = m_2 n_2^0/(m_1 n_1^0 + m_2 n_2^0), \tag{2.12}$$

and the functions ϕ_n are the Hermite polynomials: 1, ξ_1, $\frac{1}{3}\xi^2 - 1$, $\cdots$.

We assume that the distribution functions belong to the Hilbert space $\mathcal{H}$ in the velocity variables with inner product

$$(g, f) = \int \frac{\exp(-\xi^2/2)}{(2\pi)^{3/2}} g \bar{f}\, d\xi. \tag{2.13}$$

Since $\{\phi_n\} \in \mathcal{H}$ ($\{\phi_n\}$ is a complete orthogonal set in $\mathcal{H}$[4]), the hydrodynamic perturbation quantities defined by (2.2) and (2.3) may be expressed by inner products. The number density, velocity, and temperature, respectively, for each gas are

$$n_1 = (g_1, \phi_0),$$
$$u_1 = (g_1, \phi_1), \tag{2.14}$$
$$T_1 = (g_1, \phi_2),$$

and

$$n_2 = (g_2, \phi_0),$$
$$u_2 = r^{-1}(g_2, \phi_1), \tag{2.15}$$
$$T_2 = (g_2, \phi_2).$$

While $N = 2$ in the Oppenheim model, it is instructive to generalize the form of the model and allow N to be a finite positive integer.

3. THE INITIAL-VALUE PROBLEM IS WELL SET

Our objective is to show that the system (2.6) with suitable initial conditions is well set mathematically by examining an equivalent system of integral equations. To this end, we introduce

$$G_1 = e^t g_1,$$
$$G_2 = \exp(\mu t) g_2, \tag{3.1}$$

and define

$$A_n = (G_1, \phi_n) = e^t (g_1, \phi_n),$$
$$\hat{A}_n = (G_2, \phi_n) = \exp(\mu t)(g_2, \phi_n). \tag{3.2}$$

The system (2.6) may be written

$$\left(\frac{\partial}{\partial t} + \xi \cdot \frac{\partial}{\partial x}\right) G_1 = \sum_{n=0}^{N} B_n \phi_n(\xi),$$

$$\left(\frac{\partial}{\partial t} + \frac{\hat{\xi}}{r} \cdot \frac{\partial}{\partial x}\right) G_2 = \sum_{n=0}^{N} \hat{B}_n \phi_n(\hat{\xi}), \tag{3.3}$$

where

$$B_0 = A_0,$$
$$B_1 = a_1 A_1 + \frac{a_3}{r} \exp[t(1-\mu)] \hat{A}_1,$$
$$B_2 = \tfrac{3}{2}(a_2 A_2 + a_4 \exp[t(1-\mu)] \hat{A}_2) \tag{3.4}$$

and

$$\hat{B}_0 = \mu \hat{A}_0,$$
$$\hat{B}_1 = r \hat{a}_1 \exp[t(\mu - 1)] A_1 + \hat{a}_3 \hat{A}_1,$$
$$\hat{B}_2 = \tfrac{3}{2}(\hat{a}_2 \exp[t(\mu - 1)] A_2 + \hat{a}_4 \hat{A}_2). \tag{3.5}$$

The initial conditions for this system are

$$G_1(x,\xi,t=0)=G_1^0(x,\xi)=g_1(x,\xi,t=0),$$
$$G_2(x,\hat{\xi},t=0)=G_2^0(x,\hat{\xi})=g_2(x,\hat{\xi},t=0). \tag{3.6}$$

By formal integration of (3.3) we obtain the system of integral equations

$$G_1=G_1^0(x-\xi t,\xi)+\int_0^t\sum_{n=0}^{N}B_n(x^*,s)\phi_n(\xi)\,ds,$$
$$G_2=G_2^0\left(x-\frac{\hat{\xi}}{\gamma}t,\hat{\xi}\right)+\int_0^t\sum_{n=0}^{N}\hat{B}_n(\tilde{x}^*,s)\phi_n(\hat{\xi})\,ds, \tag{3.7}$$

where

$$x^*=x-\xi(t-s) \tag{3.8}$$

and

$$\tilde{x}^*=x-(\hat{\xi}/\gamma)(t-s). \tag{3.9}$$

We take moments of (3.7), replacing the umbral variable $\hat{\xi}$ by ξ, and obtain

$$A_m=(G_1,\phi_m)=\int_\xi \omega\phi_m G_1^0(x-\xi t,\xi)\,d\xi$$
$$+\int_0^t\int_\xi\sum_{n=0}^{N}B_n(x^*,s)\omega\phi_m\phi_n\,d\xi\,ds,$$
$$\hat{A}_m=(G_2,\phi_m)=\int_\xi\omega\phi_m G_2^0\left(x-\frac{\xi}{\gamma}t,\xi\right)d\xi \tag{3.10}$$
$$+\int_0^t\int_\xi\sum_{n=0}^{N}\hat{B}_n(\tilde{x}^*,s)\omega\phi_m\phi_n\,d\xi\,ds.$$

We define

$$F(x,t)=(A_0,\ldots,A_N,\hat{A}_0,\ldots,\hat{A}_N)$$

and denote by F^0 the vector whose components are moments of $G_1^0(x-\xi t,\xi)$ and $G_2^0(x-(\xi/\gamma)t,\xi)$. The mapping (3.10) may be written

$$\mathcal{F}=\mathcal{L}(F)=\int_0^t\int_\xi M(\xi,s)F[(x^*,\tilde{x}^*)s]\,d\xi\,ds+F^0 \tag{3.11}$$

where $M(\xi,s)$ is a $(2N+2)\times(2N+2)$ matrix of functions.

Let S be the space of all functions $f=f(x,t)$ such that $\partial f/\partial x_j$, $j=1,2,3$, exist and are continuous functions of t and x for all $t\geq 0$; and for each f there exists a continuous function $M(t)$ such that $|f|$ and $|\partial f/\partial x_j|\leq M(t)$ for all $t\geq 0$. We denote by S^{2N+2} the $(2N+1)$-fold direct product of S with itself.

We require that (1) $G_i^0(x,\xi)\in C^1$ in x, (2) $G_i^0(x,\xi)\in C^0$ in ξ, and (3) G_i^0 and $\nabla G_i^0=O(\exp|\xi|^\alpha)$ uniformly in x for some $\alpha<2$. For G_i^0 thus specified, the moments of $G_1^0(x-\xi t,\xi)$ and $G_2^0(x-(\hat{\xi}/\gamma)t,\xi)$, designated by A_n^0 and $\hat{A}_n^0$, belong to S and hence $F^0=(A_0^0,\ldots,A_N^0,\hat{A}_0,\ldots,\hat{A}_N^0)$ belongs to S^{2N+2}. Further, for the specified initial distributions, the mapping $\mathcal{L}$ defined by (3.11) is a mapping from S^{2N+2} into S^{2N+2}.

We define

$$|F|_x=\sum_{n=0}^{N}\left(\max_x|A_n|+\max_x|\hat{A}_n|\right)$$
$$+\sum_{n=0}^{N}\left(\sum_{j=1}^{3}\max_x\left|\frac{\partial A_n}{\partial x_j}\right|+\sum_{j=1}^{3}\max_x\left|\frac{\partial\hat{A}_n}{\partial x_j}\right|\right)$$

and introduce a norm for S^{2N+2}

$$\|F\|_{t_0}=\max_{0\leq t\leq t_0}|F|_x.$$

Then, for $0\leq\mu<1$,

$$\|\mathcal{L}(F)-\mathcal{L}(F')\|_t=\|\int_0^t\int_\xi M(\xi,s)\{F[(x^*,\tilde{x}^*),s]$$
$$-F[(x^*,\tilde{x}^*),s]\}\,d\xi\,ds\|_t \tag{3.12}$$
$$\leq\int_0^t Pe^{s(1-\mu)}\|F-F'\|_t\,ds,$$

where P is a finite positive constant

$$P=C\sum_{m,n=0}^{N}\int_\xi\omega|\phi_m||\phi_n|\,d\xi \tag{3.13}$$

with C an upper bound for the absolute values of the constant coefficients in the matrix M. Therefore,

$$\|\mathcal{L}(F)-\mathcal{L}(F')\|_t\leq\frac{P}{1-\mu}[\exp(t(1-\mu))-1]\|F-F'\|_t. \tag{3.14}$$

Since there exists a T such that

$$0<\frac{P}{1-\mu}[\exp(T(1-\mu))-1]<1,$$

we have a contraction mapping for $t\leq T$. If $\mu=1$ then from (3.12), $T<1/P$ provides a contraction mapping. Therefore, by the contraction mapping theorem there exists a unique fixed point $F^*=(A_0^*,\ldots,A_N^*,\hat{A}_0^*,\ldots,\hat{A}_N^*)$ of the mapping $\mathcal{F}=\mathcal{L}(F)$. We define

$$G_1^*=G_1^0(x-\xi t,\xi)+\int_0^t\sum_{n=0}^{N}B_n^*(x^*,s)\phi_n(\xi)\,ds,$$
$$G_2^*=G_2^0(x-(\hat{\xi}/\gamma)t,\hat{\xi})+\int_0^t\sum_{n=0}^{N}\hat{B}_n^*(\tilde{x}^*,s)\phi_n(\hat{\xi})\,ds, \tag{3.15}$$

where B_n^* and $\hat{B}_n^*$ are expressed in terms of the components A_n^* and $\hat{A}_n^*$ of the fixed point F^*. Since (G_1^*,G_2^*) satisfies (3.3) and (3.6), we have existence and uniqueness of solutions for $0\leq t\leq T$. We take $G_1^*(x,\xi,T)$ and $G_2^*(x,\hat{\xi},T)$ as the initial value at $t=T$ and again show that there is a contraction mapping for $T\leq t\leq T_1$ where $T_1>T$. By proceeding in this manner, we show existence and uniqueness of solutions for all $t:0\leq t<\infty$. As a consequence of the contraction mapping, we also have continuous dependence of the solution on the initial data. Thus for the prescribed initial distributions, the system is well set mathematically.

4. USE OF TRANSFORMS

We solve the system (3.3) with initial conditions (3.6) by first taking a Fourier transform in x, followed by a Laplace transform in t. The transformed system is solved, a Laplace inversion is carried out, followed by a Fourier inversion.

We denote by $|S|^{2N+2}$ the subspace of elements of S^{2N+2} such that the components of the elements and the Fourier transforms of the components are absolutely integrable in x and the transform space, respectively. In addition to the three previous requirements for the initial distributions, we require that (1) the initial distributions and their x gradients are absolutely integrable functions of x and (2) the Fourier transforms of the initial distributions and the components of their x

gradients are absolutely integrable in the transform space. With these specifications on the initial distributions: (1) The moments of G_i^0 and ∇G_i^0 and the Fourier transforms of these moments are absolutely integrable in x and the transform space, respectively, and (2) the operations of taking the Fourier transforms and taking the moments of G_i^0 and ∇G_i^0 are commutative (see Ref. 1 for simple-gas models). We may repeat the previous contraction mapping argument and show that $\mathcal{J} = \mathcal{L}(F)$ has a unique fixed point $\in |S|^{2N+2}$.

Let k be the Fourier variable and denote the transformed variable by a superscript T. The system (3.3) and (3.6) can be written

$$\left(\frac{\partial}{\partial t} - ik\cdot\xi\right)G_1^T = \sum_{n=0}^{N} B_n^T\phi_n(\xi),$$
$$\left(\frac{\partial}{\partial t} - i\frac{k}{r}\cdot\hat{\xi}\right)G_2^T = \sum_{n=0}^{N} \hat{B}_n^T\phi_n(\hat{\xi}), \tag{4.1}$$

where

$$G_1^T = e^t g_1^T, \quad G_2^T = e^{\mu t} g_2^T \tag{4.2}$$

and

$$A_n^T = A_n^T(k,t) = (G_1^T, \phi_n) = e^t(g_1^T, \phi_n),$$
$$\hat{A}_n^T = \hat{A}_n^T(k,t) = (G_2^T, \phi_n) = e^{\mu t}(g^T, \phi_n), \tag{4.3}$$

$$G_1^{0T}(k,\xi) = G_1^T(k,\xi,0) = g_1^T(k,\xi,0),$$
$$G_2^{0T}(k,\hat{\xi}) = G_2^T(k,\hat{\xi},0) = g_2^T(k,\hat{\xi},0). \tag{4.4}$$

We consider the following equivalent system:

$$\frac{\partial}{\partial t}G_1' = \sum_{n=0}^{N}\exp(-ik\cdot\xi t)B_n'\phi_n(\xi),$$
$$\frac{\partial}{\partial t}G_2' = \sum_{n=0}^{N}\exp[-i(k/r)\cdot\hat{\xi}t]\hat{B}_n'\phi_n(\hat{\xi}), \tag{4.5}$$

where

$$G_1' = \exp(-ik\cdot\xi t)G_1^T,$$
$$G_2' = \exp[-i(k/r)\cdot\hat{\xi}t]G_2^T; \tag{4.6}$$

$$A_n'(k,t) = (G_1'\exp(ik\cdot\xi t), \phi_n),$$
$$\hat{A}_n'(k,t) = (G_2'\exp[i(k/r)\cdot\hat{\xi}t], \phi_n), \tag{4.7}$$

$$G_1^{0\prime}(k,\xi) = G_1^{0T}(k,\xi),$$
$$G_2^{0\prime}(k,\hat{\xi}) = G_2^{0T}(k,\hat{\xi}). \tag{4.8}$$

By formal integration of (4.5) we obtain

$$G_1' = G_1^{0\prime}(k,\xi) + \int_0^t \sum_{n=0}^{N}\exp(-ik\cdot\xi s)B_n'\phi_n(\xi)\,ds,$$
$$G_2' = G_2^{0\prime}(k,\hat{\xi}) + \int_0^t \sum_{n=0}^{N}\exp[-i(k/r)\cdot\hat{\xi}s]\hat{B}_n'\phi_n(\hat{\xi})\,ds. \tag{4.9}$$

Taking moments of (4.9), we have

$$A_m' = \int_\xi \exp(ik\cdot\xi t)\,\omega\phi_m G_1^{0\prime}(k,\xi)\,d\xi$$
$$+ \int_0^t\int_\xi \sum_{n=0}^{N}\exp[ik(t-s)\cdot\xi]B_n'\omega\phi_m\phi_n\,d\xi\,ds, \tag{4.10}$$

$$\hat{A}_m' = \int_\xi \exp[i(k/r)\cdot\xi t]\omega\phi_m G_2^{0\prime}(k,\xi)\,d\xi$$
$$+ \int_0^t\int_\xi \sum_{n=0}^{N}\exp[i(k/r)(t-s)\cdot\xi]\hat{B}_n'\omega\phi_m\phi_n\,d\xi\,ds.$$

We now investigate whether the transformed quantities are such that we can apply the Laplace transform. This requires estimates of bounds for the quantities involved and these bounds are not rountinely obtained. We define

$$\|F_t'\| = \sum_{n=0}^{N}\max_k|F_n'|$$

and

$$\big|\,|F'|_{t_0}\big| = \max_{0\le t\le t_0}\|F_t'\|.$$

We have from (4.10)

$$\|A_T'\| \le \|A_0'\| + P\int_0^T\|A_t'\|\,dt + P\int_0^T\exp[t(1-\mu)]\,\|\hat{A}_t'\|\,dt \tag{4.11}$$

and

$$\|\hat{A}_T'\| \le \|\hat{A}_0'\| + P\int_0^T\exp[t(\mu-1)]\,\|A_t'\|\,dt + P\int_0^T\|\hat{A}_t'\|\,dt \tag{4.12}$$

where $P>0$ is defined by (3.13). From the continuity of the norm, there exist t_1 and $t_2 \in [0,T]$ such that

$$\|A_{t_1}'\| = \big|\,|A'|_T\big|$$

and

$$\|\hat{A}_{t_2}'\| = \big|\,|\hat{A}'|_T\big|.$$

Thus for $0 \le \mu < 1$

$$\big|\,|A'|_T\big| = \big|\,|A_{t_1}'|\,\big| \le \|A_0'\| + PT\,\big|\,|A'|_T\big| + \frac{P}{1-\mu}(\exp[T(1-\mu)]-1)\,\big|\,|\hat{A}'|_T\big| \tag{4.13}$$

and

$$\big|\,|\hat{A}'|_T\big| = \|\hat{A}_{t_2}'\| \le \|\hat{A}_0'\| + \frac{P}{1-\mu}(1-\exp[T(\mu-1)])\,\big|\,|A'|_T\big| + PT\,\big|\,|\hat{A}'|_T\big|. \tag{4.14}$$

From (4.13) and (4.14) we have

$$(1-PT)\,\big|\,|A'|_T\big| \le \|A_0'\| + \frac{P}{1-\mu}(\exp[T(1-\mu)]-1)\,\big|\,|\hat{A}'|_T\big| \tag{4.15}$$

and

$$(1-PT)\,\big|\,|\hat{A}'|_T\big| \le \|\hat{A}_0'\| + \frac{P}{1-\mu}(1-\exp[T(\mu-1)])\,\big|\,|A'|_T\big|. \tag{4.16}$$

Using (4.16) in (4.15), we have

$$\left(1 - PT - \frac{P^2(\exp[T(1-\mu)]-1)(1-\exp[T(\mu-1)])}{(1-\mu)^2(1-PT)}\right)$$
$$\times\,\big|\,|A'|_T\big| \le \|A_0'\| + \frac{P(\exp[T(1-\mu)]-1)}{(1-\mu)(1-PT)}\,\|\hat{A}_0'\|. \tag{4.17}$$

We examine the function contained in the term on the left side of (4.17)

$$f(T)=P+\frac{P^2(\exp[T(1-\mu)]-1)(1-\exp[T(\mu-1)])}{T(1-\mu)^2(1-PT)}. \tag{4.18}$$

We observe that $f(T)$ is continuous for $0<T<1/P$, $\lim_{T\to 0^+}f(T)=P$, and $f(T)\geq P$. Therefore, on the interval $0<T\leq\delta<1/P$, $f(T)$ has a minimum P and a maximum β. Hence, for $T<T_1=\min(\delta, 1/\beta)$

$$1-PT\geq 1-f(T)T\geq 1-\beta T>0 \tag{4.19}$$

and

$$1/[1-f(T)T]\leq 1/(1-\beta T). \tag{4.20}$$

We need three additional estimates. We have

$$\left(\frac{1}{1-f(T)T}\right)\frac{P}{1-\mu}\ \frac{(\exp[T(1-\mu)]-1)}{(1-PT)}\leq 1 \tag{4.21}$$

and

$$\left(\frac{1}{1-f(T)T}\right)\ \frac{P}{1-\mu}\ \frac{(1-\exp[T(\mu-1)])}{(1-PT)}\leq 1 \tag{4.22}$$

for $0\leq T<T_2$ where $T_2\leq T_1$. Finally, since $0<1-\beta T<1$ (for $T>0$) there exists an integer $N_0>1$ such that

$$1+\frac{1}{1-\beta T}\leq\frac{1}{(1-\beta T)^{N_0}}. \tag{4.23}$$

Let T and μ be fixed, $0<T\leq T_2$ and $0\leq\mu<1$. We consider the intervals $[0,T]$, $[T,2T]$, $[2T,3T]$, etc., and iterate using (4.17) and a corresponding relationship derived from (4.16) for $||\hat{A}'|_T|$, and the inequalities (4.19) through (4.23) and obtain

$$||A'|_{nT}|\leq\frac{\alpha\exp[nT(1-\mu)]}{(1-\beta T)^{nN_0}}\leq\frac{\alpha\exp(nT)}{(1-\beta T)^{nN_0}} \tag{4.24}$$

and

$$||\hat{A}'|_{nT}|\leq\alpha/(1-\beta T)^{nN_0} \tag{4.25}$$

for all integers $n\geq 0$ where $\alpha=\max(\|A_0'\|, \|\hat{A}_0'\|)$. We may make a separate calculation using (4.11) and (4.12) and show that these bounds are also valid for $\mu=1$.

For every $t\geq 0$ there exists an integer n such that $(n-1)T<t\leq nT$ and thus

$$\|A_t'\|\leq||A'|_t|\leq||A'|_{nT}|\leq$$

$$\frac{\alpha\exp[nT(1-\mu)]}{(1-\beta T)^{nN_0}}\leq\frac{\alpha\exp(nT)}{(1-\beta T)^{nN_0}}$$

$$\leq\frac{\alpha}{(1-\beta T)^{N_0}}\times\exp\left[T+\left(1+\frac{N_0\beta}{1-\beta T}\right)t\right] \tag{4.26}$$

and

$$\|\hat{A}_t'\|\leq||\hat{A}'|_t|\leq||\hat{A}'|_{nT}|\leq\frac{\alpha}{(1-\beta T)^{nN_0}}$$

$$\leq\frac{\alpha}{(1-\beta T)^{N_0}}\exp\left(\frac{N_0\beta}{1-\beta T}t\right). \tag{4.27}$$

Therefore, each of the components A_n' and $\hat{A}_n'$ can grow at most exponentially in time. Since A_n' and $\hat{A}_n'$ are continuous functions of time, we have the existence of the Laplace transforms of these quantities. Further, by (4.9) G_1' and G_2' can grow at most exponentially in time and are continuous and we may apply the Laplace transform to them as well.

5. THE TRANSFORMED SYSTEM AND THE DISPERSION RELATION

We take the Fourier transform in space (k the Fourier variable) and the Laplace transform in time (σ the Laplace variable) of the system (2.6). Denoting the transformed quantities by a superscript T, we have

$$g_1^T=\frac{g_1^{0T}}{\sigma-ik\cdot\xi+1}+\frac{\sum_{n=0}^N b_n^T\phi_n}{\sigma-ik\cdot\xi+1},$$

$$g_2^T=\frac{g_2^{0T}}{\sigma-ik/\gamma\cdot\hat{\xi}+\mu}+\frac{\sum_{n=0}^N \hat{b}_n^T\phi_n}{\sigma-ik/\gamma\cdot\hat{\xi}+\mu}, \tag{5.1}$$

where b_n^T and $\hat{b}_n^T$ are defined in terms of the inner products (g_1^T,ϕ_n) and (g_2^T,ϕ_n). We take moments of (5.1) and obtain a $(2N+2)\times(2N+2)$ linear system for $V^T=(V_1^T,\ldots,V_{2N+2}^T)$

$$(I-K)V^T=L, \tag{5.2}$$

where V_n^T are transforms of the moment quantities $n_1, u_1, T_1, \ldots, n_2, u_2, T_2, \cdots$ and K and L are defined by inner products of ϕ_n with terms of (5.1). The quantities, $(\phi_m, \phi_n/(\sigma-ik\cdot\xi+1))$ and $(\phi_m, \phi_n/(\sigma-ik/\gamma\cdot\xi+\mu))$, in the matrix $I-K$ can be evaluated in terms of the complex error function.

Formally, we have

$$V^T=(I-K)^{-1}L. \tag{5.3}$$

V may be obtained by a Laplace inversion followed by a Fourier inversion

$$V(x,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-ik\cdot x)\,dk\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{\exp(\sigma t)}{2\pi i}(I-K)^{-1}L\,d\sigma. \tag{5.4}$$

We postulate the existence of plane wave solutions to (2.6); that is, solutions of the form

$$g_1=q_1(\xi)\exp(\sigma t-ik\cdot x),$$
$$g_2=q_2(\hat{\xi})\exp(\sigma t-ik\cdot x), \tag{5.5}$$

where q_1 and $q_2\in\mathcal{H}$. We define

$$c_n=(q_1,\phi_n),\quad \hat{c}_n=(q_2,\phi_n). \tag{5.6}$$

When (5.5) and (5.6) are substituted into (2.6), the conjecture (5.5) leads to the system (5.2) with L identically zero. In order that

$$(I-K)V^T=0 \tag{5.7}$$

has a nontrivial solution we must have

$$\det[(I-K)(\sigma,k)]=0. \tag{5.8}$$

This is the dispersion relation and it defines the functional roots $\sigma=\sigma(k)$.

We assume plane wave solutions and that $\sigma=\sigma(k)$ is a root of the dispersion relation. For a one-dimensional problem (2.6) becomes

$$(\sigma - ik\xi_1 + 1)q_1 = c_0\phi_0 + \left(a_1c_1 + a_3\frac{\hat{c}_1}{\gamma}\right)\phi_1 + \tfrac{3}{2}(a_2c_2 + a_4\hat{c}_2)\phi_2,$$

$$\left(\sigma - i\frac{k}{\gamma}\hat{\xi}_1 + \mu\right)q_2 = \mu\hat{c}_0\phi_0 + \left(\hat{a}_1c_1 + \hat{a}_3\frac{\hat{c}_1}{\gamma}\right)\gamma\phi_1 + \tfrac{3}{2}(\hat{a}_2c_2 + \hat{a}_4\hat{c}_2)\phi_2. \tag{5.9}$$

Since q_1 and $q_2 \in \mathcal{H}$ and $\{\phi_n\}$ is a complete orthogonal set in $\mathcal{H}$

$$q_1 = \sum_{n=0}^{\infty} c_n\frac{\phi_n}{(\phi_n, \phi_n)}, \quad q_2 = \sum_{n=0}^{\infty} \hat{c}_n\frac{\phi_n}{(\phi_n, \phi_n)} \tag{5.10}$$

We take inner products of the equations in (5.9) with q_1 and q_2, respectively, and obtain

$$\sigma(q_1, q_1) - i(k\xi_1 q_1, q_1) = -(q_1, q_1) + \left(\sum_{n=0}^{2} b_n^{\mathcal{H}}(\phi_n, q_1)\right),$$

$$\sigma(q_2, q_2)\left(-i\frac{k}{\gamma}\hat{\xi}_1 q_2, q_2\right) = -\mu(q_2, q_2) + \left(\sum_{n=0}^{2} \hat{b}_n^{\mathcal{H}}(\phi_n, q_2)\right). \tag{5.11}$$

This system provides two relationships for $\mathrm{Re}\sigma$

$$\mathrm{Re}\sigma = \left[-\sum_{n=3}^{\infty}|c_n|^2 + |c_1|^2(-1 + a_1) + |d_2|^2(-1 + a_2) + \mathrm{Re}\left(\bar{c}_1\frac{\hat{c}_1}{\gamma}\right)a_3 + \mathrm{Re}(\bar{d}_2\hat{d}_2)a_4\right](q_1, q_1)^{-1}, \tag{5.12}$$

$$\mathrm{Re}\sigma = \left[-\mu\sum_{n=3}^{\infty}|\hat{c}_n|^2 + |\hat{c}_1|^2(-\mu + \hat{a}_3) + |\hat{d}_2|^2(-\mu + \hat{a}_4) + \mathrm{Re}\left(c_1\frac{\bar{\hat{c}}_1}{\gamma}\right)\hat{a}_1\gamma^2 + \mathrm{Re}(d_2\bar{\hat{d}}_2)\hat{a}_2\right](q_2, q_2)^{-1},$$

where $d_2 = \sqrt{3/2}\,c_2$, $\hat{d}_2 = \sqrt{3/2}\,\hat{c}_2$, and $\{\phi_n\}$ is assumed orthonormal for $n \geq 3$. We multiply the first equation by $n_1^0(q_1, q_1)$, the second by $n_2^0(q_2, q_2)$, and add to get

$$\mathrm{Re}\sigma = -\left[n_1^0\sum_{n=3}^{\infty}|c_n|^2 + \mu n_2^0\sum_{n=3}^{\infty}|\hat{c}_n|^2 + pn_1^0M_2\left|c_1 - \frac{\hat{c}_1}{\gamma}\right|^2 + pn_1^0N_2|d_2 - \hat{d}_2|^2\right] \times [n_1^0(q_1, q_1) + n_2^0(q_2, q_2)]^{-1}. \tag{5.13}$$

From (5.13) we have

$$\mathrm{Re}\sigma \leq 0. \tag{5.14}$$

Using the inequality $2(|x|^2 + |y|^2) \geq |x - y|^2$, we have for $0 \leq p \leq \mu/2$ with $\mu \leq 1$

$$\begin{aligned} n_1^0(|c_1|^2 + |d_2|^2) + \mu n_2^0(|\hat{c}_1|^2 + |\hat{d}_2|^2) &\geq 2pn_1^0M_2\left(|c_1|^2 + \left|\frac{\hat{c}_1}{\gamma}\right|^2\right) + 2pn_1^0N_2(|d_2|^2 + |\hat{d}_2|^2) \\ &\geq pn_1^0M_2\left|c_1 - \frac{\hat{c}_1}{\gamma}\right|^2 + pn_1^0N_2|d_2 - \hat{d}_2|^2, \end{aligned} \tag{5.15}$$

which when used in (5.13) implies

$$\mathrm{Re}\sigma > -\left(\frac{n_1^0(q_1, q_1) + \mu n_2^0(q_2, q_2)}{n_1^0(q_1, q_1) + n_2^0(q_2, q_2)}\right) = -1 + \delta(\mu). \tag{5.16}$$

Thus for plane wave solutions with $\sigma = \sigma(k)$ a root of the dispersion relation and $0 \leq p \leq \mu/2$, we have

$$-1 + \delta(\mu) < \mathrm{Re}\sigma \leq 0. \tag{5.17}$$

The assumption that the normalized cross-collision frequency p is less than or equal to one-half the normalized collision frequency μ is physically reasonable.

We now examine the matrix I-K for a one-dimensional problem. After integrations have been carried out with respect to ξ_2 and ξ_3, the elements of I-K contain integrals of the form

$$M(\lambda) = \frac{\lambda}{(2\pi)^{1/2}}\int \frac{\exp(-\xi_1^2/2)\,d\xi_1}{\lambda - i\xi_1}, \tag{5.18}$$

$$M(\hat{\lambda}) = \frac{\hat{\lambda}}{(2\pi)^{1/2}}\int \frac{\exp(-\xi_1^2/2)\,d\xi_1}{\hat{\lambda} - i\xi_1}, \tag{5.19}$$

where

$$\lambda = \frac{\sigma + 1}{k} \tag{5.20}$$

and

$$\hat{\lambda} = \frac{\sigma + \mu}{k/\gamma}. \tag{5.21}$$

The integrals $M(\lambda)$ and $M(\hat{\lambda})$ have the imaginary axes in the λ and $\hat{\lambda}$ planes, respectively, as natural branch cuts and each integral defines two different functions (one in each half-plane). The analytic continuation of any one of these functions across the branch cut does not lead to the other corresponding function. Therefore, we have four different functions in $I - K$ determined by $\mathrm{Re}\lambda > 0$, $\mathrm{Re}\lambda < 0$, $\mathrm{Re}\hat{\lambda} > 0$, and $\mathrm{Re}\hat{\lambda} < 0$.

In order to define the Laplace inversion, we require $\mathrm{Re}\sigma > 0$. Hence, by (5.20) and (5.21) the branches of $M(\lambda)$ and $M(\hat{\lambda})$ depend on the sign of k. We designate these functions by $M(\lambda)^+$, $M(\hat{\lambda})^+$ for $k > 0$ and $M(\lambda)^-$, $M(\hat{\lambda})^-$ for $k < 0$. Having specified the branches of $M(\lambda)$ and $M(\hat{\lambda})$ so that $\mathrm{Re}\sigma > 0$, we analytically continue these branches across the branch cuts. We may then find roots $\sigma(k)$ for all k such that $\det(I - K)$ vanishes. However, by (5.17) the roots $\sigma(k)$ such that $\mathrm{Re}\sigma(k) \notin (-1 + \delta, 0]$ do not correspond to plane waves. (The analytic continuation of the dispersion relation was proposed by Thurber.[5])

If we assume $k > 0$, then the dispersion relation is a function of $M(\lambda)^+$ and $M(\hat{\lambda})^+$ and the analytic continuations of these functions. The roots of the dispersion relation lie in three regions of the σ plane which we may appropriately call: the hydrodynamic region ($-\mu < \mathrm{Re}\sigma \leq 0$) where the dispersion relation asymptotically approaches the dispersion relation for the hydrodynamic conservation equations; the semihydrodynamic region ($-1 < \mathrm{Re}\sigma \leq -\mu$) where one gas has hydrodynamic properties and the other has rarefied properties; and the rarefied region ($\mathrm{Re}\sigma \leq 1$) where both gases have rarefied properties. These regions correspond, respectively, to the use in the dispersion relation of $M(\lambda)^+$ and $M(\hat{\lambda})^+$; $M(\lambda)^+$ and the analytic continuation of $M(\hat{\lambda})^+$; and the analytic continuations of both $M(\lambda)^+$ and $M(\hat{\lambda})^+$.

6. SUMMARY

The initial-value problem for the linearized Oppenheim model was shown to have the following properties: (1) it is well set mathematically, (2) it may justifiably be solved by the use of Fourier–Laplace transforms, (3) the roots of the dispersion relation lie in three regions of the σ plane which are related to physical properties of the component gases, and (4) the roots $\sigma(k)$ of the dispersion relation for plane wave solutions are bounded by $-1+\delta < \mathrm{Re}\sigma \leq 0$. The latter result has the important implication that the system is stable.

The theory developed in this investigation can be extended to more sophisticated models. The structure of the Boltzmann equations for gas mixtures may ultimately be revealed through studies of kinetic models.

ACKNOWLEDGMENT

I would like to thank Professor James K. Thurber for suggesting this problem and for his encouragement.

[1] L. Sirovich and J. K. Thurber, Appl. Math. **25**, 175 (1967).
[2] A. Oppenheim, Phys. Fluids **8**, 992 (1965).
[3] D. E. Greene, "Wave Propagation and Other Spectral Problems in a Binary Gas Mixture as Described by Kinetic Models to the Boltzmann Equations," Dissertation, Purdue University, 1973).
[4] M. N. Kogan, *Rarefield Gas Dynamics* (Plenum, New York, 1969), p. 113.
[5] L. Sirovich and J. K. Thurber, "Sound Propagation According to the Kinetic Theory of Gases," in *Rarefied Gas Dynamics* (Academic, New York, 1963), Vol. I, p. 159.

Vestigial effects of singular potentials in diffusion theory and quantum mechanics *

H. Ezawa†, J. R. Klauder, and L. A. Shepp

Bell Laboratories, Murray Hill, New Jersey 07974
(Received 14 February 1974)

Repulsive singular potentials of the form $\lambda V(x) = \lambda|x-c|^{-\alpha}$, $\lambda > 0$, in the Feynman–Kac integral are studied as a function of α. For $\alpha > 2$ such potentials completely suppress the contribution to the integral from paths that reach the singularity, and thus, unavoidably, certain vestiges of the potential remain even after the coefficient $\lambda \downarrow 0$. For $2 \geqslant \alpha \geqslant 1$ careful definition by means of suitable counter terms at the point of singularity (similar in spirit to renormalization counter terms in field theory) can lead to complete elimination of effects of the potential as $\lambda \downarrow 0$. For $\alpha < 1$ no residual effects of the potential exist as $\lambda \downarrow 0$. In order to prove these results we rely on the theory of stochastic processes using, in particular, local time and stochastic differential equations. These results established for the Feynman–Kac integral conform with those known in the theory of differential equations. In fact, a variety of vestigial effects can arise from suitable choices of counter terms, and these correspond in a natural way to various self-adjoint extensions of the formal differential operator.

1. INTRODUCTION

Averages of various expressions in Wiener measure, such as

$$F(T) \equiv \int \exp[-\lambda \int_0^T V(x(t))\,dt]\,d\mu_W(x)$$
$$\equiv \langle \exp[-\lambda \int_0^T V(x(t))\,dt] \rangle, \tag{1.1}$$

arise in a number of contexts, specifically in diffusion theory and in the imaginary time formulation of quantum theory. In Eq. (1.1), the Wiener measure μ_W is a normalized Gaussian measure on continuous paths $x(t)$, $0 \leqslant t \leqslant T$, where $x(0) = 0$, with mean zero and covariance $= \min(t, t')$ (standard Wiener process). We are interested in studying F for singular potentials V, such as $V(x) = |x-c|^{-\alpha}$, $\alpha > 0$, when $\lambda > 0$. Examples where $c = 0$ and $c \neq 0$ are both of interest. In the latter case and for sufficiently large α, it is conceivable that those paths that reach $x = c$ may not contribute to F at all since for such paths the appropriate integral in the exponent diverges.[1] If this behavior applies to a set of paths having nonzero measure, then it follows that $F(T) \not\to 1$ as $\lambda \downarrow 0$, and more fundamentally, that the basic stochastic process has been unalterably modified. Should this situation arise in a quantum mechanical context, it carries the interesting consequence that once turned on the effects of the repulsive singular potential cannot be completely turned off.[2] These are examples of what we mean by vestigial effects.

In the related Schrödinger problem with Hamiltonian

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\lambda}{|x-c|^{\alpha}}$$

it is known[3] that for $\alpha \leqslant 2$ it is possible to choose appropriate boundary conditions at the singularity so that the associated Hamiltonian operator converges strongly as $\lambda \downarrow 0$ to the free particle Hamiltonian. For $\alpha > 2$ this is impossible: no choice of boundary conditions permits convergence to the free particle Hamiltonian as $\lambda \downarrow 0$. As far as possible we wish to reproduce these results in the path space formulation by exploiting in that approach what plays the role of various boundary conditions in the differential equation approach. Not unexpectedly the role of boundary conditions is subsumed by *regularizations of the potential at the singularity* (e.g., by the introduction of counter terms). Specifically, we approach a given potential $V(x) = |x-c|^{-\alpha}$ through a sequence of bounded, continuous potentials $V_\epsilon(x)$, $\epsilon > 0$, for which we require pointwise convergence for all $x \neq c$ such that

$$\lim_{\epsilon \downarrow 0} V_\epsilon(x) = |x-c|^{-\alpha}, \quad x \neq c. \tag{1.2}$$

and, as it turns out for $\alpha \leqslant 2$, it is the freedom in choosing such sequences that corresponds to different boundary conditions and eventually to (possibly) distinct self-adjoint extensions of the Hamiltonian.

Along with a sequence of regularized potentials $V_\epsilon(x)$ we consider the associated averages

$$F_\epsilon(T) \equiv \langle \exp[-\lambda \int_0^T V_\epsilon(x(t))\,dt] \rangle \tag{1.3}$$

each of which is unambiguously defined. Instead of (1.1) we henceforth adopt the prescription

$$F(T) \equiv \lim_{\epsilon \downarrow 0} F_\epsilon(T), \tag{1.4}$$

provided that the limit exists. Very different results for $F(T)$ may arise for different choices of regularization even though each choice converges pointwise to the same potential except at the singularity.

The question of the behavior as $\lambda \downarrow 0$ may be phrased more precisely in terms of path space measures. Let us introduce the measures ν_ϵ^λ, where

$$d\nu_\epsilon^\lambda \equiv \exp[-\lambda \int_0^T V_\epsilon(x(t))\,dt]\,d\mu_W \tag{1.5}$$

and define, when it exists in the topology of weak convergence of measures, the measure

$$\nu^\lambda \equiv \lim_{\epsilon \downarrow 0} \nu_\epsilon^\lambda. \tag{1.6}$$

While ν_ϵ^λ is equivalent to μ_W, this need not be the case for ν^λ; it may be desirable or even necessary to choose different regularizations for different λ. We may say that the effects of the interaction disappear as $\lambda \downarrow 0$ provided the weak limit obeys

$$\lim_{\lambda \downarrow 0} \nu^\lambda = \mu_W, \tag{1.7}$$

and otherwise not.

Our basic results may now be stated: For potentials $V(x) = |x-c|^{-\alpha}$, $\alpha \leq 2$, regularizations exist such that (1.7) holds; for $\alpha > 2$ no such regularizations exist. While these results agree with those found using differential equation techniques, as desired, it is informative to probe their anatomy in the path space picture more deeply. Specifically, to obtain (1.7), nonnegative regularizations may be employed for $\alpha < 1$, while for $\alpha \geq 1$ this is not the case.[4] Moreover, in the interval $1 \leq \alpha < 3/2$, ν^λ is equivalent to μ_W for all λ, while in the interval $3/2 \leq \alpha \leq 2$, ν^λ is inequivalent to μ_W or to any other $\nu^{\lambda'}$, $\lambda' \neq \lambda$. For $\alpha > 2$ (or with nonnegative regularizations for $\alpha \geq 1$), $\nu^\lambda \to \mu'_{W,c}$ a measure appropriate to the absorbing Brownian motion[5] (also called absorbing Wiener process) in which all paths that reach $x = c$ are thereafter disregarded.[6]

One of our prime tools of analysis exploits a well-known and important equivalence demonstrated by Kac.[7] For bounded and continuous $V(x)$ he has shown that the quantity

$$F(T) = \langle \exp[-\lambda \int_0^T V(x(t))\,dt] \rangle \tag{1.8}$$

may be expressed as

$$F(T) = \int \psi(x, T)\,dx, \tag{1.9}$$

where $\psi(x, T)$ is that solution of the differential equation of generalized diffusion,

$$\frac{\partial \psi(x,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 \psi(x,t)}{\partial x^2} - \lambda V(x)\,\psi(x,t), \tag{1.10}$$

determined by the initial condition

$$\psi(x, 0) = \delta(x). \tag{1.11}$$

Clearly this equivalence can be applied to the regularized forms $V_\epsilon(x)$ to yield $F_\epsilon(T)$, and where analytically tractable this technique, treated in detail in Appendices A and B, provides valuable information on the explicit behavior for small ϵ.

Another prime tool of our analysis is the use of local time and stochastic differential equation techniques.[8] Recently,[9] we have been able to show how to realize a normalized form of the measure ν_ϵ^λ in (1.5) as a set of continuous paths on path space, much as Wiener measure is realized by a similar set of continuous paths. An alternative way, equivalent to that in Eq. (1.7), in which to ascertain that the influence of the potential disappears is to study the modified paths (determined by ν_ϵ^λ) and to show in the limits $\epsilon \downarrow 0$ and $\lambda \downarrow 0$ that they reduce to the Wiener paths. We shall find this to be an especially convenient method when the measures $\nu^\lambda = \lim \nu_\epsilon^\lambda$ and μ_W are mutually inequivalent.

The discussion in this paper is confined solely to one-dimensional systems. However, this work has been motivated, in large measure, by a potential applicability of these concepts and methods to fundamental problems in quantum field theory. An initial discussion of this application has already been given,[2] and we hope the present work serves to stimulate further research in these directions.[10]

2. ANALYSIS OF REGULARIZED SINGULAR POTENTIALS: RANDOM VARIABLE VIEWPOINT

Local time

In this section we shall find it convenient to employ the so-called *local time*

$$t^*(y) \equiv \lim_{h \downarrow 0} m[s : y \leq x(s) \leq y + h,\ 0 \leq s \leq T]/h, \tag{2.1}$$

where $x(s)$ denotes a sample path and where m denotes Lebesgue measure.[11] For benefit of the reader unfamiliar with local time we indicate its formal definition as well, namely

$$t^*(y) \equiv \int_0^T \delta(x(s) - y)\,ds.$$

Clearly $t^*(y)$ is nonnegative and satisfies

$$\int_{-\infty}^{\infty} t^*(y)\,dy = T.$$

For almost every path $t^*(y)$ has compact support [$t^*(y) \equiv 0$ for $y \geq \max x(s)$ or $y \leq \min x(s)$; both bounds almost surely exist], and it has been shown that $t^*(y)$ is continuous in y.[11] Additional properties of $t^*(y)$ will be introduced as needed.

The basic random variable in (1.5) may be expressed in terms of $t^*(y)$ as

$$Q_\epsilon \equiv \int_0^T V_\epsilon(x(t))\,dt = \int_{-\infty}^{\infty} V_\epsilon(y)\,t^*(y)\,dy,$$

which shows that the study of the random variable Q_ϵ is at the same time a study of the random field $t^*(y)$ for various "smearing functions" $V_\epsilon(y)$, a point of view not uncommon in field theory contexts. In quantum field theory, we recall, one studies field operators smeared by test functions, and as a matter of fact, under certain circumstances such smeared operators may be regarded as random variables.

Case $\alpha < 1$

We note first, for $\alpha < 1$, that

$$Q \equiv \int_{-\infty}^{\infty} |y-c|^{-\alpha}\,t^*(y)\,dy < \infty, \quad \text{a. s.},\ ^{12}$$

since $t^*(y)$ is continuous and has compact support, hence is bounded, almost surely, and $|y-c|^{-\alpha}$ is integrable at c provided $\alpha < 1$. Consider next any regularization sequence $V_\epsilon(y)$ such that on each compact set C

$$\int_C |V_\epsilon(y) - |y-c|^{-\alpha}|\,dy \to 0 \tag{2.2}$$

as $\epsilon \downarrow 0$. As a consequence, as $\epsilon \downarrow 0$,

$$|Q_\epsilon - Q| \leq \int |V_\epsilon(y) - |y-c|^{-\alpha}|\,t^*(y)\,dy \to 0, \quad \text{a. s.};$$

namely,

$$\lim_{\epsilon \downarrow 0} Q_\epsilon = \lim_{\epsilon \downarrow 0} \int_0^T V_\epsilon(x(t))\,dt$$

$$= \int_0^T |x(t) - c|^{-\alpha}\,dt = Q, \quad \text{a. s.}.$$

To convert these facts into properties of the measures requires for $\lambda \geq 0$ that $\exp(-\lambda Q_\epsilon) \leq G$ uniformly in ϵ where $\langle G \rangle < \infty$. This condition imposes a certain restriction on the negative excursions of $V_\epsilon(y)$, but one that is difficult to specify in detail. [For example, if $V_\epsilon(y) \geq -M$ uniformly, then $\exp(-\lambda Q_\epsilon) \leq \exp(\lambda M T)$ for $\lambda \geq 0$.] With a uniform bound G, it follows that $\nu_\epsilon^\lambda \to \nu^\lambda$ weakly, where $d\nu^\lambda = \exp(-\lambda Q)\,d\mu_W$, and finally $\nu^\lambda \to \mu_W$ weakly.

Nonnegative regularizations

The preceding discussion applies to rather general regularizations $V_\epsilon(x)$. Nevertheless, it is useful to direct the discussion temporarily to regularizations that in addition satisfy the condition $V_\epsilon(x) \geq 0$. A convenient example of this type is given by

$$V_\epsilon(x) = (|x-c| + \epsilon)^{-\alpha}$$

which we shall refer to as the *basic regularization*.

Elsewhere[1] we have proven a theorem related to our present discussion. Suitably rephrased that result is given by the following:

Theorem: Let $x(t)$ be a standard Wiener process, $t^*(y)$ the local time as defined in (2.1), and $f(y)$ a nonnegative measurable function. Then

$$\int f(y)t^*(y)\,dy = \int_0^T f(x(t))\,dt < \infty, \quad \text{a. s.},$$

if and only if, for each compact set C,

$$\int_C f(y)\,dy < \infty.$$

The application of this theorem to singular potentials in which $\alpha < 1$ is direct and confirms our previous result. Let us instead determine its implications for $\alpha \geq 1$. Consider, initially, the basic regularization with

$$Q_\epsilon = \int (|y-c| + \epsilon)^{-\alpha} t^*(y)\,dy.$$

For the set of paths that do not reach c in time $t < T$, dominated convergence leads to convergence of Q_ϵ as $\epsilon \downarrow 0$ to

$$Q = \int |y-c|^{-\alpha} t^*(y)\,dy.$$

For the set of paths that reach c in some time $t < T$,

$$\lim_{\epsilon \downarrow 0} Q_\epsilon \geq \int |y-c|^{-\alpha} t^*(y)\,dy$$

by Fatou's lemma, which for $\alpha \geq 1$ is almost surely infinite [since $t^*(c) > 0$, which holds in a neighborhood of c by continuity]. For more general nonnegative regularizations $V_\epsilon(x)$ let us assume that for some m and M,

$$m(|y-c| + \epsilon)^{-\alpha} \leq V_\epsilon(y) \leq M(|y-c| + \epsilon)^{-\alpha}$$

besides the fact $V_\epsilon(y) \to |y-c|^{-\alpha}$. Then almost surely

$$Q_\epsilon = \int V_\epsilon(y)t^*(y)\,dy \to Q = \int |y-c| \quad t^*(t)\,dy. \tag{2.3}$$

The variable Q in (2.3) is almost surely finite for those paths that never reach c and almost surely infinite for those paths that reach c. If $c = 0$, however, *all* paths "reach" c since $x(0) = 0$, and one expects for $\alpha \geq 1$ that $Q = \infty$, a. s. Indeed, we know from our previous work[1] that, for $\alpha \geq 1$,

$$\lim_{\epsilon \downarrow 0} \int_0^T (|x(t)| + \epsilon)^{-\alpha}\,dt = \infty, \quad \text{a. s.}.$$

As a consequence, $F_\epsilon \to 0$ as $\epsilon \downarrow 0$, where

$$F_\epsilon = \langle \exp[-\lambda \int_0^T (|x(t)| + \epsilon)^{-\alpha}\,dt] \rangle$$

for $\lambda > 0$ and $\alpha \geq 1$. The calculation in Appendix A explicitly shows for $\alpha = 1$ and $\alpha = 2$ that for fixed $\lambda > 0$ and for $\epsilon \downarrow 0$ asymptotically

$$\alpha = 1: \quad F_\epsilon \sim \text{const}\,(\ln \epsilon^{-1})^{-1}, \tag{2.4a}$$

$$\alpha = 2: \quad F_\epsilon \sim \text{const}\,\epsilon^\theta, \tag{2.4b}$$

where $\theta \equiv \frac{1}{2}(\sqrt{1+8\lambda} + 1)$, and const denotes an ϵ-independent, nonzero factor.

With nonnegative regularizations, it follows that $\exp(-\lambda Q_\epsilon) \leq 1$ and therefore ν^λ is absolutely continuous with respect to μ_W. In particular, if $c = 0$, then $\nu^\lambda \equiv 0$ for all $\lambda > 0$, and quite clearly $\nu^\lambda \not\to \mu_W$ as $\lambda \downarrow 0$.

For $c \neq 0$, $\nu^\lambda \not\equiv 0$, as noted previously below (2.3), and in fact $\nu^\lambda \to \mu'_{W,c}$, which is defined as Wiener measure on the set of paths that never reach $x = c$ and which has no weight on the complementary set. We recall[5] that there is a finite probability

$$p_c = \sqrt{2/\pi T} \int_0^{|c|} \exp(-x^2/2T)\,dx \tag{2.5}$$

that throughout the interval $0 \leq s \leq T$ paths satisfy

$$x(s) \lesseqgtr c, \quad \text{when} \quad c \gtrless 0.$$

Consequently,

$$\int d\mu'_{W,c} = p_c < 1,$$

but this simple fact hardly does justice to the fundamental difference that exists between $\mu'_{W,c}$ and μ_W. The modification of the process described here is just the one to which reference was made in Sec. 1.

In partial summary, we have seen above that for $\alpha < 1$ regularizations exist, indeed nonnegative regularizations, such that $\nu^\lambda \to \mu_W$ as $\lambda \downarrow 0$, a sufficient condition being given by (2.2). We have also seen that for $\alpha \geq 1$ no nonnegative regularization exists such that $\nu^\lambda \to \mu_W$; instead, nonnegative regularizations, e.g., the basic regularization, lead to $\mu'_{W,c}$ which is the measure for absorbing Brownian motion.

We next consider alternative prescriptions to determine if the property $\nu^\lambda \to \mu_W$ can be arranged to hold for $\alpha \geq 1$.

Case $1 \leqslant \alpha < 3/2$

We recast the expression for Q_ϵ in the form

$$Q_\epsilon = \int_{-\infty}^{\infty} V_\epsilon(y)\,t^*(y)\,dy$$

$$= \int_{|y-c| \leq 1} V_\epsilon(y)\,t^*(y)\,dy + \int_{|y-c|>1} V_\epsilon(y)\,t^*(y)\,dy.$$

The latter integral converges as $\epsilon \downarrow 0$ to

$$\int_{|y-c|>1} |y-c|^{-\alpha}\,t^*(y)\,dy, \quad \text{a. s.},$$

for any α. The former integral we write in the form

$$\int_{|y-c| \leq 1} V_\epsilon(y)\ t^*(y)\,dy = \int_{|y-c| \leq 1} V_\epsilon(y)[t^*(y) - t^*(c)]\,dy + t^*(c) \int_{|y-c| \leq 1} V_\epsilon(y)\,dy.$$

We impose on the regularization the requirement that

$$\lim_{\epsilon \downarrow 0} \int_{|y-c| \leq 1} V_\epsilon(y)\,dy = K, \tag{2.6}$$

where $-\infty < K < \infty$, which evidently controls the last term above (see below for examples). Now, continuity properties of $t^*(y)$ imply[11] that for any fixed, nonrandom $\gamma < \frac{1}{2}$ there exists a nonnegative random variable $\mathcal{R}_\gamma$, $\mathcal{R}_\gamma < \infty$, a. s., such that

$$|t^*(y) - t^*(c)| \leq |y-c|^\gamma \mathcal{R}_\gamma$$

in the range $|y-c| \leq 1$. Consequently, we find

$$\left| \int_{|y-c|\leq 1} [V_\epsilon(y) - |y-c|^{-\alpha}]\,[t^*(y) - t^*(c)]\,dy \right|$$

$$\leq R_\gamma \int_{|y-c|\leq 1} |V_\epsilon(y) - |y-c|^{-\alpha}|\,|y-c|^\gamma\,dy.$$

If we next impose on the regularization the condition

$$\int_{|y-c|\leq 1} |V_\epsilon(y) - |y-c|^{-\alpha}|\,|y-c|^\gamma\,dy \to 0, \tag{2.7}$$

we have established that

$$\lim_{\epsilon\downarrow 0} \int_{|y-c|\leq 1} V_\epsilon(y)\,[t^*(y) - t^*(c)]\,dy$$

$$= \int_{|y-c|\leq 1} |y-c|^{-\alpha}[t^*(y) - t^*(c)]\,dy, \quad \text{a.s.}$$

This procedure leads to convergence for $\alpha < 3/2$ since $\gamma < \frac{1}{2}$ can be chosen such that $\alpha - \gamma < 1$. (However, the above procedure is *not* valid for $\alpha \geq 3/2$.)

As an example of a suitable regularization for $\alpha = 1$ we may choose

$$V_\epsilon(x) = (|x-c| + \epsilon)^{-1} - b_\epsilon(|x-c| + \epsilon)^{-2} \tag{2.8}$$

where to satisfy (2.6)

$$b_\epsilon = \epsilon \ln \epsilon^{-1} + O(\epsilon). \tag{2.9}$$

For $1 < \alpha < 3/2$, we may choose

$$V_\epsilon(x) = (|x-c| + \epsilon)^{-\alpha} - b_{\epsilon,\alpha}(|x-c| + \epsilon)^{-\alpha-1}$$

where (2.6) requires

$$b_{\epsilon,\alpha} = \alpha\epsilon/(\alpha - 1) + O(\epsilon^\alpha).$$

The terms $O(\epsilon)$ and $O(\epsilon^\alpha)$ influence the value of K in (2.6) and correspond to distinct self-adjoint extensions of the corresponding Schrödinger differential operator.

Combining the results presented above, we have determined in the interval $1 \leq \alpha < 3/2$ that

$$Q \equiv \lim_{\epsilon\downarrow 0} Q_\epsilon = \int_{|y-c|>1} |y-c|^{-\alpha} t^*(y)\,dy + Kt^*(c)$$

$$+ \int_{|y-c|\leq 1} |y-c|^{-\alpha}[t^*(y) - t^*(c)]\,dy,$$

almost surely, provided that conditions (2.6) and (2.7) hold. Only the first term is necessarily nonnegative.

With regard to integrability of the path space distributions, we note that Fatou's lemma ensures

$$\int \lim_{\epsilon\downarrow 0} \exp(-\lambda Q_\epsilon)\,d\mu_W \leq \lim_{\epsilon\downarrow 0} \int \exp(-\lambda Q_\epsilon)\,d\mu_W \equiv F.$$

If $F < \infty$, then $\exp(-\lambda Q)$ has finite μ_W integral, i.e., $\langle \exp(-\lambda Q)\rangle \leq F < \infty$. If this holds true for all $\lambda \geq 0$, this is sufficient for uniform (in ϵ) integrability[13] of $\exp(-\lambda Q_\epsilon)$ which assures us that in fact equality holds, i.e., $\langle \exp(-\lambda Q)\rangle = F < \infty$.

We have analyzed the case $\alpha = 1$ and $c = 0$ in detail in Appendix B by Feynman–Kac techniques. With $V_\epsilon(x)$ as given in (2.8), it is shown that

$$F \equiv \lim_{\epsilon\downarrow 0} \langle \exp[-\lambda \int_0^T V_\epsilon(x(t))\,dt] \rangle \tag{2.10}$$

satisfies $0 < F < \infty$, for any T and all $\lambda > 0$, if and only if (2.9) holds true.

A similar calculation using Feynman–Kac techniques for the interval $1 < \alpha < 3/2$ has also been carried out, but is not included in the present paper. This analysis confirms the uniform (in ϵ) integrability of the measure for $1 < \alpha < 3/2$.

The results stated above establish the stated properties in the range $1 \leq \alpha < 3/2$, and we now turn our attention to developing techniques to treat larger values of α.

3. ANALYSIS OF REGULARIZED SINGULAR POTENTIALS: PATH SPACE VIEWPOINT

Preliminaries

Preparatory to studying cases where $\alpha \geq 3/2$ it is convenient to rephrase our basic problem in the language of stochastic differential equations. Consider the Radon–Nikodym derivative

$$\frac{d\mu_Y}{d\mu_W} = N_\epsilon^\lambda(T) \exp[-\lambda \int_0^T V_\epsilon(x(t))\,dt] \tag{3.1}$$

where $N_\epsilon^\lambda(T)$ is a nonrandom positive factor chosen to normalize μ_Y; the measure μ_Y is nothing more than a normalized form of ν_ϵ^λ as evident from Eq. (1.5). Elsewhere[9] we have shown that μ_Y may be interpreted as a probability measure for a certain Markov random process of continuous sample paths $Y(t)$, $0 \leq t \leq T$, each of which satisfies $Y(0) = 0$. In a one-to-one fashion, each path $Y(t)$ of the Y-process is effectively generated by a corresponding path $W(t)$ of a standard Wiener process by a stochastic differential equation

$$dY(t) = a(Y(t), t)\,dt + dW(t) \tag{3.2a}$$

or more properly in integral form as

$$Y(t) = \int_0^t a(Y(s), s)\,ds + W(t). \tag{3.2b}$$

Equation (3.2) has a unique continuous solution with probability one[13,14] if

$$|a(x,s) - a(y,s)| \leq \text{const}\,|x-y|$$

and

$$|a(x,s)| \leq \text{const}\,(1 + |x|),$$

in the interval $0 \leq s \leq T$; but these conditions are not necessary. In fact, it suffices to have $a(x,s)$ continuous along with the second condition.[15]

The connection between the drift term $a(x,t)$ and the potential $V(x)$ (assumed bounded and continuous for present purposes) is as follows.[9] Let $B(x,t)$ satisfy the differential equation

$$\frac{\partial B}{\partial t} = -\frac{1}{2}\frac{\partial^2 B}{\partial x^2} + \lambda V(x) B, \tag{3.3}$$

for $0 \leq t \leq T$, subject to the final value condition $B(x,T) \equiv 1$ for all $x \in R$. Then it follows that

$$a(x,t) \equiv \frac{\partial B(x,t)/\partial x}{B(x,t)} \tag{3.4}$$

and the normalization factor in (3.1) is given by

$$N \equiv B(0,0)^{-1}.$$

Note that the equation for B is just the equation of generalized diffusion with time running backwards. A simple mathematical (or physical!) argument[9] shows that $B(x,t)$ is bounded, continuous, and strictly positive in $R\times[0,T]$.

The preceding picture applies for smooth potentials, such as $V_\epsilon(x)$, $\epsilon>0$, for which a set of paths appropriate to the Y-process may be determined from the stochastic equation, at least in principle. Assume that these continuous paths converge as $\epsilon\downarrow 0$, and that the resultant, ϵ-limiting paths are also continuous. Finally, if as $\lambda\downarrow 0$, the ϵ-limiting paths, say $Y(t)$, converge to Wiener path $W(t)$, then we may assert that all traces of the interaction vanish in the limit $\lambda\downarrow 0$. If instead the paths $Y(t)\not\to W(t)$ as $\lambda\downarrow 0$, then the interaction has left an indelible imprint that cannot be removed.

Two examples

Two relatively simple examples enable one to gain proper perspective on the limiting behavior of sample paths. If $B(x,t)\equiv 1$ on $R\times[0,T]$, then $V\equiv 0$, $a\equiv 0$, $Y(t)=W(t)$, and $\mu_Y=\mu_W$. This self-evident behavior simply puts us on notice that $B(x,t)\to 1$ or $a(x,t)\to 0$ on $R\times[0,T]$ is a clue that $Y(t)\to W(t)$ and μ_Y(or ν^λ)$\to\mu_W$.

The other example describes the absorbing Brownian motion and is more interesting. Let $c\neq 0$, and without loss of generality assume $c<0$. Choose $B(x,t)=\mathrm{erf}(\xi)$, where $\xi\equiv|x-c|/\sqrt{2(T-t)}$, defined on $R\times[0,T]$ except at the single point $x=c$, $t=T$ where ξ is indeterminate.[16] For all $x\neq c$, $V\equiv 0$ and

$$a(x,t)=(x-c)^{-1}E(\xi), \tag{3.5}$$

where

$$E(\xi)\equiv 2\xi\exp(-\xi^2)/\sqrt{\pi}\ \mathrm{erf}(\xi).$$

With such a drift term $Y(t)\neq W(t)$. Less evident is the fact that $\mu_Y=\mu'_{W,c}/p_c$, where p_c is given by (2.5), and thus the Y-process is an absorbing Wiener process. In the standard picture $\mu'_{W,c}$ arises from dropping those Wiener paths that reach $x=c$ at any $t\leq T$; the measure is normalized as a final step to give a probability measure. In the nonstandard picture provided by (3.2) and (3.5), the Y paths are deflected just the right amount to yield the normalized distribution $\mu'_{W,c}/p_c$. As such, the Y paths necessarily satisfy $Y(t)-c>0$ for all $t\geq 0$, which is surely an essential feature of an absorbing Wiener process.

Although we are unable to solve explicitly for $Y(t)$ with the drift expression (3.5), *the most essential characteristics of such paths are dictated by the behavior of the drift term near the singularity* and hold for any smooth function $E(\xi)$ so long as $E(\xi)\approx E(0)=1$ for $|\xi|\ll 1$. Fortunately, the stochastic equation for $E(\xi)$ replaced by 1 is well known and describes the three-dimensional Bessel process.[14] Specifically, the stochastic equation

$$dY(t)=(Y(t)-c)^{-1}\,dt+dW(t)$$

is solved (uniquely[14]) by

$$Y(t)-c=\sqrt{W_1^2(t)+W_2^2(t)+(W_3(t)-c)^2},$$

where W_1, W_2, and W_3 are three, independent, standard Wiener processes all conditioned to start at zero at $t=0$, and where $dW\equiv[W_1dW_1+W_2dW_2+(W_3-c)\,dW_3]/(Y-c)$. At $t=0$, $Y(t)-c=-c>0$. Couple this with the fact that $W_1^2(t)+W_2^2(t)>0$ with probability 1 for $t>0$,[14] and we conclude that $Y(t)-c>0$ with probability 1 for all $t\geq 0$. By analogy the solutions with the relevant $a(x,t)$ given by (3.5) also have the property that $Y(t)-c>0$ with probability one for all $t\geq 0$, namely that the paths never cross c. In fact, even the statistics of the Bessel process near the origin are approximately those with the relevant $a(x,t)$, which offers still further insight into the paths appropriate to absorbing Brownian motion.

Approximate "solutions"

Unfortunately, for a given $V(x)$, explicit expressions for B or a are nearly nonexistent. However, since we are ultimately interested in the double limit $\epsilon\downarrow 0$, $\lambda\downarrow 0$, we may choose one of a family of "equivalent" potentials all leading to the same limiting behavior [such as $V(x)+v(x,t)$ where $V(x)$ is the potential of interest and $v(x,t)$ is locally integrable and bounded below at infinity]. Indeed we can choose a simple analytic "solution" $B(x,t)$ that *defines* [by (3.3)] a potential, generally time dependent, that faithfully corresponds to the singularity of the potential of interest.

In fact, we shall go one step further and faithfully represent the singularity up to a time-dependent factor, a modification that in no way influences the ultimate limiting behavior. Briefly, in what follows we choose "solutions" of the form

$$B(x,t)\equiv\exp[\mu(t)W(x)]$$

with $\mu(t)>0$ save for $\mu(T)=0$ [so that $B(x,T)=1$]. It follows that $a(x,t)\equiv\mu(t)W'(x)$ and

$$2\lambda V(x)\equiv\mu W''(x)+\mu^2W'^2(x)+2\dot{\mu}W(x).$$

In our case the singularity always appears in the first two terms, while the last term is always locally integrable. While any smooth function $\mu(t)$ would suffice, we shall, for convenience, arbitrarily let $\mu(t)=\text{const}\equiv\mu>0$ for $0\leq t\leq .99T$, and let $\mu(t)$ decrease for $.99T\leq t\leq T$ so that $\mu(T)=0$. Since the last term in V is unimportant, we confine our discussion to the interval $0\leq t\leq .99T$ where $\dot{\mu}\equiv 0$.

A. Equivalent processes

Behavior for $\alpha<1$

In the framework of the preceding discussion let

$$B(x,t)\equiv\exp[\mu(|x-c|^\gamma+\epsilon^\gamma)^{(1+\beta)}/\gamma(1+\beta)]$$

denote a "solution" where $\beta>0$, $\gamma>1$, and $\mu=\text{const}>0$ for $0\leq t\leq .99T$, and μ falls smoothly for $.99T\leq t\leq T$ so that $\mu(T)=0$ ensuring that $B(x,T)=1$. In this section the function μ will be frequently used and invariably it is so defined. For reasons discussed above we do not concern ourselves in detail with the behavior near $t=T$, but instead concentrate on the interval $0\leq t\leq .99T$. In that time interval,

$$a(x,t)\equiv\mu\ \mathrm{sgn}(x-c)\,|x-c|^{\gamma-1}\,(|x-c|^\gamma+\epsilon^\gamma)^\beta$$

and

$$2\lambda V_\epsilon(x) \equiv \mu\beta\,|x-c|^{2\gamma-2}(|x-c|^\gamma+\epsilon^\gamma)^{\beta-1} + \mu(\gamma-1)|x-c|^{\gamma-2}(|x-c|^\gamma+\epsilon^\gamma)^\beta + \mu^2|x-c|^{2\gamma-2}(|x-c|^\gamma+\epsilon^\gamma)^{2\beta}.$$

These admittedly complicated expressions have been chosen with a special purpose. Useful simplifications would arise if $\gamma \equiv 1$, but strictly speaking that option is not open to us [since $V_\epsilon(x)$ is not integrable, and since $a(x,t)$ is not continuous which we shall find useful in discussing the stochastic equations]. Instead, to avail ourselves of those simplifications we choose γ to be a function of ϵ that *rapidly* approaches 1 as $\epsilon \downarrow 0$. That is, we do not simply choose $\gamma = 1+\epsilon$, but rather something really dramatic like $\gamma = 1+\exp(-\epsilon^{-137})$ which will enable us to characterize V_ϵ in an especially transparent fashion.

With the proposed behavior for γ, we can *effectively* set $\gamma = 1$ already with $\epsilon < .1$ so that the preceding expression for a reads

$$a(x,t) = \mu\,\mathrm{sgn}(x-c)(|x-c|+\epsilon)^\beta$$

and the one for V_ϵ reads

$$2\lambda V_\epsilon(x) = \mu\beta(|x-c|+\epsilon)^{\beta-1} + 2\mu\delta(x-c)\epsilon^\beta + \mu^2(|x-c|+\epsilon)^{2\beta}.$$

Here we have introduced $2\delta(x-c)$ to represent the limiting form

$$\lim_{\gamma \downarrow 1}(\gamma-1)\,|x-c|^{\gamma-2} = 2\delta(x-c),$$

valid for continuous test functions of compact support. In this form, it is easy to see that $V_\epsilon(x)$ is a regularization of $|x-c|^{\beta-1}$, $\beta>0$, the latter two terms either vanishing as $\epsilon \downarrow 0$ or remaining completely "harmless" (i.e., not influencing our general conclusions). Hence, apart from such "harmless" terms, we may interpret the "solution" $B(x,t)$ as applying to $V = |x-c|^{-\alpha}$, where $\alpha = 1-\beta < 1$, and where $\lambda = \mu\beta/2 > 0$. While a general discussion of the stochastic equation is given later, it is fairly clear as $\lambda \downarrow 0$ (here arranged by $\mu \downarrow 0$) that $Y(t) \to W(t)$ and $\mu_Y \to \mu_W$, as found earlier.

So convenient is the picture provided by γ rapidly approaching unity with ϵ that we shall henceforth adopt such a procedure; indeed, we shall go so far as to *omit* the intermediate stage of discussion and *only present the resultant expressions that arise as* $\gamma \downarrow 1$.

Behavior for $1 \leqslant \alpha < 3/2$

Consider first the open interval $1 < \alpha < 3/2$ and choose the "solution"

$$B(x,t) = \exp[-\mu(|x-c|+\epsilon)^{1-\beta}/(1-\beta)]$$

with μ as before, but now with $0 < \beta < 1/2$. In the interval $0 \leqslant t \leqslant .99T$ it follows that

$$a(x,t) = -\mu\,\mathrm{sgn}(x-c)(|x-c|+\epsilon)^{-\beta}$$

and

$$2\lambda V_\epsilon(x) = \beta\mu(|x-c|+\epsilon)^{-\beta-1} - 2\mu\delta(x-c)\epsilon^{-\beta} + \mu^2(|x-c|+\epsilon)^{-2\beta} \tag{3.6}$$

Since $2\beta < 1$ the last term in V_ϵ is "harmless" and its "null" effects have just been established. We set $\lambda = \beta\mu/2 > 0$ and note that we deal here with a regularization of $|x-c|^{-\alpha}$ for $1 < \alpha < 3/2$. The contribution of the δ function blows up as $\epsilon \downarrow 0$; nevertheless, *this term just precisely regularizes the first term in the sense of Eq.* (2.6). The idealization that $\gamma = 1$ has enabled us to bring the regularizing term into clear evidence. In addition, Eq. (2.7) is satisfied, apart, of course, from the last "harmless" term in (3.6).

We defer a discussion of the stochastic equation but do note that the paths $Y(t)$ exist and are unique for $\epsilon > 0$, and pass to continuous paths as $\epsilon \downarrow 0$. Finally, as $\lambda \downarrow 0$ ($\mu \downarrow 0$ here) the paths $Y(t) \to W(t)$ and all traces of the potential disappear, as one would expect from our former analysis.

For $\alpha = 1$ choose

$$B(x,t) = \exp\{\mu(|x-c|+\epsilon)[\ln(|x-c|+\epsilon)-1]\},$$

with μ as before. Then, for $0 \leqslant t \leqslant .99T$,

$$a(x,t) = \mu\,\mathrm{sgn}(x-c)\ln(|x-c|+\epsilon)$$

and

$$2\lambda V_\epsilon(x) = \mu(|x-c|+\epsilon)^{-1} + 2\mu\delta(x-c)\ln\epsilon + \mu^2[\ln(|x-c|+\epsilon)]^2.$$

The last term is "harmless" while the second term provides just the correct regularization for the first term in the sense of (2.6). When $\epsilon \downarrow 0$ followed by $\lambda \downarrow 0$ (here $\lambda = \mu/2$), it follows rather clearly that the paths $Y(t) \to W(t)$, etc., as is appropriate.

Additional remarks

Remark 1: The analysis given above for $1 \leqslant \alpha < 3/2$ does not contain the arbitrary parameter K that was encountered earlier [cf. Eq. (2.6)]. This is readily corrected if we take any of our given "solutions" $B(x,t) \equiv B_{\text{old}}(x,t)$ and introduce $B_{\text{new}}(x,t)$ by

$$B_{\text{new}}(x,t) \equiv \exp[k\mu(|x-c|+\epsilon)]\,B_{\text{old}}(x,t)$$

where μ is as before and k is a constant to be chosen. The so modified B leads to

$$a_{\text{new}} = a_{\text{old}} + k\mu\,\mathrm{sgn}(x-c)$$

and

$$2\lambda V_{\epsilon\ \text{new}} = 2\lambda V_{\epsilon\ \text{old}} + 2k\mu\delta(x-c) + 2k\mu\,\mathrm{sgn}(x-c)a_{\text{old}} + k^2\mu^2.$$

Apart from additional "harmless" terms, we have evidently been able to affect the integral of the potential in the vicinity of the singularity. In each case k can be chosen so that (2.6) holds for any pregiven K.

For convenience we shall omit from future discussion the arbitrariness illustrated here.

Remark 2: We briefly outline the "solution" for $1 < \alpha < 3/2$ corresponding to nonnegative regularizations and which leads to absorbing Brownian motion. (An analogous discussion for $\alpha = 1$ is omitted.) Let

$$B(x,t) = (|x-c|+\epsilon)^\sigma \exp[\mu(|x-c|+\epsilon)^{1-\beta}/(1-\beta)] \tag{3.7}$$

where μ is as before, $0 < \beta < 1/2$, and $\sigma \equiv 1$ for $0 \leqslant t \leqslant .99T$, while σ falls smoothly for $.99T \leqslant t \leqslant T$ such that $\sigma(T) = 0$. We note that *by itself* the first factor is a simplified "solution" descriptive of (the essential fea-

tures of) absorbing Brownian motion. The complete "solution" (3.7) leads, in the interval $0 \leq t \leq .99T$, to

$$a(x,t) = \operatorname{sgn}(x-c)[(|x-c|+\epsilon)^{-1} + \mu(|x-c|+\epsilon)^{-\beta}]$$

and, for $x \neq c$,

$$2\lambda V_\epsilon(x) = \mu(2-\beta)(|x-c|+\epsilon)^{-1-\beta} + \mu^2(|x-c|+\epsilon)^{-2\beta}.$$

In the limit $\epsilon \downarrow 0$, we have already observed [in connection with Eq. (3.5) and subsequent discussion] that the drift term $a(x,t)$ is such that with probability 1 no path ever reaches the singularity and thus the behavior of V at $x=c$ is immaterial. Consequently, the present "solution" may be interpreted as a regularized form of $|x-c|^{-\alpha}$, $1<\alpha<3/2$, with $\lambda = \mu(1-\beta/2) > 0$, such that as $\lambda \downarrow 0$ (i.e., $\mu \downarrow 0$) absorbing Brownian motion, and not standard Brownian motion arises. The big, bold clue to this behavior can be read directly from the expression for the drift term!

B. Inequivalent processes

The reason Eq. (3.6) fails to apply for $\alpha \geq 3/2$ is that for $2\beta \geq 1$ the last term in the potential is no longer "harmless." This fact suggests the introduction of one or more *counter terms* chosen to *cancel* the "harmful" terms and to ensure that only "harmless" terms remain. With this simple argument as motivation, we now treat cases where $\alpha \geq 3/2$. In order to avoid logarithmic terms in the initial analysis we confine ourselves to the restricted set of α values that satisfy

$$1 + \frac{J-1}{J} < \alpha < 1 + \frac{J}{J+1}$$

for some $J = 2, 3, 4, \cdots$. Observe that such α respect the general condition $3/2 < \alpha < 2$.

Case $3/2 < \alpha < 2$ (no logarithmic terms)

The "solution" for B is a straightforward generalization of those given earlier. Let

$$B(x,t) = \exp\left(-\sum_{j=1}^{J} f_j \mu^j (|x-c|+\epsilon)^{(1-\beta_j)}/(1-\beta_j)\right), \tag{3.8}$$

where $f_1 \equiv 1$ and the remaining f_j are constants to be determined, μ is as before and μ^j is the jth power of μ, and β_j are positive parameters ordered so that $1 > \beta_1 > \beta_2 > \cdots > \beta_J > 0$, where $J = 2, 3, \cdots$ is chosen so that

$$(J-1)/J < \beta_1 \equiv \alpha - 1 < J/(J+1). \tag{3.9}$$

Final specification of f_j and β_j, $j \geq 2$, appears below.

From the "solution" given above we find, for $0 \leq t \leq .99T$, that

$$a(x,t) \equiv -\sum_{j=1}^{J} f_j \mu^j (|x-c|+\epsilon)^{-\beta_j} \operatorname{sgn}(x-c) \tag{3.10}$$

and (from the fact that $2\lambda V = \partial a/\partial x + a^2$)

$$2\lambda V_\epsilon(x) \equiv \sum_{j=1}^{J} f_j \beta_j \mu^j (|x-c|+\epsilon)^{-1-\beta_j} - 2\delta(x-c)\sum_{j=1}^{J} f_j \mu^j \epsilon^{-\beta_j} + \sum_{n,m=1}^{J} f_n f_m \mu^{n+m}(|x-c|+\epsilon)^{-\beta_n-\beta_m}. \tag{3.11}$$

We assume the leading term in the potential, namely

$$\beta_1 \mu (|x-c|+\epsilon)^{-1-\beta_1},$$

is the term of interest with $\lambda = \beta_1\mu/2$, and we choose the remaining parameters to cancel all potentially "harmful" terms. Since this cancellation must hold identically in μ, we require that

$$1 + \beta_j = \beta_n + \beta_m, \quad \text{for } n+m=j,$$

and

$$f_j \beta_j = -\sum_{n+m=j} f_n f_m,$$

for all j, $2 \leq j \leq J$. The solution of the β equation is simply

$$\beta_n = 1 - (1-\beta_1)n, \quad n = 1, \ldots, J. \tag{3.12}$$

The f_j are determined uniquely but no equally simple solution can be given for them in the general case.

The cancellation between first and last terms in the potential is not complete and the remainder is given by

$$\sum_{n+m \geq J+1} f_n f_m \mu^{n+m}(|x-c|+\epsilon)^{-\beta_n-\beta_m}.$$

But *all such terms are "harmless"* since

$$\beta_n + \beta_m = 2 - (1-\beta_1)(n+m) \leq 2 - (1-\beta_1)(J+1) < 1,$$

as follows from (3.9) and (3.12). It is of course this very property that dictates the number of counter terms in the first place.

In summary, therefore, the conditions imposed imply that the "solution" (3.8) corresponds to

$$2\lambda V_\epsilon(x) = \beta_1\mu(|x-c|+\epsilon)^{-1-\beta_1} - 2\delta(x-c)\sum_{j=1}^{J} f_j \mu^j \epsilon^{-\beta_j} + \text{h.t.}, \tag{3.13}$$

where h.t. denotes "harmless terms," and $\lambda \equiv \beta_1\mu/2$. The essential distinction for $\alpha \geq 3/2$, when compared to $\alpha < 3/2$, is that *λ-dependent regularizations are required*, as manifested by the power series in μ that appears as a coefficient of $\delta(x-c)$. A moment's thought will convince the reader that this fact prohibits the almost sure convergence of

$$Q_\epsilon = \int_0^T V_\epsilon(x(t))\, dt,$$

as $\epsilon \downarrow 0$, whenever $\alpha \geq 3/2$, which fact means that in the limit $\epsilon \downarrow 0$ the measures μ_γ for distinct λ values are mutually singular for $c=0$ (or for the subset of paths that reach c if $c \neq 0$).

Finally, we observe that with the drift term (3.10) the sample paths pass to Wiener paths in the appropriate limits since the characteristic clue for absorbing Brownian motion is absent. (This fact will be discussed further below).

Case $3/2 \leq \alpha < 2$ (logarithmic terms)

We complete the analysis for $\alpha < 2$ by considering those cases where

$$(J-1)/J = \beta_1 = \alpha - 1, \quad J = 2, 3, \cdots.$$

In this case $B(x,t)$ is as above except that the *last* factor (where $j=J$) is given by

$$\exp\{f_J \mu^J (|x-c|+\epsilon)[\ln(|x-c|+\epsilon) - 1]\} \tag{3.14}$$

rather than by the form implicit in (3.8). As a consequence, the formulas for a and V_ϵ are changed so that

$$a(x,t)=f_J\mu^J \ln(|x-c|+\epsilon)\ \mathrm{sgn}(x-c) + \{\text{Eq. (3.10) with } J \text{ replaced by } J-1\} \tag{3.15}$$

and

$$\begin{aligned}2\lambda V_\epsilon(x)=&f_J\mu^J(|x-c|+\epsilon)^{-1}+2\delta(x-c)f_J\mu^J\ln\epsilon\\&+[f_J\mu^J\ln(|x-c|+\epsilon)]^2\\&+2f_J\mu^J\ln(|x-c|+\epsilon)\,\mathrm{sgn}(x-c)\\&\times\{\text{Eq. (3.10) with } J \text{ replaced by } J-1\}\\&+\{\text{Eq. (3.11) with } J \text{ replaced by } J-1\}.\end{aligned} \tag{3.16}$$

The previous equations for β_j and f_j hold for all j, where now $2\leq j\leq J-1$. (If $J=2$ those equations are empty.) The relation for $j=J$ is replaced by

$$1=\beta_n+\beta_m,\quad n+m=J,$$

$$f_J=-\sum_{n+m=J} f_nf_m.$$

Since $\beta_1=(J-1)/J$ the solution for β_n is given by $\beta_n=1-n/J$, $n=1,\ldots,J-1$, and f_n is determined accordingly. Again the remaining terms are "harmless" being of the form $[\ln(|x-c|+\epsilon)]^2$,

$$\ln(|x-c|+\epsilon)(|x-c|+\epsilon)^{-\beta_j},\ \beta_j<1,$$

or

$$(|x-c|+\epsilon)^{-\beta_n-\beta_m},\ n+m\geq J+1,$$

where

$$\beta_n+\beta_m=2-(n+m)/J\leq 1-1/J<1.$$

In summary, if $\beta_1+1\equiv\alpha=1+(J-1)/J$, $J=2,3,\cdots$, and the relevant conditions for β_j and f_j hold, then the "solution" $B(x,t)$ in (3.8) as modified by (3.14) applies to the potential

$$2\lambda V_\epsilon(x)=\beta_1\mu(|x-c|+\epsilon)^{-1-\beta_1} - 2\delta(x-c)\left(\sum_{j=1}^{J-1} f_j\mu^j\epsilon^{-\beta_j}-f_J\mu^J\ln\epsilon\right)+\text{h.t.} \tag{3.17}$$

With this regularization the drift term $a(x,t)$ in (3.15) reduces to zero in the appropriate limits establishing that all traces of the interaction vanish.

Apart from a discussion of the stochastic equations, this concludes our analysis for the range $3/2\leq\alpha<2$.

Case $\alpha=2$

Nonperturbative Analysis: For $\alpha=2$ choose

$$B(x,t)=(|x-c|+\epsilon)^\theta \tag{3.18}$$

where $\theta=\text{const}$ for $0\leq t\leq .99T$, and θ goes smoothly to zero thereafter so that $\theta(T)=0$. In the interval $0\leq t\leq .99T$,

$$a(x,t)=\theta\ \mathrm{sgn}(x-c)(|x-c|+\epsilon)^{-1} \tag{3.19}$$

and

$$2\lambda V_\epsilon(x)=\theta(\theta-1)(|x-c|+\epsilon)^{-2}+2\theta\delta(x-c)\epsilon^{-1}. \tag{3.20}$$

Assume that paths are found from the stochastic equation, and the limit $\epsilon\downarrow 0$ is taken. With $\lambda\equiv\theta(\theta-1)/2$, we observe that two ways for $\lambda\downarrow 0$ are possible. In one such way, $\lambda\downarrow 0$ by $\theta\downarrow 0$, which has the effect of reducing the drift term to zero and leading to a vanishing of the interaction effects. In the other way, $\lambda\downarrow 0$ by $\theta\downarrow 1$, for which $a(x,t)\to(x-c)^{-1}$, appropriate to the absorbing Brownian motion (in our approximate "solution" sense, of course). In addition, from our analysis of nonnegative regularizations in Sec. 2 we know that absorbing Brownian motion also arises as $\lambda\downarrow 0$ by $\theta\downarrow 1$ with just the basic regularization and without requiring the δ-function term in (3.20).

In summary, with the "solution" (3.18) and $\theta<0$ the regularization ensures the effects of the potential vanish as $\lambda\downarrow 0$ ($\theta\uparrow 0$). Solving for θ we may express this special regularization in the form

$$V_\epsilon(x)=(|x-c|+\epsilon)^{-2}-\frac{4\epsilon^{-1}\delta(x-c)}{1+\sqrt{1+8\lambda}}, \tag{3.21}$$

which illustrates an involved dependence on the coupling λ. The singularity in this expression at $\lambda=-1/8$ arises simply from the fact that for real θ, $\lambda=\theta(\theta-1)/2\geq -1/8$, but this fact need not concern us here. On the other hand, there is another restriction on θ that limits the validity of (3.21).

It is of fundamental importance to understand that θ is *not* arbitrary and that *we must require* $\theta>-1$. Although $B(x,t)$ in (3.18) is only an approximate "solution," it is essentially accurate near the singularity $x=c$ and in the range $0\leq t\leq .99T$. Clearly, after $\epsilon\downarrow 0$, $B(x,t)$ is *not* locally integrable at the singularity *unless* $\theta>-1$, and this holds for all t, $0\leq t\leq .99T$.

The importance of this fact may be seen as follows. Let

$$p_Y(x,t)\equiv\int\delta(x-x(t))\,d\mu_Y(x) \tag{3.22}$$

denote the normalized density of Y paths at $(x,t)\in R\times[0,T]$. Then it follows that[9]

$$p_Y(x,t)=B(x,t)\,\psi(x,t)/B(0,0) \tag{3.23}$$

where $\psi(x,t)$ is the function determined by Eqs. (1.10) and (1.11). Of course, B and ψ are closely related; if $\psi(x,t;z)$ denotes the solution of (1.10) subject to $\psi(x,0;z)=\delta(x-z)$, then $\psi(x,t)=\psi(x,t;0)$ and $B(x,t)=\int\psi(x,T-t;z)\,dz$. Conversely, in order to be acceptable, two functions $\psi(x,t)$ and $B(x,t)$ that satisfy the proper differential equation and boundary conditions must necessarily also satisfy $B(x,t)\psi(x,t)\in L^1$ for almost all t, $0\leq t\leq T$, since $p_Y(x,t)$ is integrable. In general, any singularity in $B(x,t)$ is not cancelled by a corresponding vanishing of $\psi(x,t)$, and thus a generally necessary condition is that $B(x,t)$ must be locally integrable for almost all t. [By symmetry, similar remarks apply to the function $\psi(x,t)$ which should be integrable according to Eq. (1.9).]

For θ in the range $-1<\theta\leq 0$, it follows that $0\leq\lambda<1$, i.e., λ is bounded above. Equation (3.21) has validity only for $0<\lambda<1$. On the other hand, larger values of λ may always be reached with the $\theta>1$ solutions. To generate a family of potentials for all $\lambda>0$ that eliminate interaction effects as $\lambda\downarrow 0$, it is possible (even if un-

esthetic) to choose $\theta > 1$ solutions for large λ values and to switch to $\theta < 0$ solutions as λ is reduced and when the integrability condition allows. Precisely the same viewpoint is needed to generate similar behaving solutions in the related Schrödinger problem.[3]

Perturbative Analysis: It is tempting to ask whether the results for $\alpha = 2$ are in any way approximated by those for $\alpha < 2$ when J, the number of "subtraction terms," becomes very large. If this approximation is to make sense, then it must apply in the limit $J \to \infty$ for which $\beta_1 = 1$, and indeed $\beta_n = 1$ for all n. The equation for the f coefficients then becomes

$$f_j = -\sum_{m+m=j} f_n f_m, \quad j \geq 2. \tag{3.24}$$

With $\lambda = \beta_1 \mu/2 = \mu/2$, we may ask whether the coefficients of the regularization δ function in (3.13) and in (3.20) are the same; namely, whether

$$\sum_{j=1}^{\infty} f_j (2\lambda)^j = -\theta = \tfrac{1}{2}[\sqrt{1+8\lambda} - 1]. \tag{3.25}$$

Since $\theta(\theta - 1) = 2\lambda$, the sought for equality requires that

$$\sum f_j (2\lambda)^j + \sum f_n f_m (2\lambda)^{n+m} = 2\lambda,$$

a relation which formally holds *identically in* λ *term by term in virtue of* (3.24). Moreover, substitution of the relation $\theta = -\sum f_j \mu^j$, coupled with $\beta_n = 1$ for all n, converts Eqs. (3.10) and (3.11) for a and V_ϵ into Eqs. (3.19) and (3.20), respectively. Even $B(x,t)$ in (3.8) can be suitably rescaled (without essential change) so that in the limit $\beta_j \to 1$, for all j, the "solution" (3.18) is recovered.

By implication of the argument above, the perturbation series for θ converges absolutely for $0 \leq \lambda < 1/8$, to yield $\theta = \frac{1}{2}[1 - \sqrt{1+8\lambda}]$. For real $\lambda \geq 1/8$ the perturbation solution may be extended by analytic continuation or by standard summation techniques for divergent power series. However, the perturbation theory approach is connected only with the solutions where $\theta < 0$, namely, those for which all interaction effects vanish as $\lambda \to 0$ and yet which make sense for $\lambda < 1$. The nonperturbative solution, on the other hand, can avail itself of the $\theta > 1$ solutions for which λ can take on any positive value. These latter solutions cannot be reached through perturbation theory from the standard Wiener process, a fact that is wholly unrelated to the convergence or nonconvergence of the perturbation series. However, these "unreachable" solutions can be reached by perturbation theory taking the *absorbing* Wiener process as the "unperturbed" starting point; this is the viewpoint advocated in Ref. 2.

Case $\alpha > 2$

For $\alpha > 2$ there is only one form of $B(x,t)$ that is locally integrable, and this form inevitably leads to absorbing Brownian motion.

In the interval $0 \leq t \leq .99T$ choose

$$B(x,t) = X^{1/2} K_{1/(\alpha-2)}\left(\frac{2\sqrt{2\lambda}}{(\alpha-2)} X^{1-\alpha/2}\right), \tag{3.26}$$

where $X \equiv |x - c| + \epsilon$ and K_ν is the usual modified Bessel function. For $.99T \leq t \leq T$, however, we let $B(x,t)$ change smoothly so as to match the condition $B(x,T) \equiv 1$. The other possible form for $B(x,t)$ involves

$$X^{1/2} I_{1/(\alpha-2)}\left(\frac{2\sqrt{2\lambda}}{(\alpha-2)} X^{1-\alpha/2}\right).$$

In the limit $\epsilon \to 0$ only the first solution is locally integrable at the singularity for any $\lambda > 0$.

The solution $B(x,t)$ in (3.26) corresponds, in the interval $0 \leq t \leq .99T$, exactly to

$$V_\epsilon(x) = (|x - c| + \epsilon)^{-\alpha}, \quad x \neq c,$$

and leads to the drift term

$$a(x,t) \equiv \frac{\partial B(x,t)/\partial x}{B(x,t)}$$

Assume that the limit $\epsilon \to 0$ has been taken and let us study the form of the drift term as $\lambda \to 0$. This means we sit at fixed $|x - c| > 0$ and study the drift term for small λ. For simplicity we assume $(\alpha - 2)^{-1} \equiv \nu > 0$ is not an integer. Then to obtain the limiting behavior as $\lambda \to 0$ it suffices to use

$$K_\nu(z) \propto z^{-\nu}[1 + O(z^{2\delta})],$$

where $\delta \equiv \min(1, \nu)$, for which

$$B(x,t) \propto X[1 + O(\lambda^\delta X^{-\delta/\nu})]$$

where $X \equiv |x - c|$. Consequently,

$$a(x,t) = (x - c)^{-1} + O(\lambda^\delta)$$

which shows that as $\lambda \to 0$ *all* such processes for $\alpha > 2$ limit to absorbing Brownian motion. A parallel argument leads to the same result for $(\alpha - 2)^{-1} = m$, $m = 1, 2, \ldots$.

C. Discussion of stochastic equations

As evident from the preceding discussion, we must deal with stochastic differential equations of the form

$$dY(t) = a(Y(t), t)\, dt + dW(t) \tag{3.27}$$

for a variety of choices of the drift term $a(x,t)$. Toward the beginning of this section, we discussed a form of the drift coefficients in which there appeared a parameter γ that rapidly approached one with ϵ [e.g., $\gamma = 1 + \exp(-\epsilon^{-137})$]. Typical of the form taken by $a(x,t)$ when the parameter γ is made explicit is the expression

$$a(x,t) = -\mu\ \mathrm{sgn}(x - c)\, |x - c|^{\gamma-1} (|x - c|^\gamma + \epsilon^\gamma)^{-\beta} \tag{3.28}$$

which is valid in the interval $1 < \alpha = \beta + 1 < 3/2$ and for $0 \leq t \leq .99T$. Inspection of the relevant expressions applicable in the range $0 < \alpha \leq 2$ ensure that in each case $a(x,t)$ is *continuous and satisfies the bound*

$$|a(x,t)|^2 \leq K(1 + x^2)$$

for some $K < \infty$. In view of the simple form (namely unity) of the diffusion coefficient, these properties for $a(x,t)$ are sufficient conditions[15] to *guarantee the existence and uniqueness of a continuous solution* $Y(t)$ with probability one for every $\epsilon > 0$. As $\epsilon \to 0$, however, the bound on $a(x,t)$ tends to infinity and there is no obvious guarantee that the resultant paths are continuous.

In order to discuss the behavior of the paths $Y(t)$ as $\epsilon \to 0$, we probe more deeply into the behavior of the

paths near the singularity by exploiting the following simple transformation. For each path $Y(t)$ and $\epsilon > 0$ let us introduce the path

$$Z(t) \equiv f(Y(t)) = (Y(t) - c)^3.$$

This transformation is evidently invertible in the form

$$Y(t) - c = Z^{1/3}(t) \equiv \operatorname{sgn}(Z(t)) \, |Z(t)|^{1/3}.$$

Since $Y(0) = 0$, $Z(0) = -c^3$ and, in addition, the "trouble point" $Y(t) = c$ has been (arbitrarily) mapped into $Z(t) = 0$. At any rate $Z(t)$ satisfies a stochastic differential equation in virtue of the fact that $Y(t)$ satisfies one. Specifically,

$$dZ(t) = f'(Y(t))\, dY(t) + \tfrac{1}{2} f''(Y(t))\, dt,$$

so that if $Y(t)$ fulfills (3.27) then

$$dZ(t) = \bar{a}(Z(t), t)\, dt + \bar{\sigma}(Z(t), t)\, dW(t), \tag{3.29a}$$

where

$$\bar{a}(Z(t), t) \equiv 3Z^{1/3}(t) + 3\,|Z(t)|^{2/3}\, a(c + Z^{1/3}(t), t), \tag{3.29b}$$

$$\bar{\sigma}(Z(t), t) \equiv 3\,|Z(t)|^{2/3}. \tag{3.29c}$$

For the typical form of $a(x, t)$ given in (3.28) this new stochastic equation becomes, in the interval $0 \leq t \leq .99T$,

$$dZ(t) = 3Z^{1/3}(t)\left(1 - \frac{\mu\,|Z(t)|^{\gamma/3}}{(|Z(t)|^{\gamma/3} + \epsilon^{\gamma})^{\beta}}\right) dt + 3\,|Z(t)|^{2/3}\, dW(t). \tag{3.30}$$

Although (3.30) itself does not have a unique solution, it does have a unique continuous solution when we require as well that $Z^{1/3}(t) + c$ satisfy (3.27) with (3.28).

In the formulation in terms of Z paths the drift and diffusion coefficients remain locally bounded as $\epsilon \downarrow 0$ and fulfill a condition of the form

$$|\bar{a}(x, t)|^2 + |\bar{\sigma}(x, t)|^2 \leq K(1 + x^2)$$

for some $K < \infty$ uniformly in ϵ. Moreover, the drift and diffusion terms are both continuous uniformly in ϵ. These properties hold not only in the example illustrated by (3.30) where $0 < \beta < \frac{1}{2}$, but in the more general cases considered involving sums of terms each of which has $\beta_j \leq 1$. In view of these facts, we are assured that the limiting equation as $\epsilon \downarrow 0$, i.e.,

$$dZ(t) = 3Z^{1/3}(t)\,[1 - \mu\,|Z(t)|^{(1-\beta)/3}]\, dt + 3\,|Z(t)|^{2/3}\, dW(t), \tag{3.31}$$

for $0 < \beta < \frac{1}{2}$ and $0 \leq t \leq .99T$, has a continuous solution with probability one. [15]

To help understand the stochastic equations for the Z paths it is helpful to consider the simple example

$$Z(t) = (W(t) - c)^3$$

for $W(t)$ a standard Brownian motion. Then it follows that

$$dZ(t) = 3Z^{1/3}(t)\, dt + 3\,|Z(t)|^{2/3}\, dW(t). \tag{3.32}$$

Observe that as $\mu \downarrow 0$ ($\lambda \downarrow 0$), Eq. (3.31) passes continuously into Eq. (3.32) suggesting that the Y paths pass to Wiener paths and that the final distribution corresponds to Brownian motion. Thus, all traces of the potential disappear.

In case the final distribution is absorbing Brownian motion we are still assured of continuous paths when $\epsilon \downarrow 0$. To illustrate this we adopt the form of $a(x, t)$ implicit in Remark 2 above. In the interval $1 < \alpha = \beta + 1 < 3/2$ this leads to a stochastic equation for $Z(t)$ of the form ($0 \leq t \leq .99T$)

$$dZ(t) = 3Z^{1/3}(t)\left(1 + \frac{|Z(t)|^{\gamma/3}}{|Z(t)|^{\gamma/3} + \epsilon^{\gamma}} + \frac{\mu\,|Z(t)|^{\gamma/3}}{(|Z(t)|^{\gamma/3} + \epsilon^{\gamma})^{\beta}}\right) dt, + 3\,|Z(t)|^{2/3}\, dW(t). \tag{3.33}$$

This equation has with probability 1 a continuous solution for every $\epsilon > 0$ that is made unique by requiring that $Z^{1/3}(t) + c$ satisfy the Y form of the stochastic equation. The limiting equation as $\epsilon \downarrow 0$ reads

$$dZ(t) = 3Z^{1/3}(t)[2 + \mu\,|Z(t)|^{(1-\beta)/3}]\, dt + 3\,|Z(t)|^{2/3}\, dW(t) \tag{3.34}$$

which has a continuous solution with probability 1. Lastly, when $\mu \downarrow 0$ ($\lambda \downarrow 0$) the resultant equation

$$dZ(t) = 6Z^{1/3}(t)\, dt + 3\,|Z(t)|^{2/3}\, dW(t) \tag{3.35}$$

is easily seen to be solved by

$$Z(t) = [W_1^2(t) + W_2^2(t) + (W_3(t) - c)^2]^{3/2},$$

which is just our Bessel process idealization of absorbing Brownian motion. Observe the extremely simple relationship in the Z-path description between Eqs. (3.32) and (3.35), which are the stochastic equations for Wiener and (idealized) absorbing Wiener processes, respectively.

We now proceed to show the existence of a limiting process as $\epsilon \downarrow 0$. For each $\epsilon > 0$ we have a unique continuous family of Y paths with probability 1, which with probability 1 satisfy the Z form of the stochastic differential equation where $Z(t) = (Y(t) - c)^3$. This means we have for each $\epsilon > 0$ a measure on path space for the Y paths (μ_Y) and another one for the Z paths (μ_Z, say). From compactness arguments we shall show convergence of a subsequence of the measures μ_Z as $\epsilon \downarrow 0$, which in turn shows convergence of a subsequence of the measures μ_Y as $\epsilon \downarrow 0$. According to (3.29) we have

$$|Z(t) - Z(t_0)| \leq \left| \int_{t_0}^{t} \bar{a}(Z(s), s)\, ds \right| + 3 \left| \int_{t_0}^{t} |Z(s)|^{2/3}\, dW(s) \right|,$$

which leads directly to the relation

$$\langle |Z(t) - Z(t_0)|^4 \rangle \leq 8\left(\langle \left| \int_{t_0}^{t} \bar{a}(Z(s), s)\, ds \right|^4 \rangle + 81 \langle \int_{t_0}^{t} |Z(s)|^{2/3}\, dW(s) \Big|^4 \rangle \right).$$

We next note that [15]

$$\langle \left| \int_{t_0}^{t} |Z(s)|^{2/3}\, dW(s) \right|^4 \rangle \leq 36(t - t_0) \int_{t_0}^{t} \langle |Z(s)|^{8/3} \rangle\, ds.$$

For Z large (i.e., $Y - c$ large) the paths are well behaved and for all intents and purposes are Wiener-like. Only near $Z \approx 0$ are the paths significantly changed, but this does not prevent us from putting a bound on the

previous averages that leads to

$$\langle |Z(t) - Z(t_0)|^4 \rangle \leq K(t - t_0)^2$$

for some $K < \infty$, uniformly in ϵ. This gives a sufficient compactness condition to ensure that a subsequence of path space distributions weakly converges to a path space distribution as $\epsilon \downarrow 0$. [17] From the convergence of the drift term, it is clear that every convergent subsequence of distributions has the same limit, and therefore that in fact the path space distributions weakly converge to a path space distribution as $\epsilon \downarrow 0$. In addition, results of Skorokhod[15] ensure that the paths $Z(t)$ converge as $\epsilon \downarrow 0$ with probability 1 to paths $Z(t)$ for $\epsilon = 0$, and that moreover those paths satisfy the appropriate limiting stochastic equation. Consequently, the Y paths satisfy their limiting stochastic equation, suitably interpreted, with probability one.

A parallel argument based on the limit $\mu \downarrow 0$ (i.e., $\lambda \downarrow 0$) leads to the weak convergence of the relevant path space distributions as well as a convergence of the associated paths with probability one. In this way we establish the claimed properties of the paths and distributions as the limits $\epsilon \downarrow 0$ and $\lambda \downarrow 0$ are taken. The ultimate distributions are those of either the Wiener process or the absorbing Wiener process depending on the ultimate form of the drift term.

SUMMARY

In quantum mechanics as well as diffusion theory there are perturbations so singular that they leave indelible imprints on systems after the coupling coefficient is reduced to zero, which we have termed vestigial effects. The simple example of a particle moving in a singular, one-dimensional potential is used to emphasize that such vestigial effects can clearly be displayed in terms of Feynman–Kac integrals on path space, their associated measures and the closely related stochastic differential equations. The vestigial effects can be controlled by adding counter terms to the potential, and this in fact constitutes one way of defining different self-adjoint extensions of a formal Hamiltonian operator. The cases with $V(x) = |x - c|^{-\alpha}$, $1 \leq \alpha \leq 2$, are already indicative of what may happen in quantum field theory where very singular perturbations abound and helpful mathematical pictures are needed.

ACKNOWLEDGMENTS

We are grateful to V. E. Beneš and J. A. Morrison for helpful discussions.

APPENDIX A

We are interested in the asymptotic behavior as $\epsilon \downarrow 0$ of

$$F_\epsilon(T) = \langle \exp(-\lambda_1 \int_0^T (|x(t)| + \epsilon)^{-1}\, dt - \lambda_2 \int_0^T (|x(t)| + \epsilon)^{-2}\, dt) \rangle, \tag{A1}$$

with

$$\lambda_1 \geq 0, \quad -\tfrac{1}{4} \leq 2\lambda_2 \leq \tfrac{3}{4}, \tag{A2}$$

which we shall obtain by solving the Feynman–Kac differential equation (1.10). In this appendix, we shall discuss the cases with $\lambda_1 = 0$, $\lambda_2 \gtrless 0$ and $\lambda_1 > 0$, $\lambda_2 > 0$. The results with the cases $\lambda_2 > 0$ have been presented in (2.4).

Let the Laplace transform on T of $\psi(x, T)$ be denoted by $\tilde{\psi}(x, s)$ and its abscissa of convergence by σ. The formula (1.9) then involves the inverse Laplace transformation,

$$F_\epsilon(T) = \frac{1}{2\pi i} \int_C ds\, \exp(sT) \int_{-\infty}^{\infty} dx\, \tilde{\psi}(x, s), \tag{A3}$$

where the contour C on the complex s plane is a straight line parallel to the imaginary axis and lying to the right of $s = \sigma$. The differential equation (1.10) and the boundary condition become

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{\lambda_1}{|x| + \epsilon} + \frac{\lambda_2}{(|x| + \epsilon)^2} + s \right) \tilde{\psi}(x, s) = 0, \tag{A4}$$

$$[d\tilde{\psi}/dx]_{x=0^-} = [d\tilde{\psi}/dx]_{x=0^+} + 2, \tag{A5}$$

and

$$\psi(x, s) \underset{x \to \pm\infty}{\to} 0 \quad (s > 0). \tag{A6}$$

The function $\psi(x, s)$ thus defined for $s > 0$ is to be continued analytically over the complex s plane.

The solutions to (A4) are the Whittaker functions, [18] $W_{k,m}(z)$ and $M_{k,m}(z)$ with

$$z = \alpha[|x| + \epsilon] \tag{A7}$$

and

$$\alpha = (8s)^{1/2}, \quad k = -2\lambda_1/\alpha, \quad m^2 - \tfrac{1}{4} = 2\lambda_2. \tag{A8}$$

We take the convention that $s^{1/2}$ be defined on the s-plane cut along the negative real axis such that $s^{1/2} = \sqrt{s}$ for $s > 0$.

We note here that, due to the restriction $\lambda_1 \geq 0$ in (A2), the parameter k ranges, if at all, only over the left-hand half of its complex plane as s varies over the cut plane of its own; this fact will be found to have a vital importance for the analyticity properties of $\tilde{\psi}(x, s)$. The restriction of λ_2 in (A2) enables us to use a real parameter μ as defined by

$$\mu(\mu + 1) = 2\lambda_2, \quad -\tfrac{1}{2} \leq \mu < 1. \tag{A9}$$

The Whittaker functions behave asymptotically as follows:

As $|z| \to \infty$, $|\arg z| < \pi/2$ (which cases are all we need),

$$M_{k,m}(z) = \frac{\Gamma(2 + 2\mu)}{\Gamma(1 - k + \mu)}\, z^{-k} \exp(z/2)[1 + O(z^{-1})],$$

$$W_{k,m}(z) = z^k \exp(-z/2)[1 + O(z^{-1})]. \tag{A10}$$

When $z \to 0$, however, two cases have to be distinguished. Namely, if $\mu \neq 0$

$$M_{k,m}(z) = z^{1+\mu} + O(z^{2+\mu}),$$

$$W_{k,m}(z) = \frac{\pi \exp(-z/2)}{\sin 2\mu\pi} \left(-\frac{k + \mu}{\Gamma(1 - k - \mu)\Gamma(2 + 2\mu)}\, z^{1+\mu} \right.$$

$$\left. + \frac{1}{\Gamma(1 - k + \mu)\Gamma(1 - 2\mu)} \{2\mu z^{-\mu} + (k + \mu) z^{1-\mu}\} \right.$$

$$+O(z^{2-|\mu|})\Big), \tag{A11}$$

and if $\mu=0$, the second function must be understood as $\lim_{\mu\to 0} W_{k,1/2+\mu}$, so that

$$M_{k,m}(z)\big|_{\mu=0} = z + O(z^2),$$

$$W_{k,m}(z)\big|_{\mu=0} = \frac{1}{\Gamma(1-k)}\,[1 - z/2 - kz\{\Psi(1-k) - 2\Psi(1) - 1\}$$

$$- kz\,\log z + O(z^2\,\log z)], \tag{A12}$$

where $\Psi(\cdot)$ is the digamma function[19] and $\Psi(1) = -0.577\cdots$ is the negative of Euler's constant.

Now, we can write down the solution to the differential equation (A4) which satisfies the boundary conditions (A5) and (A6); it is

$$\tilde{\psi}(x,s) = N_\epsilon\, W_{k,m}(\alpha[|x| + \epsilon]) \tag{A13}$$

with the normalization constant

$$N_\epsilon = \{\alpha\cdot[-dW_{k,m}(z)/dz]_{z=\alpha\epsilon}\}^{-1}. \tag{A14}$$

Let, for $s>0$,

$$\int_{-\infty}^{\infty} \tilde{\psi}(x,s)\,dx = \frac{2}{\alpha^2}\,\frac{1}{[-dW_{k,m}(z)/dz]_{z=\alpha\epsilon}} \int_{\alpha\epsilon}^{\infty} W_{k,m}(t)\,dt$$

$$\equiv \epsilon^2 f(\alpha\epsilon, k), \tag{A15}$$

exhibiting that the s-dependence of this function comes only through

$$\alpha\epsilon = (8\epsilon^2 s)^{1/2} \quad \text{and} \quad k = -2\lambda_1/(8s)^{1/2}. \tag{A16}$$

Then, (A3) takes the form

$$F_\epsilon(T) = \frac{1}{2\pi i}\int_C \epsilon^2 f(\alpha\epsilon, k)\exp(sT)\,ds \tag{A17}$$

and we are interested in the limit as $\epsilon \downarrow 0$.

Before starting the evaluation of the integral, we have to study the analyticity of the integrand $f(\alpha\epsilon, k)$ on the complex s plane, thereby fixing the contour C of the integration. It is enough for our purpose to look at the positive real axis $s>0$, because, being a Laplace transform, $f(\alpha\epsilon, k)$ should be analytic on the part $\mathrm{Re}\, s > \sigma$ of the s plane if it is finite on the portion $s>\sigma$ of the real axis. The function $f(\alpha\epsilon, k)$ as defined by (A15) has three factors. All the first factor $2/\alpha^2 = 1/(4s)$ can possibly do is to produce a pole at $s=0$. [But, see (A30) and (B7).] Under the restriction (A2) of λ_1 and λ_2, the third factor is analytic all over the cut s plane except possibly at $s=0$, as one sees from the integral representation, valid for $\mathrm{Re}(1-k+\mu)>0$,

$$W_{k,m}(z) = [\Gamma(1-k+\mu)]^{-1}\, z^{1+\mu}\, 2^{-1-2\mu}$$

$$\times \int_0^\infty \exp(-\tfrac{1}{2} z\,\cosh\theta)\,\sinh^{1+2\mu}\theta\,\coth^{2k}(\tfrac{1}{2}\theta)\,d\theta, \tag{A18}$$

and the range of k as remarked earlier.

The analyticity of the second factor depends critically on λ_1 and λ_2. In the case of $\lambda_1,\ \lambda_2 \geq 0$, we shall show shortly that the derivative can have no zeros when $s \geq 0$. This implies, when combined with the analyticity of the other two factors, that $\sigma = 0$, which in turn implies that $f(\alpha\epsilon, k)$, being a Laplace transform with $\sigma=0$, is analytic everywhere on the right-hand half of the s plane. To prove $dW_{k,m}(z)/dz \neq 0$, $z \geq 0$, we look at (A4) to notice that $W_{k,m}(z) = N_\epsilon \psi(x)$ with $z = \alpha(x+\epsilon)$ is convex everywhere towards the x axis, i.e., $[d^2W_{k,m}(z)/dz^2]/W_{k,m}(z) > 0$, $z>0$. Then, $dW_{k,m}(z)/dz$ cannot change sign because it is continuous and has to vanish as $z\to\infty$.

Thus, in the case of $\lambda_1 \geq 0$, $\lambda_2 \geq 0$, we have found that $\sigma = 0$ and therefore that the contour C of the integral (A17) can be put on the imaginary axis of the s plane.

When $\lambda_1 = 0$, $\lambda_2 < 0$, the derivative vanishes at one point, say $z = z_0 > 0$ giving a pole to $f(\alpha\epsilon, 0)$. To see this, observe from (A18) that $W_{0,m}(z) > 0$ for $z>0$, which, if combined with the differential equation (A4), implies that $d^2W_{0,m}(z)/dz^2$ changes sign once and only once as z varies over the positive real axis. Then, taking into account that $dW_{0,m}(z)/dz > 0$, $d^2W_{0,m}(z)/d^2z < 0$ in the neighborhood of $z=0$ and that $W_{0,m}(z)\to 0$ as $z\to\infty$, one sees that $dW_{0,m}(z)/dz$ should vanish once and only once on the positive real z axis. In this case, $\sigma = (z_0/\epsilon)^2/8$.

Among the different cases specified by (A2) to be considered, the ones with $\lambda_1 = 0$ admit rigorous and simple arguments based upon the Tauberian theorem of the Laplace transformation. Let us discuss this case first.

The case of $\lambda_1 = 0$, $\lambda_2 > 0$

When $\lambda_1 = 0$, we have $k=0$ and f depends on s through $\alpha\epsilon = (8\epsilon^2 s)^{1/2}$ only. Because $\sigma = 0$ in this case, we can, by a change of variable to $u = \epsilon^2 s$, rewrite (A17) as

$$F_\epsilon(T) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} f([8u]^{1/2}, 0)\exp(uT/\epsilon^2)\,du, \tag{A19}$$

which is a function of T/ϵ^2 only. Note that $T/\epsilon^2 \to \infty$ as $\epsilon \to 0$ and the Tauberian theorem[20] provides the asymptotic evaluation of the integral.

In general, let the Laplace transform on t of $F(t)$ be $\tilde{F}(u)$ and the abscissa of convergence be σ. If,

(a) $F(t) \geq 0$, $t \geq 0$,

(b) $\sigma \geq 0$,

(c) $\tilde{F}(u) \sim C u^{-\gamma}$, $(C>0,\ \gamma>0)$ as $u \to 0$,

and further

(d) $F(t)$ is monotone decreasing,

then

$$F(t) \sim [C\gamma/\Gamma(1+\gamma)]t^{\gamma-1} \quad \text{as} \quad t\to\infty.$$

That $F(t) \equiv F_\epsilon(T)$, $t = T/\epsilon^2$ satisfies the conditions (a) and (b) is clear. The condition (d) is obvious from the definition (A1). The condition (c) for $F(u) \equiv f([8u]^{1/2}, 0)$ can be checked by the help of (A11):

$$f([8u]^{1/2}, 0) \sim C u^{-\gamma} \quad (u \to 0) \tag{A20}$$

with

$$\gamma = (1-\mu)/2$$

and

$$C = \frac{2^{(3\mu+1)/2}}{\pi^{1/2}}\,\frac{\Gamma(\mu)\Gamma(1+\mu/2)\Gamma((1-\mu)/2)}{\Gamma(2\mu+1)}.$$

where the formula

$$\int_0^\infty W_{0,m}(t)\,dt=\frac{2}{\pi^{1/2}}\ \Gamma\left(1+\frac{\mu}{2}\right)\Gamma\left(\frac{1-\mu}{2}\right) \tag{A21}$$

has been used.

By the theorem, thus, we can conclude that

$$F_\epsilon(T)\sim B\,\epsilon^{1+\mu}/T^{(1+\mu)/2}\ \text{ as } T/\epsilon^2\to\infty \tag{A22}$$

where $B=C/\Gamma([1-\mu]/2)$. This is a particular case of (2.4b).

The case of $\lambda_1=0$, $\lambda_2<0$

As we have seen before, the function $f(\alpha\epsilon,0)$ has a pole, say at $\alpha\epsilon=z_0$, or $s=(z_0/\epsilon)^2/8$, and is otherwise analytic all over the cut s plane; we should note that the behavior of $f(\alpha\epsilon,0)$ at $s=0$ as determined in (A20) is valid also here.

The use of the variable $u=\epsilon^2 s$ gives

$$F_\epsilon(T)=\frac{1}{2\pi i}\int_{C'} f([8u]^{1/2},0)\exp(uT/\epsilon^2)\,du, \tag{A23}$$

where C' is a contour parallel to the imaginary u axis and lying to the right of $\sigma=z_0^2/8$. Deforming the contour into $C_1'+C_2'$, where C_1' encircles the pole and C_2' is on the imaginary axis,

$$F_\epsilon(T)=A\exp[z_0^2T/(8\epsilon^2)]+\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} f([8u]^{1/2},0)\times\exp(uT/\epsilon^2)\,du.$$

The second term can be evaluated in the same way as in (A19) with the result $B\epsilon^{1+\mu}/T^{(\mu+1)/2}$. The coefficient of the first term is the residue at $u=z_0^2/8$ of $f([8u]^{1/2},0)$, i.e.,

$$A=\frac{1}{2z_0}\int_{z_0}^\infty W_{0,m}(t)\,dt\Big/\left[-\frac{d^2W_{0,m}(z_0)}{dz_0^2}\right]. \tag{A24}$$

Because $dW_{0,m}/dz>0$ as $z\downarrow 0$ and $z=z_0$ is the only place the derivative vanishes on the positive z axis, we see that $-d^2W_{0,m}(z_0)/dz_0>0$ and consequently $A>0$ as it should.

We can now conclude that, if $\lambda_1=0$, $\lambda_2<0$, then

$$F_\epsilon(T)\sim A\ \exp(aT/\epsilon^2)\to\infty\ \text{ as }\ \epsilon\to 0, \tag{A25}$$

where A and $a\equiv z_0^2/8$ are constants as determined by λ_2.

It may be interesting to remark that, if $0<-\mu\ll 1$ then (A11) gives

$$z_0\approx -2\mu,$$

which is close to 0. Consequently,

$$-d^2W_{0,m}(z_0)/dz_0^2\approx-\mu/z_0^2=1/(-4\mu)$$

by (A11) again, and

$$\int_{z_0}^\infty W_{0,m}(t)\,dt\approx 2$$

by (A21). Then, (A25) becomes

$$F_\epsilon(T)=2\ \exp[2^{-1}(\mu/\epsilon)^2T],\quad(\lambda_1=0,\ 0<-\lambda_2\ll 1). \tag{A26}$$

It is amusing to compare the results of this subsection with the simple and universal upper bound on $F_\epsilon(T)$ given by replacing all paths $x(t)$ by zero which leads to

$$F_\epsilon(T)=\langle\exp[-\lambda_2\textstyle\int_0^T(|x(t)|+\epsilon)^{-2}\,dt]\rangle \le\exp(|\lambda_2|T/\epsilon^2).$$

The case of $\lambda_1>0$, $\lambda_2\geqslant 0$

In this case, it will be found convenient to divide the complex s plane into two regions with a big circle of radius $R=\lambda_1/(4\epsilon)$: As $\epsilon\downarrow 0$, either $|\alpha\epsilon|\le\sqrt{2\lambda_1\epsilon}\to 0$ or $|k|\le\sqrt{2\lambda_1\epsilon}\to 0$ depending upon whether s lies within or outside the circle.

Let us first look at the contribution $F_\epsilon^{\rm in}(T)$ to the integral (A17) from that portion of the contour C lying inside the circle R. Here, the inverse derivative factor in (A15) can be evaluated by using the asymptotic forms as $z\to 0$ of Whittaker functions, namely (A11) or (A12):

$$1\Big/\left[-\frac{dW_{km}(z)}{dz}\right]_{z=\alpha\epsilon} =\begin{cases}[\Gamma(1-k+\mu)/\mu\Gamma(1+2\mu)]\ (\alpha\epsilon)^{1+\mu}+O([\alpha\epsilon]^{2+\mu}) & (\mu>0)\\ \Gamma(1-k)/[k\log\alpha\epsilon+\frac{1}{2}+O(\alpha\epsilon\log\alpha\epsilon)] & (\mu=0)\end{cases}; \tag{A27}$$

in the second line, we notice, $|k\log\alpha\epsilon|$ grows indefinitely as $s\to 0$ and becomes very small when s approaches the circle R, yet the denominator as a whole can never vanish. On the other hand, the integral in (A15) is given by

$$\int_{\alpha\epsilon}^\infty W_{k,m}(t)\,dt=\frac{\Gamma(2+\mu)\Gamma(1-\mu)}{\Gamma(2-k)}\ F(1-\mu,2+\mu,2-k;\tfrac{1}{2})+\Delta_\epsilon \tag{A28}$$

for $(-2<)\ \mu<1$, where F denotes the Gauss hypergeometric function ${}_2F_1$ [not to be confused with $F_\epsilon(T)$] and where the error term[21] Δ_ϵ introduced by replacing the lower bound of the integral by 0 is $O(\epsilon^{1-\mu})$ and $O(\epsilon^2\log\epsilon)$ for $\mu>0$ and $\mu=0$, respectively.

Let us verify that the approximate expressions above do give $f(\alpha\epsilon,k)$ the same analyticity as expected from the general argument presented before.

In view of the range of k as remarked earlier, the gamma functions in (A27) and (A28) are analytic everywhere in the cut s plane. The hypergeometric function in (A28) is also analytic as manifested by Euler's integral representation, valid when $|\mu|<1$ and $\mathrm{Re}\,k<0$:

$$F(1-\mu,2+\mu,2-k;\tfrac{1}{2}) =\frac{\Gamma(2-k)}{\Gamma(1-\mu)\Gamma(1-k+\mu)}\int_0^t t^{-\mu}(1-t)^{-k+\mu}\times(1-t/2)^{-(2+\mu)}\,dt. \tag{A29}$$

Thus, we see from (A15) that $f(\alpha\epsilon,k)$ is analytic everywhere on the cut s plane except possibly at $s=0$, even in the approximation that the error terms in (A27) and (A28) are disregarded.

As $s \to 0$, one has $|k| \to \infty$ and (A29) shows that[22]

$$F(1-\mu,\ 2+\mu,\ 2-k;\ \tfrac{1}{2}) \underset{\mathrm{Re}\,k \to -\infty}{\to} 1,$$

for in this limit the contribution to the integral comes from $l \sim 1$ reducing it to the beta function $B(1-\mu, 1-k+\mu)$. Then, a short calculation leads to

$$\epsilon^2 f(\alpha\epsilon, k) \underset{s\to 0}{\sim} \begin{cases} \dfrac{\Gamma(2+\mu)\Gamma(1-\mu)}{\mu\,\Gamma(1+2\mu)} \dfrac{2}{(2\lambda_1)^{1-\mu}} \epsilon^{1+\mu} & (\mu > 0) \\ \dfrac{2}{(2\lambda_1)^2} \dfrac{1}{\log[(8s)^{1/2}/\epsilon]} & (\mu = 0). \end{cases} \tag{A30}$$

We see that the singularity at $s=0$ is present only when $\mu = 0$ and it is indeed very weak.

Now, we can estimate the contribution $F_\epsilon^{\mathrm{in}}(T)$ to the integral (A17) from that part of the contour C which lies inside the big circle R.

Let us divide the contour C further with a circle having a fixed (ϵ-independent), yet sufficiently large radius $R_0 \gg \lambda_1^2/8$, so that

$$F_\epsilon^{\mathrm{in}}(T) = \frac{1}{2\pi i}\left(\int_{-iR_0}^{iR_0} + \int_{iR_0}^{iR} + \int_{-iR}^{-iR_0}\right) \epsilon^2 f(\alpha\epsilon, k) \exp(sT)\, ds. \tag{A31}$$

The first integral is obviously $O(\epsilon^{1+\mu})$ and $O(1/\log[1/\epsilon])$ when $\mu > 0$ and $\mu = 0$, respectively; the smallness here is due mainly to the inverse derivative factor (A27). That the second and the third integrals are negligible compared to the first can be seen by using (A27), (A28) and the fact that (A29) is approximately constant when $|k| < \lambda_1/(2R_0)^{1/2} \ll 1$. In fact, if $\mu > 0$, one sees, e.g., that

$$\int_{iR_0}^{iR} \epsilon^2 f(\alpha\epsilon, k) \exp(sT)\, ds = \mathrm{const}\,\epsilon^{1+\mu} \int_{iR_0}^{iR} s^{-(1-\mu)/2} \exp(sT)\, ds$$
$$= \mathrm{const}\,\epsilon^{1+\mu}\ O(R_0^{-(1-\mu)/2}) \quad (R_0 \to \infty) \tag{A32}$$

with the aid of the asymptotic estimate

$$\int_{iR_0}^{iR} s^{-\gamma} \exp(sT)\ ds = \left[\frac{1}{T}\, s^{-\gamma} \exp(sT)\right]_{iR_0}^{iR} + \frac{\gamma}{T} \int_{iR_0}^{iR} \times s^{-(\gamma+1)} \exp(sT)\, ds, \tag{A33}$$

as established by integration by parts; the second term here is bounded by $[s^{-\gamma}/T]_{R_0}^{R}$. A similar estimate may be made for the case of $\mu = 0$.

Now, let us turn to the contribution $F_\epsilon^{\mathrm{out}}(T)$ to the integral (A17) from the portion of C outside the big circle R, where $|k| \leq \sqrt{2\lambda_1\epsilon} \to 0$ as $\epsilon \downarrow 0$:

$$F_\epsilon^{\mathrm{out}}(T) = \frac{1}{2\pi i}\left(\int_{iR}^{i\infty} + \int_{-i\infty}^{-iR}\right) \epsilon^2 f(\alpha\epsilon, k) \exp(sT)\, ds. \tag{A34}$$

When $\mu > 0$, we may approximately set $k=0$ and change the variable of integration to $u = \epsilon^2 s$,

$$F_\epsilon^{\mathrm{out}}(T) = \frac{1}{2\pi i}\left(\int_{-i\infty}^{i\infty} - \int_{-i\epsilon^2 R}^{i\epsilon^2 R}\right) f([8u]^{1/2}, 0) \exp(uT/\epsilon^2)\, du,$$

recognizing that the first integral here is nothing but the one (A19) already evaluated with the result $[C/\Gamma(\gamma)]\epsilon^{1+\mu}/T^{(1+\mu)/2}$, $\gamma = (1-\mu)/2$; see (A22). To evaluate the second, we may invoke (A20) on the ground that $\epsilon^2 R = \lambda_1\epsilon/4 \to 0$ as $\epsilon \downarrow 0$, obtaining

$$\frac{1}{2\pi i} \int_{-i\epsilon^2 R}^{i\epsilon^2 R} f([8u]^{1/2}, 0) \exp(uT/\epsilon^2)\, du = C \int_{-i\lambda_1\epsilon/4}^{i\lambda_1\epsilon/4} u^{-\gamma} \times \exp(uT/\epsilon^2)\, du, \tag{A35}$$

which, upon returning to the original variable $s = u/\epsilon^2$, turns out to be

$$C\,\epsilon^{2(1-\gamma)} \int_{-iR}^{iR} s^{-\gamma} \exp(sT)\, ds = [C/\Gamma(\gamma)]\epsilon^{1+\mu}\{T^{-(1+\mu)/2} + O(R^{-\gamma})\},$$

the first term being the value at $R \to \infty$ and the error committed being estimated similarly to (A33). Thus, the main contributions of order $\epsilon^{1+\mu}$ cancel out, so that

$$F_\epsilon^{\mathrm{out}}(T) = o(\epsilon^{1+\mu})$$

which is of higher order in ϵ than is $F_\epsilon^{\mathrm{in}}(T)$.

When $\mu = 0$, the approximation $k=0$ implies $W_{k,m}(z) \sim W_{0,1/2}(z) = \exp(-z/2)$, so that we can go back to (A15) and (A17), and write

$$F_\epsilon^{\mathrm{out}}(T) = \frac{1}{2\pi i}\left(\int_{iR}^{i\infty} + \int_{-i\infty}^{-iR}\right) \frac{1}{s} \exp(sT)\, ds.$$

Hence

$$F_\epsilon^{\mathrm{out}}(T) = O\left(\frac{1}{R}\right) = O(\epsilon),$$

which is again of higher order in ϵ than $F_\epsilon^{\mathrm{in}}(T)$.

Summing up, thus, we can conclude for $F_\epsilon(T) = F_\epsilon^{\mathrm{in}}(T) + F_\epsilon^{\mathrm{out}}(T)$ that

$$F_\epsilon(T) = \mathrm{const} \begin{cases} \epsilon^{1+\mu} & (\lambda_1 > 0,\ \mu > 0) \\ 1/\log[1/\epsilon] & (\lambda_1 > 0,\ \mu = 0) \end{cases} \tag{A36}$$

as indicated in (2.4). The first line of (A36) is valid in fact for $\lambda_1 \geq 0$, $\mu > 0$ as one sees from (A22).

APPENDIX B

This appendix is to show, for the case of the example (2.8), that there exists a regularization with parameter b_ϵ that leaves the average

$$F_\epsilon(T) = \langle \exp\{-\lambda_1 \int_0^T [(|x(t)| + \epsilon)^{-1} - b_\epsilon(|x(t)| + \epsilon)^{-2}]\, dt\}\rangle, \tag{B1}$$

nonvanishing in the limit $\epsilon \downarrow 0$ as indicated in (2.10). We assume that $b_\epsilon \downarrow 0$ in the limit because it is a regularization; consequently, we have $\mu \downarrow 0$ for the parameter μ defined as previously by

$$\mu(\mu+1) = 2\lambda_2 = -2\lambda_1 b_\epsilon \quad (\mu \geq -1/2).$$

The average (B1) can be expressed as the inverse Laplace transform (A17). Here, however, the integra-

tion contour C may no longer be taken to be the imaginary axis of the s plane, for the potential function has a negative part which may produce some singularities in $f(\alpha\epsilon, k)$ in the right-hand half of the s plane.

Here again, it is convenient to divide the complex s plane into two regions with a big circle of radius $R=\lambda_1/4\epsilon$.

Let us first look at the region outside the circle, where $|k| \leq \sqrt{2\lambda_1\epsilon} \to 0$ as $\epsilon \downarrow 0$ implying $W_{k,m}(z) \sim W_{0,m}(z)$. Moreover, since $\mu \downarrow 0$ in the limit, we have

$$W_{k,m}(z) \sim W_{0,1/2}(z) = \exp(-z/2),$$

so that

$$\epsilon^2 f(\alpha\epsilon, k) \sim 1/s \qquad (s > R = \lambda_1/4\epsilon) \tag{B2}$$

which has no singularities in the region considered.

In the inside region $|\alpha\epsilon| \leq \sqrt{2\lambda_1\epsilon} \to 0$ as $\epsilon \downarrow 0$. For those factors comprising $\epsilon^2 f(\alpha\epsilon, k)$ in (A15), we get, on the one hand from (A11),[23]

$$\left[-\frac{dW_{k,m}(z)}{dz}\right]_{z=\alpha\epsilon} = \frac{1}{\Gamma(1-k)}\,\frac{2\lambda_1}{(8s)^{1/2}}\,[D_0(\epsilon)+D_1(s) + O(\epsilon\log\epsilon,\ \mu^2\epsilon^{-1}\log\epsilon)] \tag{B3}$$

where $k=-2\lambda_1/(8s)^{1/2}$ as before, and

$$D_0(\epsilon) = \mu/(2\lambda_1\epsilon) - \log\epsilon, \tag{B4}$$

$$D_1(s) = \log(-k) - 1/(2k) - \Psi(1-k) - \log 2\lambda_1 - 2\gamma$$

with $\gamma = -\Psi(1) = 0.577$ being Euler's constant. On the other hand, we have

$$\int_{\alpha\epsilon}^{\infty} W_{k,1/2}(t)\,dt = \frac{2}{\Gamma(1-k)}\,[1 + k\{\Psi(1-k/2) - \Psi(\tfrac{1}{2}-k/2)\} + O(\mu,\epsilon)]. \tag{B5}$$

In fact, from (A28) we get

$$\int_{\alpha\epsilon}^{\infty} W_{k,1/2}(t)\,dt = \frac{1}{\Gamma(2-k)}\,F(1,2,2-k;1/2) + O(\mu,\epsilon),$$

of which the hypergeometric function can be evaluated in the following way: Use one of the Gauss recurrence relations

$$aF(a+1,b,c;x) = cF(a,b,c;x) - (c-a)F(a,b,c+1;x)$$

to derive

$$F(1-\mu, 2+\mu, 2-k;x) = [\mu(\mu+1)]^{-1} \times [k(1-k)F(-\mu, 1+\mu, -k;x) + (1-k)(\mu+k)F(-\mu, 1+\mu, 2-k;x) - 2k(1-k)F(-\mu, 1+\mu, 1-k;x)]$$

and then go to the limit $\mu \to 0$ using

$$F(a, 1-a, c; 1/2) = 2^{1-c}\sqrt{\pi}\ \Gamma(c)/\left[\Gamma\left(\frac{a+c}{2}\right)\Gamma\left(\frac{c-a+1}{2}\right)\right];$$

then we obtain

$$F(1,2,2-k;1/2) = 2(1-k)\,[1 + k\{\Psi(1-k/2) - \Psi(\tfrac{1}{2}-k/2)\}]$$

which we were unable to find in the available tables of mathematical formulas.[18]

Thus, substituting (B3) and (B5) into (A15), we get

$$\epsilon^2 f(\alpha\epsilon, k) = -\frac{k}{\lambda_1^2}\left[1 + k\left\{\Psi\left(1-\frac{k}{2}\right) - \Psi\left(\frac{1}{2}-\frac{k}{2}\right)\right\}\right] \Big/ [D_0(\epsilon) + D_1(s)] \tag{B6}$$

in the approximation to neglect those error terms which should eventually vanish in the limit $\epsilon \downarrow 0$. Note that this function goes over to the asymptotic form (B2) already within the circle R if $|k| \ll 1$, or $|s| \gg \lambda_1^2/2$. Thus, (B6) can be used all over the cut s plane.

We can now see that the function $\epsilon^2 f(\alpha\epsilon, k)$ is analytic all over the cut s plane except possibly for poles due to the zeros of its denominator, $D_0(\epsilon) + D_1(s)$. To see this, it is enough to recall that $\lambda_1 > 0$ implies $\mathrm{Re}\,k \leq 0$, in which region the digamma functions comprising its numerator and denominator are all analytic. Despite the factor $-k = \lambda_1/(2s)^{1/2}$ in front, (B6) remains finite as $s \to 0$:

$$\epsilon^2 f(\alpha\epsilon, k) \underset{s\to 0}{\to} [\lambda_1^2\{D_0(\epsilon) - (\log 2\lambda_1 + 2\gamma)\}]^{-1}, \tag{B7}$$

for $s \to 0$ means $|k| \to \infty$ and

$$\Psi(x) = \log(x-1) + \frac{1}{2(x-1)} - \frac{1}{12(x-1)^2} + O\left(\frac{1}{(x-1)^3}\right) \qquad (|x| \to \infty).$$

In order to decide on the possibility of poles, let us examine how the denominator of (B6) behaves on the positive real s axis. Asymptotically we have

$$D(s) \to D_0(\epsilon) - (\log 2\lambda_1 + 2\gamma) \equiv D(0) \quad (s \to 0)$$

and

$$D(s) \sim D_0(\epsilon) + (2s)^{1/2}/(2\lambda_1) \qquad (s \to \infty).$$

The latter is an increasing function of s. As a matter of fact, $D(s)$ is monotone increasing over the entire range of s from 0 to ∞ as one sees from the positivity of the weight function multiplying $\exp(kt)$ in

$$D(s) = D_0(\epsilon) - \log 2\lambda_1 + \int_0^{\infty}\left(\frac{1}{e^t-1} - \frac{1}{t} + \frac{1}{2}\right)\exp(kt)\,dt,$$

which is constructed by using Binet's formula

$$\Psi(x) = \log x - \int_0^{\infty}\left(\frac{1}{e^t-1} - \frac{1}{t} + 1\right)\exp(-xt)\,dt \qquad (\mathrm{Re}\,x > 0)$$

and $\Psi(1+x) = \Psi(x) + (1/x)$. Thus, $D(s)$ has a zero, and in fact one simple zero (say, at $s = s_0$) on the positive real s axis if and only if[24]

$$D(0) = D_0(\epsilon) - (\log 2\lambda_1 + 2\gamma) < 0. \tag{B8}$$

This is a necessary and sufficient condition for the function $\epsilon^2 f(\alpha\epsilon, k)$ to have a pole on the positive real axis.

We remark here for later reference that the residue at the pole, if there is one, is positive:

$$\mathrm{Res}[\epsilon^2 f(\alpha\epsilon, k)]_{s=s_0} = [N(s)\,dD(s)/ds)]_{s=s_0} > 0, \tag{B9}$$

where $N(s)$ denotes the numerator of (B6). In fact, the right-hand side is positive not only at s_0, but also for any $0 \leq s < \infty$, for $dD(s)/ds > 0$ follows from the monotonicity of $D(s)$ established above and $N(s) > 0$ from its integral representation

$$\frac{N(s)}{(-k/\lambda^2)} = 1 + (1-2x)\int_0^\infty \frac{\exp[(1-2x)t/2]}{\exp(t/2)+1}\,dt$$
$$= \int_0^\infty \frac{\exp(-2xt)}{(1+\exp(-t/2))^2}\,dt > 0,$$

where $x \equiv (1-k)/2 \geq 1/2$ and the first line derives from

$$\Psi(z) = \int_0^\infty \left(\frac{\exp(-t)}{t} - \frac{\exp(-tx)}{1-\exp(-t)}\right)dt$$

as applied to the numerator of (B6), the second line being obtained by integration by parts.

Now, we can turn to the discussion of $F_\epsilon(T)$, that is, the inverse Laplace transform (A17). There arise different cases depending on how $\mu \downarrow 0$ as $\epsilon \downarrow 0$.

Let us begin with the simplest cases where $\epsilon^2 f(\alpha\epsilon, k)$ has no poles on the right-hand half of the s plane. In such cases, the contour C of the integral (A17) can be put on the imaginary s axis, which we divide into three regions: $|s| < R_0$, $R_0 < |s| < R$, and $|s| > R$ with $R = \lambda_1/4\epsilon$ and an ϵ-independent $R_0 \gg \lambda_1^2/8$. The limit of the contribution $F_\epsilon^{(1)}$ from the first region depends critically on the behavior of $D_0(\epsilon)$ as $\epsilon \downarrow 0$. If μ was taken to be a constant ($|\mu| \ll 1$ as the foregoing argument requires), then $D_0(\epsilon) \sim \mu/(2\lambda_1\epsilon)$ and $F_\epsilon^{(1)}$ would vanish like $\sim\epsilon \downarrow 0$ in conformity with the previous result (A36). However, if it is arranged that $D_0(\epsilon)$ approaches a certain constant $-K$ as $\epsilon \downarrow 0$, then $F_\epsilon^{(1)}$ has a nonvanishing limit. This is, in fact, the case if the regularization counter term is chosen such that

$$\mu = 2\lambda_1\epsilon[\log\epsilon - K]. \tag{B10a}$$

By (B8), we note, the condition of no pole requires that

$$K < -(\log 2\lambda_1 + 2\gamma). \tag{B10b}$$

When $F_\epsilon^{(1)}$ is nonvanishing in the limit, estimates similar to the one in Appendix A shows that the contributions to the integral (A17) from the second and the third regions do not outweigh $F_\epsilon^{(1)}$. Thus, under the conditions (B10) we have

$$F_\epsilon(T) \to \text{const} \neq 0 \quad \text{as } \epsilon \downarrow 0. \tag{B11}$$

Among the cases where the pole comes in, two will be of particular interest. In either case, we move the contour of integration C to $C_1' + C_2'$, where C_1' encircles the pole and C_2' is on the imaginary axis.

(i) $\mu = \mu_0\epsilon^{1-\delta}$ with $\mu_0 < 0$, $0 < \delta < 1$.

As $\epsilon \downarrow 0$, we have

$$D(0) = (\mu_0/2\lambda_1)\epsilon^{-\delta} - \log(2\lambda_1\epsilon) - 2\gamma \to -\infty \tag{B12}$$

and the position s_0 of the pole and the residue are given approximately by

$$s_0 = \mu_0^2/(2\epsilon^{2\delta}) \quad \text{and} \quad \text{Res}[\epsilon^2 f(\alpha\epsilon, k)] = 2. \tag{B13}$$

To make it certain that the pole lies within the circle R, however, we must change our R to $R = \lambda_1/(2\epsilon^{2\rho})$, $\rho > \delta$, taking advantage of the fact that the whole argument so far remains valid as long as $8\epsilon^2 R \to 0$ and $\lambda_1^2/2R \to 0$ as $\epsilon \downarrow 0$; these conditions impose $0 < \rho < 1$ and the existence of such a $\rho > \delta$ is guaranteed by our presumption $0 < \delta < 1$.

Thus,

$$F_\epsilon(T) \sim 2\exp[2^{-1}(\mu_0/\epsilon^\delta)^2 T] \quad (\epsilon \downarrow 0), \tag{B14}$$

because the contribution from the contour C_2' vanishes as in (B10) in the limit $\epsilon \downarrow 0$. Note that, as $\delta \uparrow 1$, this $F_\epsilon(T)$ for $\lambda_1 > 0$, $\mu = \mu_0\epsilon^{1-\delta}$, ($\mu_0 < 0$) approaches the one, (A26), for $\lambda_1 = 0$, $\mu = \text{const}\,(0 < -\mu \ll 1)$.

(ii) $\mu = 2\lambda_1\epsilon[\log\epsilon - K]$ with $-(\log 2\lambda_1 + 2\gamma) < K < \infty$, $K \neq 0$. (B15)

This means $D_0(\epsilon) = -K$ and

$$D(0) = -K - (\log 2\lambda_1 + 2\gamma) < 0.$$

In this case, we can only write

$$F_\epsilon(T) = \text{Res}[\epsilon^2 f(\alpha\epsilon, k)]_{s=s_0}\exp(s_0 T) + \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \epsilon^2 f(\alpha\epsilon, k)\exp(sT)\,ds, \tag{B16}$$

where the pole s_0 should be determined as the zero of

$$D(s) = D_1(s) - K \tag{B17}$$

and the residue determined by (B9); such a pole exists for any value of $K > -(\log 2\lambda_1 + 2\gamma)$ and it indeed lies in the circle R. We notice that the function $\epsilon^2 f(\alpha\epsilon, k)$ is now independent of ϵ: In fact, it is given by (B6) with the denominator $D(s)$ in (B17) and this does cover the asymptotic behavior (B2) outside the circle R. It is clear nevertheless that the first term dominates over the second at least at large T. Therefore, $F_\epsilon(T)$ cannot vanish identically.

Denote the first term in (B16) by $F_\epsilon^{\text{pol}}(T)$.

If, in particular, $0 < K \ll 1$, we note, $s_0 \approx 6\lambda_1^2 K$ and

$$F_\epsilon^{\text{pol}}(T) = 6\exp[6\lambda_1^2 KT].$$

If, on the contrary, $K \gg 1$, then $s_0 \approx 2\lambda_1^2 K^2$ and

$$F_\epsilon^{\text{pol}}(T) = 2\exp[2\lambda_1^2 K^2 T]. \tag{B18}$$

*This paper, originally scheduled for September 1974, was delayed in publication through no fault of the authors.
†On leave of absence from the Department of Physics, Gakushuin University, Tokyo, Japan.
[1]L.A. Shepp, J.R. Klauder, and H. Ezawa, Ann. Inst. Fourier, Grenoble **24**, (2), 189 (1974).
[2]J.R. Klauder, Acta Phys. Austr., Suppl. **XI**, 341 (1973); Phys. Lett. **47B**, 523 (1973).
[3]See, e.g., E.A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill, New York, 1945); T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, New York, 1966).
[4]B. Simon, J. Funct. Anal. **14**, 295 (1973); B. DeFacio and C.L. Hammer, J. Math. Phys. **15**, 1071 (1974).
[5]See, e.g., S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943); M.S. Bartlett, *An Introduction to Stochastic Processes* (Cambridge U.P., Cambridge, 1966).
[6]The relation of these results to certain properties in quantum field theory should not go unnoticed. There one deals with superrenormalizable theories with fields both locally equivalent and nonequivalent to the free field; with renormalizable fields; and with nonrenormalizable fields. It is conjectured that in the latter case the behavior is similar to that for $\alpha > 2$—namely, as the interaction is turned off, the limiting theory is not the free theory (see Ref. 2).
[7]M. Kac, *Proceedings Second Berkeley Symposium on Mathematical Statistics and Probability* (University of California Press, 1951), p. 189.

[8]The concepts of local time and stochastic equations were already used by Symanzik in his pioneering study of Euclidean quantum field theory: K. Symanzik, *Proceedings of the International School of Physics "Enrico Fermi"*, Varenna Course XLV, edited by R. Jost (Academic, New York, 1969).

[9]H. Ezawa, J.R. Klauder, and K.A. Shepp, Ann. Phys. (N.Y.) **88**, 588 (1974).

[10]It is interesting to note that Umezawa and co-workers [H. Matsumoto, N.J. Papastamatiou, and H. Umezawa, Phys. Lett. **46B**, 73 (1973), and to be published; H. Umezawa, Lectures at the School on Renormalization and Invariance in Quantum Field Theory, Capri, July, 1973] have studied spontaneously-broken symmetry in field theory by exploiting functional integrals having auxiliary terms in the Lagrangian which, although formally vanishing in a suitable limit, serve to pick out one or another broken-symmetry solution.

[11]K. Itô and H. McKean, *Diffusion Processes and Their Sample Paths* (Springer-Verlag, New York, 1965), Sec. 2.8. Note our definition differs by a factor two from that given here.

[12]The notation a.s. stands for "almost surely", meaning that the statement is true with the possible exception of a set of points (paths) of probability measure 0 in the sample space considered. In other words, the statement is true with probability 1.

[13]J. L. Doob, *Stochastic Processes* (Wiley, New York, 1953).

[14]H. McKean, *Stochastic Integrals* (Academic, New York, 1969).

[15]A.V. Skorokhod, *Studies in the Theory of Random Processes* (Addison-Wesley, Reading, Mass., 1965).

[16]This function $B(x,t)$ is obtained[9] from the fundamental solution for absorbing Brownian motion, Ref. 5, $\rho(x,y,t) \equiv \{\exp[-(x-y)^2/2t] - \exp[-(x-y-2c)^2/2t]\}/\sqrt{2\pi t}$, or $(x-c)(y-c) > 0$, by $B(x,t) = \int \rho(x,y,T-t)\,dy$.

[17]I.V. Girsanov, Dokl. Akad. Nauk SSSR **138**, 18 (1961) [Soviet Math. Dokl. **2**, 506 (1961)].

[18](a) A useful reference for these functions is the book by L.J. Slater, *Confluent Hypergeometric Functions* (Cambridge U.P., Cambridge, 1960). (b) Reference is made also to some tables of mathematical formulas: M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables* (Dover, New York, 1968); S. Moriguchi, K. Udagawa, and S. Hitotumatu, *Mathematical Formulas*, (Iwanami Shoten, Tokyo, 1960), Vol. III (in Japanese).

[19]Here is a minor departure from the customary notation $\psi(\cdot)$ for the digamma function [see Ref. 18(b)].

[20]G. Doetsch, *Theorie und Anwendung der Laplace-Transform* (Springer-Verlag, Berlin, 1937; Dover edition, New York, 1943).

[21]For $\mu \geq 1$, a drastically different evaluation of the integral applies. The other places where our restriction to $\mu < 1$ is vital are (A32) and (A35).

[22]This behavior of the hypergeometric function can be seen also from its series definition.

[23]We use the notation $O(a,b) \equiv O(a) + O(b)$.

[24]If $\lambda_1 \neq 0$, then $D_0(\epsilon) \sim \mu/2\lambda_1\epsilon \to -\infty$ overwhelms $-\log 2\lambda_1 \to \infty$; hence $D(0) < 0$ and $\epsilon^2 f(\alpha\epsilon, k)$ has a pole in accordance with the assertion given previously.

Matrix elements of the generators of $IU(n)$ and $IO(n)$ and respective deformations to $U(n,1)$ and $O(n,1)$

M. K. F. Wong

Fairfield University, Fairfield, Connecticut 06430

Hsin-Yang Yeh

Moorhead State College, Moorhead, Minnesota 56560
(Received 15 November 1974)

The unitary continuous representations of $U(n,1)$ and $O(n,1)$ are discussed from the point of view of deformation of $IU(n)$ and $IO(n)$. It is shown that there are two general ways of writing the matrix elements of the infinitesimal generators of the groups $U(n,1)$ and $O(n,1)$. The first one is to write them as either pure real or pure imaginary. The second one is to write them as complex. We show how these different ways are related to each other.

I. INTRODUCTION

The infinitesimal method has been a very successful tool in the investigation of unitary representations of Lie groups. In the case of the compact groups $U(n)$ and $O(n)$, the first successful attempt was made by Gel'fand and Zetlin[1] when they determined the matrix elements of the infinitesimal generators of the groups. In the case of noncompact groups, $U(n,1)$ and $O(n,1)$ have been studied by many authors. In particular, the matrix elements of the generators of $U(n,1)$ have been determined by Gel'fand and Graev[2] and by Ottoson.[3] Those of $O(n,1)$ have been determined by Hirai,[4] Ottoson,[5] Schwarz,[6] and Wong.[7] There is, however, another approach regarding the representations of $U(n,1)$ and $O(n,1)$, and that is through the deformation of $IU(n)$ and $IO(n)$. This was first done by Chakrabarti.[8] Similar results were obtained by Wolf[9] through multiplier representations. On the other hand, Rosen and Roman[10] have discussed in detail the Lie algebra of these groups.

In an attempt to unify these investigations, we came across an apparent problem. The problem is: The matrix elements of the infinitesimal generators of $U(n,1)$ and $O(n,1)$ obtained by Chakrabarti are complex, while those obtained by the other authors are either pure real or pure imaginary. We shall show in Secs. III and IV that there is no contradiction between these results. We have thus reached the following conclusion: There are two general ways of expressing the matrix elements of the generators of $U(n,1)$ and $O(n,1)$. The first one is to write them as either pure real or pure imaginary. This is a matter of definition of the generators. One can see this already in the case of the compact group $O(n)$. The original Gel'fand–Zetlin matrix elements for $O(n)$ were in terms of the matrix A_{ik}, which has 1 at the ith row and kth column and -1 at the kth row and ith column. As a result, $A_{2k+1,2k}$, for example, has matrix elements which are pure real. On the other hand, the later papers by Pang and Hecht[11] and by Wong[12] used J_{ij}, where J_{ij} has i at the ith row and jth column and $-i$ at the jth row and ith column. As a result, their $J_{2k+1,2k}$ has matrix elements which are pure imaginary. We see therefore that this is purely a matter of definition of the generators of the group. This difference of definition, however, has an influence on at least two properties of the generators. The first influence is on the commutation relations of the generators. The second influence is on the properties of the generators under Hermitian conjugation. We shall see in subsequent sections that for $U(n,1)$ the difference of these two properties persists in the different definitions of the generators given by Rosen and Roman on the one hand and by Gel'fand and Graev and Ottoson on the other.

The second way is to write the matrix elements of the generators as complex. This is done by Chakrabarti.[8] This, in principle, corresponds to adding a phase factor to the matrix elements. We shall show how Chakrabarti's results can be reconciled with the results of Gel'fand and Graev, and Ottoson in the case of $U(n,1)$ and with Hirai, Ottoson, Schwarz, and Wong in the case of $O(n,1)$.

II. REPRESENTATIONS OF $IU(n)$ AND DEFORMATION TO $U(n,1)$

$IU(n)$ is a group which is made of the semidirect product of $U(n)$ and $I(2n)$. The generators of $U(n)$ are labeled by A^i_j $(i,j=1,2,\ldots,n)$ and the generators of $I(2n)$ by I^i_{n+1}, I^{n+1}_i $(i=1,2,\ldots,n)$. The commutation relations are

$$[A^i_j,A^k_l]=\delta^i_l A^k_j-\delta^k_j A^i_l, \tag{1}$$

$$[A^i_j,I^k_{n+1}]=-\delta^k_j I^i_{n+1}, \tag{2}$$

$$[A^i_j,I^{n+1}_k]=\delta^i_k I^{n+1}_j, \tag{3}$$

$$[I^i_{n+1},I^j_{n+1}]=[I^{n+1}_i,I^{n+1}_j]=[I^{n+1}_i,I^j_{n+1}]=0 \tag{4}$$

with

$$(A^i_j)^*=A^j_i, \tag{5}$$

$$(I^i_{n+1})^*=I^{n+1}_i \quad (i,j,k,l=1,2,\ldots,n). \tag{6}$$

Chakrabarti has shown that the matrix elements of I^n_{n+1} are given by

$$\begin{aligned}\langle h_{jn}-1\,|\,I^n_{n+1}\,|\,h\rangle &= \kappa\left(\frac{\Pi^n_{j=2}(h_{jn+1}-h_{jn}-i+j+1)\Pi^{n-1}_{i=1}(h_{in-1}-h_{jn}-i+j)}{\Pi_{\substack{1\le i\le n\\ i\ne j}}(h_{in}-h_{jn}-i+j+1)(h_{in}-h_{jn}-i+j)}\right)^{1/2}\\ &= \langle h\,|\,I^{n+1}_n\,|\,h_{jn}-1\rangle^*\end{aligned} \tag{7}$$

Without loss of generality, we can choose κ to be equal to 1. The (infinite-dimensional) basis is labeled by $(n$

$-1)$ numbers in the first row, followed by the familiar Gel'fand basis for $U(n)$,

$$\begin{vmatrix} & h_{2n+1} & h_{3n+1} & \cdots & & h_{nn+1} \\ h_{1n} & & h_{2n} & \cdots & h_{n-1n} & h_{mn} \\ h_{1n-1} & \cdots & & & h_{n-1n-1} & \\ & \cdots & & & & \\ h_{11} & & & & & \end{vmatrix}$$

with the usual inequalities

$$h_{ij+1} \geq h_{ij} \geq h_{i+1j+1} \quad (i,j=1,\ldots,n)$$

and

$$h_{1n} \geq h_{2n+1} \geq h_{2n} \geq \cdots \geq h_{nn+1} \geq h_{mn} \tag{8}$$

but allowing the two extreme numbers to tend to infinity:

$$h_{1n} \to \infty, \quad h_{mn} \to -\infty.$$

The matrix element in (7) differs from the Gel'fand–Zetlin matrix element in A^n_{n+1} by a factor of

$$[-(h_{1n+1}-h_{jn}+j)(h_{n+1n+1}-h_{jn}-n+j)]^{1/2}. \tag{9}$$

The group $U(n)$ is then extended to $U(n)\otimes U(1)$ by introducing an extra parameter ξ and the generator A^{n+1}_{n+1}, such that

$$A^{n+1}_{n+1}|h\rangle = \left(\xi + \sum_{i=2}^{n} h_{in+1} - \sum_{i=1}^{n} h_{in}\right)|h\rangle. \tag{10}$$

The deformation to $U(n,1)$ is then obtained by taking the semidirect product of $U(n)\otimes U(1)$ with I_{2n}: $[U(n)\otimes U(1)]\times I_{2n} \to U(n,1)$. If one defines

$$A^i_{n+1} = \pm[\Delta, I^i_{n+1}] + i\epsilon I^i_{n+1}, \tag{11}$$

$$A^{n+1}_i = \pm[\Delta, I^{n+1}_i] + i\epsilon I^i_{n+1} \tag{12}$$

with

$$\Delta \equiv \frac{1}{2\sqrt{\Delta_{(2)}}}\left[\sum_{i,j=1}^{n} A^i_j A^j_i + \left(\frac{\Delta_{(3)}}{\Delta_{(2)}} + n\right) A^{n+1}_{n+1}\right], \tag{13}$$

$$\Delta_{(2)} \equiv \sum_{i=1}^{n} I^{n+1}_i I^i_{n+1}, \tag{14}$$

$$\Delta_{(3)} \equiv \sum_{i,j=1}^{n} I^{n+1}_i A^i_j I^j_{n+1} + A^{n+1}_{n+1}\Delta_{(2)}, \tag{15}$$

one finds that

$$A^i_{n+1} = -(A^{n+1}_i)^+, \tag{16}$$

$$[A^i_{n+1}, A^j_{n+1}] = [A^{n+1}_i, A^{n+1}_j] = 0, \tag{17}$$

and

$$[A^{n+1}_i, A^j_{n+1}] = A^j_i - \delta^j_i A^{n+1}_{n+1}, \tag{18}$$

In other words, the generators A^i_j $(i,j=1,\ldots,n+1)$ now generate the algebra of $U(n,1)$, according to the definition of Gel'fand and Graev.

The nonzero matrix elements of A^n_{n+1} and A^{n+1}_n turn out to be complex:

$$\begin{aligned}\langle h_{jn}-1|A^n_{n+1}|h\rangle &= [\tfrac{1}{2}(\xi-n)+i\epsilon-(h_{jn}-j)]\langle h_{jn}-1|I^n_{n+1}|h\rangle \\ &= -\langle h|A^{n+1}_n|h_{jn}-1\rangle^* \quad (j=1,\ldots,n).\end{aligned} \tag{19}$$

III. RECONCILIATION OF CHAKRABARTI'S RESULTS WITH THOSE OF GEL'FAND AND GRAEV

We know, however, from the results of Gel'fand and Graev, that the matrix elements of A^n_{n+1} for $U(n,1)$ are pure imaginary. To reconcile the two results, we now calculate the value of $A^n_{n+1}A^{n+1}_n$ from Chakrabarti, obtaining

$$\begin{aligned}&\sum_h \langle h_{jn}-1|A^n_{n+1}|h\rangle\langle h|A^{n+1}_n|h_{jn}-1\rangle \\ &\quad = \sum_h -[(\tfrac{1}{2}\xi - \tfrac{1}{2}n - h_{jn}+j)^2+\epsilon^2]\langle h_{jn}-1|I^n_{n+1}|h\rangle^2.\end{aligned} \tag{20}$$

We know that the principal continuous series of Gel'fand and Graev is given by

$$h_{1n+1} = -n/2 + z, \tag{21}$$

$$h_{n+1n+1} = n/2 + z^*, \tag{22}$$

where z is a complex number and z^* is the complex conjugate of z. Comparing (10) with (21) and (22), we obtain

$$\xi = 2\,\mathrm{Re}z\,. \tag{23}$$

Let us now make the identification

$$\epsilon = \mathrm{Im}z\,. \tag{24}$$

Then the first term on the right-hand side of (20) becomes

$$\begin{aligned}&-[(\mathrm{Re}z - n/2 - h_{jn}+j)^2 + (\mathrm{Im}z)^2] \\ &\quad = -[(\mathrm{Re}z - n/2 - h_{jn}+j+i\,\mathrm{Im}z) \\ &\qquad \times (\mathrm{Re}z - n/2 - h_{jn}+j-i\,\mathrm{Im}z)] \\ &\quad = -[(z-n/2-h_{jn}+j)(z^*-n/2-h_{jn}+j)] \\ &\quad = -(h_{1n+1}-h_{jn}+j)(h_{n+1n+1}-h_{jn}-n+j).\end{aligned} \tag{25}$$

But the last expression in (25) is just the square of the factor suppressed [see (9)]. We see therefore that Chakrabarti's result (19) is in agreement with that of Gel'fand and Graev, except that Gel'fand and Graev now make a further demand that, in view of (16), one requires that the matrix elements of A^n_{n+1} be pure imaginary. Thus the matrix elements of A^n_{n+1}, according to Gel'fand and Graev, are

$$\begin{aligned}&\langle h_{jn}-1|A^n_{n+1}|h\rangle \\ &\quad = \left(-\frac{\prod_{i=1}^{n+1}(h_{in+1}-h_{jn}-i+j+1)\prod_{i=1}^{n-1}(h_{in-1}-h_{jn}-i+j)}{\prod_{\substack{1\leq i\leq n \\ i\neq j}}(h_{in}-h_{jn}-i+j+1)(h_{in}-h_{jn}-i+j)}\right)^{1/2} \\ &\quad = -\langle h|A^{n+1}_n|h_{jn}-1\rangle^*.\end{aligned} \tag{26}$$

This is a pure imaginary quantity because the factor under the square root in (26) is negative, due to the branching laws of $U(n,1)$.

We would like to mention here that, in this connection, there are two different ways of defining the generators of $U(n,1)$. One way is according to Gel'fand and Graev: Eqs. (1), (5), (16), (17), and (18). In this case the commutation relations are exactly the same as for the generators of $U(n+1)$. However, Eq. (16) is different from the corresponding equation for $U(n+1)$. As a result, the matrix elements of A^i_{n+1}, A^{n+1}_i, $i=1,\ldots,n$, are pure imaginary. The second way of defining the

generators of $U(n,1)$ is according to Rosen and Roman, where instead of Eqs. (1), (16), and (18), we have

$$A^i_{n+1}=(A^{n+1}_i)^* \tag{27}$$

and

$$[A^i_j,A^k_l]=g^i_l A^k_j-g^k_j A^i_l, \tag{28}$$

where

$$g^1_1=g^2_2=\cdots=g^n_n=-g^{n+1}_{n+1}=1,$$
$$g^i_j=0, \quad \text{for } i\neq j. \tag{29}$$

According to this definition the generators of $U(n,1)$ under Hermitian conjugation, Eq. (27), behave the same way as the generators of $U(n+1)$. However, the commutation relations (28) are different. If one uses this definition, then the matrix elements of A^i_{n+1}, A^{n+1}_i $(i=1,\ldots,n)$ are real, but they differ from those of the generators of $U(n+1)$, i.e., the Gel'fand–Zetlin results, by a factor of $\sqrt{-1}$.

Speaking of the definition by Rosen and Roman, we would also like to point out that the connection Chakrabarti makes of his result with those of Rosen and Roman, i.e.,

$$E_{ij}=A^i_j-A^j_i, \quad F_{ij}=i(A^i_j+A^j_i) \tag{30}$$

is valid only for $i,j=1,2,\ldots,n$. For $i=j=n+1$, one has to make the identification

$$E_{n+1,j}=i(A^{n+1}_j-A^j_{n+1}), \quad F_{n+1,j}=-(A^{n+1}_j+A^j_{n+1}),$$
$$E_{i,n+1}=i(A^i_{n+1}-A^{n+1}_i), \quad F_{i,n+1}=-(A^i_{n+1}+A^{n+1}_i),$$

and

$$F_{n+1,n+1}=-2iA^{n+1}_{n+1} \tag{31}$$

in order that the commutation relations (42), (43), and (44) of Rosen and Roman may be satisfied, i.e.,

$$[E_{\mu\nu},E_{\rho\sigma}]=g_{\mu\rho}E_{\nu\sigma}-g_{\nu\rho}E_{\mu\sigma}+g_{\mu\sigma}E_{\rho\nu}-h_{\nu\sigma}E_{\rho\mu}, \tag{32}$$
$$[F_{\mu\nu},F_{\rho\sigma}]=g_{\mu\rho}E_{\nu\sigma}+g_{\nu\rho}E_{\mu\sigma}-g_{\mu\sigma}E_{\rho\nu}-g_{\nu\sigma}E_{\rho\mu}, \tag{33}$$
$$[E_{\mu\nu},F_{\rho\sigma}]=g_{\mu\rho}F_{\nu\sigma}-g_{\nu\rho}F_{\mu\sigma}+g_{\mu\sigma}F_{\rho\nu}-g_{\nu\sigma}F_{\rho\mu}, \tag{34}$$

where $g_{11}=\cdots=g_{nn}=-g_{n+1,n+1}=1$.

One sees therefore that if one uses the $E_{\mu\nu}$ and $F_{\mu\nu}$ of Rosen and Roman as the infinitesimal generators, then the matrix elements of $E_{n+1,j}$, for example, are real and under Hermitian conjugation:

$$E_{n+1,j}{}^*=E_{j,n+1}. \tag{35}$$

We therefore conclude that another way of expressing the matrix elements of the infinitesimal generators of $U(n,1)$ is by means of the $E_{\mu\nu}$ and $F_{\mu\nu}$ of Rosen and Roman. In that case the matrix elements of $E_{n+1,j}$ are real, and under Hermitian conjugation, $E_{n+1,j}{}^*=E_{j,n+1}$.

IV. $IO(n)\to O(n,1)$

$IO(n)$ is actually the Euclidean group in n dimensions, consisting of combining rotation and translation in an n-dimensional Euclidean space. For example, $IO(2)$ consists of rotation and translation in a plane. There are three parameters: one for rotation and two for translation. This is called E_3 by Miller,[13] where the number 3 refers to the number of parameters. Miller's E_6 is the same as $IO(3)$. The matrix elements of E_6, as found by Miller (Theorem 6.3, Eq. 6.30), are in agreement with Chakrabarti's results for $IO(3)$ upon the following identification:

$$m=m_{12}, \quad u=m_{13}, \quad s=m_{24}, \quad \omega=\kappa=1. \tag{36}$$

For the $IO(n)$ group the generators obey the following commutation relations:

$$[J_{ab},j_{cd}]=i(\delta_{ac}J_{bd}+\delta_{bd}J_{ac}-\delta_{ad}J_{bc}-\delta_{bc}J_{ad}), \tag{37}$$
$$[J_{ab},I_{n+1\,c}]=i(\delta_{ac}I_{n+1\,b}-\delta_{bc}I_{n+1\,a}), \tag{38}$$
$$[I_{n+1\,a},I_{n+1\,b}]=0 \tag{39}$$
$$(a,\ b,\ c,\ d=1,\ldots,n).$$

Chakrabarti has shown that the matrix elements of $I_{2k+1\,2k}$ for $IO(2k)$ are made up of representations with $(k-1)$ numbers in the first row, followed by the Gel'fand pattern for $O(2k)$:

$$|h\rangle=\left|\begin{array}{ccccc} & h_{2k+1\,2} & \cdots & h_{2k+1\,k-1} & h_{2k+1\,k} \\ h_{2k\,1} & h_{2k\,2} & & h_{2k\,k-1} & h_{2k\,k} \\ \cdots & & & & \\ h_{31} & & & & \\ h_{21} & & & & \end{array}\right\rangle$$

with

$$\langle h_{2k\,j}+1\,|I_{2k+1\,2k}|h\rangle=\langle h\,|I_{2k+1\,2k}\,|h_{2k\,j}+1\rangle^*=\frac{i}{2}\left(\frac{\Pi^k_{\beta=2}(l_{2k+1\,\beta}-l_{2k\,j}-1)(l_{2k+1\,\beta}+l_{2k\,j})\Pi^{k-1}_{\alpha=1}(l_{2k-1\,\alpha}-l_{2k\,j}-1)(l_{2k-1\,\alpha}+l_{2k\,j})}{\Pi^k_{\alpha\neq j}(l^2_{2k-1\,\alpha}-l^2_{2k\,j})(l^2_{2k\,\alpha}-l^2_{2k\,j}-2l_{2k\,j}-1)}\right)^{1/2}$$
$$=-\langle h_{2k\,j}+1\,|I_{2k\,2k+1}|h\rangle, \tag{40}$$

where

$$l_{2k}=h_{2k}+k-\alpha, \quad l_{2k-1}=h_{2k-1}+k-\alpha. \tag{41}$$

For $IO(2k-1)$ the basis vectors are

$$|h\rangle=\left|\begin{array}{ccccc} & h_{2k\,2} & \cdots & h_{2k\,k-1} & h_{2k\,k} \\ h_{2k-1\,1} & h_{2k-1\,2} & & h_{2\,k-1\,k-1} & \\ \cdots & & & & \\ h_{31} & & & & \\ h_{21} & & & & \end{array}\right\rangle \tag{42}$$

with

$$\langle h_{2k-1\,j}+1\,|I_{2k-1\,2k}|h\rangle=-i\left(\frac{\Pi^k_{\beta=2}(l^2_{2k\,\beta}-l^2_{2k-1\,j})}{l^2_{2k-1\,j}(4l^2_{2k-1\,j}-1)}\right.$$
$$\left.\times\frac{\Pi^{k-1}_{\alpha=1}(l^2_{2k-2\,\alpha}-l^2_{2k-1\,j})}{\Pi^{k-1}_{\alpha\neq j}(l^2_{2k-1\,\alpha}-l^2_{2k-1\,j})[(l^2_{2k-1\,\alpha}-1)^2-l^2_{2k-1\,j}]}\right)^{1/2}, \tag{43}$$

$$\langle h\,|I_{2k-1\,2k}\,|h\rangle=\frac{\Pi^k_{\beta=2}l_{2k\,\beta}\Pi^k_{\alpha=1}l_{2k-2\,\alpha}}{\Pi^{k-1}_{\alpha=1}l_{2k-1\,\alpha}(l_{2k-1\,\alpha}-1)}. \tag{44}$$

The deformation to $O(n,1)$ is given by

$$J_{n\,n+1}=(i/\sqrt{\Delta_{(2)}})[\Delta/2, I_{n\,n+1}]+\lambda I_{n\,n+1}, \tag{45}$$

where

$$\Delta_{(2)}|h\rangle=\sum_{k=1}^{n} I_{n+1\,k}I_{n+1\,k})|h\rangle=1|h\rangle \tag{46}$$

and

$$\Delta=\sum_{i<j=1}^{n} J_{ij}^2. \tag{47}$$

Notice that we have added a factor of $\frac{1}{2}$ to Δ in Eq. (45). This is necessary in order to obtain the correct commutation relations for $O(n,1)$:

$$[J_{n+1\,a}, J_{n+1\,b}]=-iJ_{ab}. \tag{48}$$

This factor has been correctly added by Wolf in his deformation formula, Eq. (4.4).[14] This also changes Chakrabarti's Eq. (6.14) to read

$$J_{j\,n+1}=\sum_{i=1}^{n}\tfrac{1}{2}(I_{i\,n+1}J_{ij}+J_{ij}I_{i\,n+1})+\lambda I_{j\,n+1} \tag{49}$$

$$(j=1,\ldots,n).$$

Accordingly the matrix elements are

$$\langle h_{2k\,j}+1|J_{2k+1\,2k}|h\rangle = \{-i(h_{2k\,j}+k-j+\tfrac{1}{2})+\lambda\}\langle h_{2k\,j}+1|I_{2k+1\,2k}|h\rangle, \tag{50}$$

$$\langle h_{2k-1\,j}+1|J_{2k-1\,2k}|h\rangle = \{-i(h_{2k-1\,j}+k-j)+\lambda\}\langle h_{2k-1\,j}+1|I_{2k-1\,2k}|h\rangle, \tag{51}$$

and

$$\langle h|J_{2k-1\,2k}|h\rangle=\lambda\langle h|I_{2k-1\,2k}|h\rangle. \tag{52}$$

Comparing this with the results of $O(n,1)$, obtained by Hirai, Ottoson, Schwarz, and Wong, we find that they agree if one makes the following identifications:

$$\text{First for } O(2k-1,1):\ \lambda=il_{2k\,1} \tag{53}$$

This is especially consistent with the results of Wong,[7] who has explicitly stated that $l_{2k\,1}$ must be either zero or pure imaginary, since λ is real.

Again, (51) gives a complex quantity. So we shall find the value of $|J_{2k-1\,2k}|^2$ from (51):

$$|\langle h_{2k-1\,j}+1|J_{2k-1\,2k}|h_{2k-1\,j}\rangle|^2=(\lambda^2+l_{2k-1\,j}^2),$$

$$|\langle h_{2k-1\,j}+1|I_{2k-1\,2k}|h_{2k-1\,j}\rangle|^2 = (-l_{2k-1}^2+l_{2k-1}^2+l_{2k-1\,j}^2)|\langle h_{2k-1\,j}+1|I_{2k-1\,2k}|h_{2k-1\,j}\rangle|^2. \tag{54}$$

(54) agrees with the results of $O(n,1)$.

Next for $O(2k,1)$: One has from the principal series

$$h_{2k+1\,1}=\tfrac{1}{2}-k+ic. \tag{55}$$

If one makes the identification

$$c=\lambda, \tag{56}$$

one obtains from (50)

$$\begin{aligned}|\langle h_{2k\,j}+1|J_{2k+1\,2k}|h\rangle|^2/|\langle h_{2k\,j}+1|I_{2k+1\,2k}|h\rangle|^2 &=\lambda^2+(l_{2k\,j}+\tfrac{1}{2})^2\\ &=-(h_{2k+1\,1}-\tfrac{1}{2}+k)^2+(l_{2kj}+\tfrac{1}{2})^2\\ &=-(l_{2k+1\,1}-\tfrac{1}{2})^2+(l_{2k\,j}+\tfrac{1}{2})^2\\ &=(l_{2k\,j}+l_{2k+1\,1})(l_{2k\,j}-l_{2k+1\,1}+1)\\ &=-(l_{2k+1\,1}-l_{2k\,j}-1)(l_{2k+1\,1}+l_{2k\,j}).\end{aligned} \tag{57}$$

Equation (57) again agrees with the results of $O(2k,1)$ obtained by Ottoson and others.

V. CONCLUSION

We see therefore that Chakrabarti's results in both $IU(n)\to U(n,1)$ and $IO(n)\to O(n,1)$ can be reconciled with the results of Gel'fand and Graev, and Ottoson and others. The representations of $U(n,1)$ and $O(n,1)$ thus obtained are continuous representations. The matrix elements obtained by Chakrabarti appear to be complex, but they can be reduced to either pure real or pure imaginary by working out their absolute value squared and then taking the square root. The results then agree with each other. We can therefore say that the matrix elements of the generators of $U(n,1)$, at least for the continuous representation, can be (a) complex or (b) pure imaginary or pure real. The first case (a) corresponds to the results obtained by Chakrabarti. The second case, i.e., pure imaginary, corresponds to the results of Gel'fand and Graev. In the case where one defines the generators according to Rosen and Roman, then one obtains the matrix elements as pure real, which, however, is just a variation of case (b).

In the case of $O(n,1)$, for the continuous representation, the matrix elements of the generators again can be either (a) complex or (b) pure imaginary, for the off-diagonal part of $J_{2k+1\,2k}$ and $J_{2k-1\,2k}$. The case where the matrix elements are pure real is just a variation of the definition of the generators from case (b). For the diagonal matrix elements of $J_{2k-1\,2k}$, it is always real. The first case (a) corresponds to Chakrabarti's results (with a correction of a factor of $\frac{1}{2}$) and the second case (b) corresponds to the results given by several authors, among whom are Hirai, Ottoson, Schwarz, and Wong.

[1] I. M. Gel'fand and M. L. Zetlin, Dokl. Akad. Nauk SSSR **71**, 825, 1017 (1950).
[2] I. M. Gel'fand and M. I. Graev, Izv. Akad. Nauk SSSR Ser. Math. **29**, 1329 (1965) [Am. Math. Soc. Transl. **64**, 116 (1967) Ser. 2].
[3] U. Ottoson, Comm. Math. Phys. **10**, 114 (1968).
[4] T. Hirai, Proc. Japan Acad. **38**, 83, 258 (1962).
[5] U. Ottoson, Comm. Math. Phys. **8**, 228 (1968).
[6] F. Schwarz, J. Math. Phys. **12**, 131 (1971).
[7] M. K. F. Wong, J. Math. Phys. **15**, 25 (1974).
[8] A. Chakrabarti, J. Math. Phys. **9**, 2087 (1968).
[9] K. B. Wolf, J. Math. Phys. **12**, 197 (1971); **13**, 1634 (1972).
[10] J. Rosen and P. Roman, J. Math. Phys. **7**, 2072 (1966).
[11] S. C. Pang and K. T. Hecht, J. Math. Phys. **8**, 1233 (1967).
[12] M. K. F. Wong, J. Math. Phys. **8**, 1899 (1967).
[13] W. Miller, Jr., *Lie Theory and Special Functions* (Academic, New York, 1968).
[14] This deformation formula was first given by A. Sankaranarayanan, Nuovo Cimento **38**, 1441 (1965).

Killing inequalities for relativistically rotating fluids*

R. O. Hansen and Jeffrey Winicour

Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
(Received 18 September 1974)

For rigidly rotating fluids in general relativity, it is shown that the angular momentum density is everywhere positive. This result depends on a global inequality satisfied by the Killing scalars. The inequality follows, via the Hopf theorem, from an elliptic equation (essentially one of the field equations) on the scalars. A derivation of the field equations in terms of the manifold of Killing orbits is presented. Possible generalizations of the result to systems with differential rotation or interior event horizons are discussed.

1. INTRODUCTION

In a general asymptotically flat space–time, the asymptotic symmetries define certain energy–momentum linkages in terms of two-dimensional integrals over surfaces at infinity.[1] The resulting total energy–momentum is unique up to the usual transformation properties of a Lorentz four-vector as in special relativity. However, the total angular momentum not only contains an arbitrary amount of momentum (corresponding to the choice of axis freedom in special relativity) but also an arbitrary amount of supermomentum resulting from the super-translational freedom associated with radiative space–times. From an asymptotic point of view, total angular momentum is less rigid a concept than total energy–momentum. However, when these surface integrals are converted to three-dimensional volume integrals over the interior, neither the energy–momentum density nor the angular momentum density have their usual degree of special relativistic uniqueness. While total energy–momentum is well defined, there is no density rigidly associated with it. Consequently, neither energy density nor angular momentum density retain the same local physical significance they possess in special relativity.

For space–times with *global* symmetries the situation is quite different. The linkages reduce to the corresponding Komar integrals[2] for which unique densities can be defined. Here we consider asymptotically flat space–times with two global commuting Killing vectors corresponding to a time translation and a spatial rotation, so that the associated components of total energy and total angular momentum and their densities are all mathematically well defined. For such systems, the energy density and angular momentum density are in close agreement with their standard forms in the special relativistic limit (see Sec. 2). This gives some assurance that these densities have useful physical meaning in general relativity. More reassuring is the positive-definite nature of the energy density in the strong curvature case given reasonable matter conditions. Similar results concerning the angular momentum density would not be expected even for axisymmetric special relativistic systems since different portions of the system could have opposing rotational motion about the same axis. However, in special relativity, the angular momentum density of a system with uniform sense of rotation about a given axis is uniformly positive (or negative). Our major result is a similar property of the angular momentum density of a uniformly rotating general relativistic fluid.

We begin in Sec. 2 with a discussion of the Komar integrals which shows that our result is not manifestly obvious as in the flat space case, but depends upon a certain global inequality involving the Killing scalars. To establish this inequality, we set up in Sec. 3 a geometrical formalism for interior solutions based upon the Geroch treatment of the manifold of Killing trajectories. In Sec. 4, we show that a certain combination of Killing scalars satisfies a two-dimensional elliptic equation whose source terms do not depend upon the material properties of the interior. This equation leads via the Hopf theorem to the desired inequality.

2. THE KOMAR INTEGRALS

Let $\xi_0{}^a$ and $\xi_1{}^a$ be commuting Killing vectors corresponding to a time translation and spatial rotation, respectively. We fix their extensions by the requirements that

$$\xi_0{}^a\xi_{0a} \to -1$$

at infinity and that solutions of

$$dx^a/d\phi = \xi_1{}^a$$

describe closed rotational orbits for the parameter range $0 \leq \phi \leq 2\pi$. The mass and angular momentum are then given by the Komar integrals over two-surfaces at infinity

$$M = -\frac{1}{8\pi}\oint \nabla^{[a}\xi_0{}^{b]}\,dS_{ab} \tag{2.1}$$

and

$$J = \frac{1}{16\pi}\oint \nabla^{[a}\xi_1{}^{b]}\,dS_{ab}. \tag{2.2}$$

The minus sign difference between the forms of these integrals arises because the Komar integral gives the covariant energy component. The factor of 2 difference is less trivial: It arises from virial effects (see below).

By means of Einstein's equations

$$G^{ab} = 8\pi T^{ab} \tag{2.3}$$

and the Gauss theorem, these integrals lead to the volume integrals over the interior

$$M = -2\int \xi_0{}^a[T_a{}^b - \tfrac{1}{2}\delta_a{}^b T]\,dS_b \tag{2.4}$$

and

$$J = \int \xi_1{}^a T_a{}^b\,dS_b, \tag{2.5}$$

where we choose our integration regions to contain the rotational orbits,[3] so that

$$\xi_1{}^b\, dS_b = 0.$$

The integrand in Eq. (2.5) is the standard angular momentum density of a special relativistic system. The special relativistic energy density, $\xi_0{}^a T_a{}^b$, does not agree with the integrand in (2.4). However, Eq. (2.4) does give the correct total energy for a stationary (but rotating) special relativistic system via the virial theorem,

$$\int \xi_0{}^b T\, dS_b = \int \xi_0{}^a T_a{}^b\, dS_b.$$

The energy densities agree to the extent that stresses are negligible compared with energy density. Furthermore, the energy density defined by (2.4) is positive for general relativistic systems without unduly negative stresses, so that it provides a useful density associated with total active gravitational mass.

For an axisymmetric rotating fluid, the stress–energy is given by

$$T^{ab} = (\mu + p)u^a u^b + p g^{ab}, \tag{2.6}$$

with

$$u^a = (-\psi)^{-1/2}(\xi_0{}^a + \Omega \xi_1{}^a), \tag{2.7}$$

where

$$\psi = \lambda_{00} + 2\Omega\lambda_{01} + \Omega^2\lambda_{11} \tag{2.8}$$

and

$$\lambda_{AB} = \xi_A{}^a \xi_{Ba}.$$

This leads to

$$M = \int [\mu + 3p - 2\Omega(\mu + p)\psi^{-1}(\lambda_{01} + \Omega\lambda_{11})]\xi_0{}^b\, dS_b \tag{2.9}$$

and

$$J = -\int (\mu + p)\psi^{-1}(\lambda_{01} + \Omega\lambda_{11})\xi_0{}^b\, dS_b. \tag{2.10}$$

The timelike nature of the hydrodynamical stream lines implies that ψ is negative, so that the sign of the angular momentum density is determined by $\lambda_{01} + \Omega\lambda_{11}$, where $\lambda_{11} > 0$ except on the axis where it vanishes. In the special relativistic limit, $\lambda_{01} \to 0$ and the density is strictly positive when the angular velocity Ω is positive. However, to decide this question in the strong curvature case, we need the interior Einstein equations.

3. THE FIELD EQUATIONS

We use a formalism developed by Geroch[4] for space-times admitting two commuting Killing vectors. Since the field equations have been given only for source-free fields, we here present a general derivation of the equations with sources.

Let (M, g_{ab}) be a space–time admitting a pair of commuting Killing vectors, $\xi_0{}^a$ and $\xi_1{}^a$. We assume that $\xi_0{}^a$ is everywhere timelike and $\xi_1{}^a$ everywhere spacelike. It is convenient to introduce upper-case Latin indices[4] with the range 0, 1,[5] and write $\xi_A{}^a$ for the Killing vectors. Upper-case Latin indices will be raised and lowered with the alternating symbol ϵ_{AB} (with $\epsilon_{00} = \epsilon_{11} = 0$, $\epsilon_{01} = -\epsilon_{10} = 1$), using the rules

$$\epsilon^{AM}\epsilon_{BM} = \delta^A{}_B, \quad p^A = \epsilon^{AM} p_M, \quad p_A = p^M \epsilon_{MA}. \tag{3.1}$$

Two points p and q in M are said to lie on the same orbit if there is a curve from p to q whose tangent is everywhere a linear combination of $\xi_0{}^a$ and $\xi_1{}^a$. The set S of orbits possesses (locally) a manifold structure. Furthermore, there is a natural, one-to-one correspondence[4] between tensor fields $T^{a\cdots b}{}_{c\cdots d}$ on S and tensor fields $T^{a\cdots b}{}_{c\cdots d}$ on M which satisfy

$$\xi_{Am} T^{m\cdots b}{}_{c\cdots d} = 0, \cdots, \ \xi_A{}^m T^{a\cdots b}{}_{c\cdots m} = 0, \tag{3.2}$$

$$\mathcal{L}_{\xi_A} T^{a\cdots b}{}_{c\cdots d} = 0. \tag{3.3}$$

Thus, we shall speak of tensor fields on M satisfying (3.2) and (3.3) as tensor fields on S.

The Killing scalars $\lambda_{AB} = \xi_A{}^m \xi_{Bm}$ are scalar fields on S; the timelike character of the orbits requires that

$$\tau^2 = -\lambda^{MN}\lambda_{MN} \tag{3.4}$$

define a positive scalar field τ^2 on S. A metric h_{ab} and alternating tensor ϵ_{ab} on S are given by

$$h_{ab} = g_{ab} + 2\tau^{-2}\lambda^{MN}\xi_{Ma}\xi_{Nb}, \tag{3.5}$$

$$\epsilon_{ab} = (1/\sqrt{2})\tau^{-1}\epsilon^{MN}\epsilon_{abmn}\xi_M{}^m \xi_N{}^n. \tag{3.6}$$

Note that indices of tensors on S may be raised and lowered using either h_{ab} or g_{ab}, with the same result. Furthermore, if $T^{a\cdots b}{}_{c\cdots d}$ is a tensor field on S, then so is

$$D_a T^{b\cdots c}{}_{d\cdots e} = h_a{}^m h^b{}_n \cdots h^c{}_p h_d{}^q \cdots h_e{}^r \nabla_m T^{n\cdots p}{}_{q\cdots r}. \tag{3.7}$$

Equation (3.7) defines the derivative operator D_a on S. The Riemann tensor $R_{abc}{}^d$ of S is given by

$$D_{[a}D_{b]}k_c = \tfrac{1}{2}R_{abc}{}^m k_m, \tag{3.8}$$

where k_a is any vector field on S.

We wish to write a collection of equations, equivalent to Einstein's equation, involving only tensor fields on S. To do this, we require one more pair of scalar fields, c_A, defined by

$$c_A = \tfrac{1}{2}\epsilon^{MN}\epsilon^{mnpq}\xi_{Mm}\xi_{Nn}\nabla_p \xi_{Aq}. \tag{3.9}$$

Following the procedure given by Geroch,[4] we obtain the equations

$$D^m(\tau^{-1}D_m\lambda_{AB}) = \tau^{-3}\lambda_{AB}(D^m\lambda^{MN})(D_m\lambda_{MN}) + 2\tau^{-3}c_A c_B - 2\tau^{-1}R_{mn}\xi_A{}^m\xi_B{}^n, \tag{3.10}$$

$$D_a c_A = -\sqrt{2}\,\tau\epsilon_a{}^m R_{mn}\xi_A{}^n, \tag{3.11}$$

$$R_{ab} = \tfrac{1}{2}\tau^{-2}(D_a\lambda^{MN})(D_b\lambda_{MN}) + \tau^{-1}D_aD_b\tau - 2\tau^{-4}h_{ab}\lambda^{MN}c_M c_N + h_a{}^m h_b{}^n R_{mn}, \tag{3.12}$$

where R_{ab} is the Ricci tensor of M.

It is convenient to separate (3.12) into its trace and trace-free parts:

$$R = \tfrac{1}{2}\tau^{-2}(D^m\lambda^{MN})(D_m\lambda_{MN}) + \tau^{-1}D^mD_m\tau - 4\tau^{-4}\lambda^{MN}c_Mc_N + h^{mn}R_{mn}, \tag{3.13}$$

$$R_{ab} - \tfrac{1}{2}h_{ab}R = \tfrac{1}{2}\tau^{-2}(D_a\lambda^{MN})(D_b\lambda_{MN}) - \tfrac{1}{4}\tau^{-2}h_{ab}(D^m\lambda^{MN})(D_m\lambda_{MN}) + \tau^{-1}D_aD_b\tau - \tfrac{1}{2}\tau^{-1}h_{ab}D^mD_m\tau + h_a{}^mh_b{}^nR_{mn} - \tfrac{1}{2}h_{ab}h^{mn}R_{mn}. \tag{3.14}$$

Equation (3.13) may be simplified somewhat. Contract (3.10) with λ^{AB}, to obtain

$$D^mD_m\tau = -2\tau^{-3}\lambda^{MN}c_Mc_N + 2\tau^{-1}\lambda^{MN}R_{mn}\xi_M{}^m\xi_N{}^n, \tag{3.15}$$

and substitute into (3.13):

$$R = \tfrac{1}{2}\tau^{-2}(D^m\lambda^{MN})(D_m\lambda_{MN}) - 6\tau^{-4}\lambda^{MN}c_Mc_N + h^{mn}R_{mn} + 2\tau^{-2}\lambda^{MN}R_{mn}\xi_M{}^m\xi_N{}^n. \tag{3.16}$$

The left-hand side of (3.14) vanishes identically; thus we have

$$D_aD_b\tau - \tfrac{1}{2}h_{ab}D^mD_m\tau + \tfrac{1}{2}\tau^{-1}(D_a\lambda^{MN})(D_b\lambda_{MN}) - \tfrac{1}{4}\tau^{-1}h_{ab}(D^m\lambda^{MN})(D_m\lambda_{MN}) + \tau(h_a{}^mh_b{}^nR_{mn} - \tfrac{1}{2}h_{ab}h^{mn}R_{mn}) = 0. \tag{3.17}$$

The Bianchi identity

$$\nabla^m(R_{am} - \tfrac{1}{2}g_{am}R) = 0 \tag{3.18}$$

takes the form

$$D^m(\tau h_m{}^nR_{np}\xi_A{}^p) = 0, \tag{3.19}$$

$$D^m[\tau(h_a{}^nh_m{}^pR_{np} - \tfrac{1}{2}h_{am}h^{np}R_{np})] + \tfrac{1}{2}h^{mn}R_{mn}D_a\tau + \tau^{-1}\lambda^{MN}D_a(R_{mn}\xi_M{}^m\xi_N{}^n) + 2\sqrt{2}\,\tau^{-2}\lambda^{MN}c_M\epsilon_a{}^mR_{mn}\xi_N{}^n = 0. \tag{3.20}$$

Equation (3.19) is the integrability condition for (3.11). The role of (3.20) is more subtle. The divergence of the left-hand side of (3.17) vanishes if (3.10), (3.11), (3.16), and (3.20) are satisfied. But the left-hand side of (3.17) is a symmetric, trace-free tensor field S_{ab} on S. If S_{ab} vanishes on a closed curve bounding some region in S, and if its divergence vanishes everywhere in the region, then S_{ab} vanishes there. Thus, if (3.10), (3.11), (3.16), and (3.20) are satisfied, and if (3.18) is satisfied on some closed curve in S, then (3.18) is satisfied everywhere in the region bounded by the curve.

Let T_{AB}, θ_{Aa}, and t_{ab} be defined by

$$T_{AB} = T_{mn}\xi_A{}^m\xi_B{}^n, \tag{3.21}$$

$$\theta_{Aa} = h_a{}^mT_{mn}\xi_A{}^n, \tag{3.22}$$

$$t_{ab} = h_a{}^mh_b{}^nT_{mn}. \tag{3.23}$$

Substituting for R_{ab} from the Einstein equation (2.3) in (3.10), (3.11), (3.16), (3.20), and (3.18), we obtain

$$D^m(\tau^{-1}D_m\lambda_{AB}) = \tau^{-3}\lambda_{AB}(D^m\lambda^{MN})(D_m\lambda_{MN}) + 2\tau^{-3}c_Ac_B - 16\pi\tau^{-1}(T_{AB} - \tfrac{1}{2}\lambda_{AB}T), \tag{3.24}$$

$$D_ac_A = -8\sqrt{2}\,\pi\tau\epsilon_a{}^m\theta_{Am}, \tag{3.25}$$

$$R = \tfrac{1}{2}\tau^{-2}(D^m\lambda^{MN})(D_m\lambda_{MN}) - 6\tau^{-4}\lambda^{MN}c_Mc_N + 8\pi(T + 4\tau^{-2}\lambda^{MN}T_{MN}), \tag{3.26}$$

$$D^m(\tau t_{am}) - \tau T_{MN}D_a(\tau^{-2}\lambda^{MN}) + 2\sqrt{2}\,\tau^{-2}\lambda^{MN}c_M\epsilon_a{}^m\theta_{Nm} = 0, \tag{3.27}$$

$$D_aD_b\tau + \tfrac{1}{2}\tau^{-1}(D_a\lambda^{MN})(D_b\lambda_{MN}) - \tfrac{1}{4}\tau^{-1}h_{ab}(D^m\lambda^{MN})(D_m\lambda_{MN}) + \tau^{-3}h_{ab}\lambda^{MN}c_Mc_N + 8\pi\tau t_{ab} = 0, \tag{3.28}$$

where

$$T = T^m{}_m = h^{mn}t_{mn} - 2\tau^{-2}\lambda^{MN}T_{MN}. \tag{3.19}$$

Equations (3.24)—(3.28) are equivalent to Einstein's equation. That is to say, a 2-manifold S with metric h_{ab} and fields λ_{AB}, c_A, T_{AB}, θ_{Aa}, and t_{ab} satisfying (3.24)—(3.27) in some region of S, and (3.28) on the boundary of that region, determines a unique space—time (M, g_{ab}), with two commuting Killing vectors, satisfying Einstein's equation.

We require the field equations only for perfect fluids, described by (2.6). Decompose the four-velocity u^a into

$$u_A = u_m\xi_A{}^m, \quad v_a = h_a{}^mu_m. \tag{3.30}$$

Substitution into the field equations gives

$$D^m(\tau^{-1}D_m\lambda_{AB}) = \tau^{-3}\lambda_{AB}(D^m\lambda^{MN})(D_m\lambda_{MN}) + 2\tau^{-3}c_Ac_B - 16\pi\tau^{-1}[(\mu+p)u_Au_B + \tfrac{1}{2}(\mu-p)\lambda_{AB}], \tag{3.31}$$

$$D_ac_A = -8\sqrt{2}\,\pi(\mu+p)\tau u_A\epsilon_a{}^mv_m, \tag{3.32}$$

$$R = \tfrac{1}{2}\tau^{-2}(D^m\lambda^{MN})(D_m\lambda_{MN}) - 6\tau^{-4}\lambda^{MN}c_Mc_N + 8\pi(\mu+p), \tag{3.33}$$

$$v_aD^m[(\mu+p)\tau v_m] + (\mu+p)\tau v^mD_mv_a - (\mu+p)\tau v^mD_av_m + \tau^{-1}(\mu+p)\lambda^{MN}D_a(u_Mu_N) + \tau D_ap - 2\sqrt{2}\,\tau^{-2}(\mu+p)\lambda^{MN}c_Mc_N\epsilon_a{}^mv_m = 0, \tag{3.34}$$

$$D_aD_b\tau + \tfrac{1}{2}\tau^{-1}(D_a\lambda^{MN})(D_b\lambda_{MN}) - \tfrac{1}{4}\tau^{-1}h_{ab}(D^m\lambda^{MN})(D_m\lambda_{MN}) + \tau^{-3}h_{ab}\lambda^{MN}c_Mc_N + 8\pi\tau[(\mu+p)v_av_b + ph_{ab}] = 0. \tag{3.35}$$

Equation (3.34) can be simplified by substituting from (3.32). This gives

$$\tau^{-1}(\mu+p)\lambda^{MN}D_a(u_Mu_N) = -\tau(h_a{}^m + v_av^m)D_mp + (\mu+p)\epsilon_a{}^mv_m(\tau\epsilon^{np}D_nv_p - 2\sqrt{2}\,\tau^{-2}\lambda^{MN}c_Mu_N), \tag{3.36}$$

$$(\mu+p)v^mD_mu_A = -u_Av^mD_mp, \tag{3.37}$$

$$D^m(\tau\mu v_m) = -pD^m(\tau v_m). \tag{3.38}$$

Equations (3.36) and (3.37) are the equations of hydrostatic support in the directions perpendicular and parallel to the flow of convective circulation, respectively.

Equation (3.38) expresses the conservation of convective flux.

We now specialize to the case of vanishing convective circulation, i.e., $v^a = 0$. The four-velocity then takes the form

$$u^a = (-\psi)^{-1/2} s^M \xi_M{}^a; \tag{3.39}$$

the field equations become

$$D^m(\tau^{-1} D_m \lambda_{AB}) = \tau^{-3}\lambda_{AB}(D^m\lambda^{MN})(D_m\lambda_{MN}) + 2\tau^{-3}c_A c_B + 8\pi\tau^{-1}[(\mu+3p)\lambda_{AB} + (\mu+p)\tau^2\psi^{-1}s_A s_B], \tag{3.40}$$

$$D_a c_A = 0, \tag{3.41}$$

$$R = \tfrac{1}{2}\tau^{-2}(D^m\lambda^{MN})(D_m\lambda_{MN}) - 6\tau^{-4}\lambda^{MN}c_M c_N + 8\pi(\mu+p), \tag{3.42}$$

$$\tfrac{1}{2}(\mu+p)\psi^{-1}D_a\psi - \tfrac{1}{2}(\mu+p)\psi^{-1}\lambda^{MN}D_a(s_M s_N) = -D_a p, \tag{3.43}$$

$$D_a D_b \tau + \tfrac{1}{2}\tau^{-1}(D_a\lambda^{MN})(D_b\lambda_{MN}) - \tfrac{1}{4}\tau^{-1}h_{ab}(D^m\lambda^{MN})(D_m\lambda_{MN}) + \tau^{-3}h_{ab}\lambda^{MN}c_M c_N + 8\pi p\tau h_{ab} = 0. \tag{3.44}$$

Roughly speaking, s^A represents the angular velocity of the system with respect to infinity,[7] and ψ the Newtonian plus centrifugal potentials. We further assume that the system rotates rigidly, so that the second term in (3.43) vanishes.

We now impose the condition that the system possess a regular axis of symmetry,[8] where $\tau = 0$. We take as our axis conditions that the manifold S be extendable to a manifold with boundary $\hat{S}$, the boundary corresponding to the axis, and that $\hat{S}$ have a regular metric $\hat{h}_{ab}$ which agrees with h_{ab} on the interior.[9] We henceforth assume that S has been so extended, and delete the carets.

Several results follow immediately from the axis assumptions. First, since the Killing vectors are linearly dependent on the axis, c_A vanishes there. Thus, in the absence of convective circulation, c_A vanishes everywhere. Next, the regularity of the left-hand side of (3.14) requires that (3.44) be satisfied on the axis. Thus, we need only satisfy (3.44) on some curve, bounding the region of interest, with end points on the axis. We take this to be a curve at infinity, on which (3.44) is again automatically satisfied by virtue of asymptotic flatness. Furthermore, since λ_{AB}, μ, p, s^A, and ψ are all well-behaved fields on M, they must have vanishing normal derivatives on the axis.[8]

Finally, we simplify our notation by identifying a Greek index with each symmetric pair of upper-case Latin indices.[4] Greek indices are raised and lowered with the symmetric metric $G_{\alpha\beta}$ defined by

$$G_{\alpha\beta} = -\epsilon_{A(C}\epsilon_{D)B}, \quad \alpha \leftrightarrow (AB), \quad \beta \leftrightarrow (CD). \tag{3.45}$$

In this spirit, we write $S_\alpha = s_A s_B$. The field equations for a stationary axisymmetric, asymptotically flat, rigidly rotating perfect fluid then take the form

$$D^m(\tau^{-1}D_m\lambda_\alpha) = \tau^{-3}\lambda_\alpha(D^m\lambda^\mu)(D_m\lambda_\mu) + 8\pi\tau^{-1}[(\mu+3p)\lambda_\alpha + (\mu+p)\tau^2\psi^{-1}S_\alpha], \tag{3.46}$$

$$R = \tfrac{1}{2}\tau^{-2}(D^m\lambda^\mu)(D_m\lambda_\mu) + 8\pi(\mu+p), \tag{3.47}$$

$$\tfrac{1}{2}(\mu+p)\psi^{-1}D_a\psi = -D_a p. \tag{3.48}$$

4. THE KILLING INEQUALITIES

We now return to the question of the sign of $\eta = \lambda_{01} + \Omega\lambda_{11}$ which determines the sign of the angular momentum density. We assume uniform fluid rotation with positive angular velocity Ω. The problem then is to show that η is positive throughout the fluid interior.

Equations (3.46)—(3.48) are the entire set of field equations for such a system. The key equation for our purpose results from skewing Eq. (3.46) with λ_β and S_γ to obtain

$$\epsilon^{\alpha\beta\gamma}\lambda_\beta S_\gamma D^m(\tau^{-1}D_m\lambda_\alpha) = 0. \tag{4.1}$$

This is equivalent to

$$N^{[\alpha}S^{\beta]}\lambda_\beta D^m(\tau^{-1}D_m\lambda_\alpha) = 0, \tag{4.2}$$

where

$$N^\alpha = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & \Omega \end{pmatrix},$$

so that $\eta = \lambda_\alpha N^\alpha$. Also, note that $\psi = \lambda_\alpha S^\alpha$. Because N^α and S^α are constant matrices, we can rewrite (4.2) in the form

$$D^m[\tau^{-1}(\psi D_m\eta - \eta D_m\psi)] = 0. \tag{4.3}$$

Viewed as an elliptic equation for $\psi^{-1}\eta$, (4.3) becomes

$$\tau^{-1}\psi^2 D^m D_m(\psi^{-1}\eta) + D^m(\tau^{-1}\psi^2)D_m(\psi^{-1}\eta) = 0. \tag{4.4}$$

This is a well-behaved equation to which the Hopf theorem[10] is applicable in the open region D bounded by the axis $\tau = 0$ and the velocity of light curve[11] $\psi = 0$. Consequently, each point of D has a neighborhood in which $\psi^{-1}\eta$ is either constant or does not have a maximum.

Consider the boundary of D. On the axis $\psi^{-1}\eta$ vanishes. On the velocity of light curve,

$$\lambda_{00} + 2\Omega\lambda_{01} + \Omega^2\lambda_{11} = 0,$$

which implies that

$$\eta = \tfrac{1}{2}\Omega^{-1}(\Omega^2\lambda_{11} - \lambda_{00}) > 0.$$

Consequently $\psi^{-1}\eta \to -\infty$ as the velocity of light curve is approached from the interior of D. Furthermore, asymptotic flatness implies that $\eta > 0$ for all points in D sufficiently far from the source. Consequently, the set of points $E \subset D$ for which $\psi^{-1}\eta > 0$ must have compact closure. If E were nonempty, then $\psi^{-1}\eta$ would attain a maximum at some interior points. But this would violate the Hopf theorem.[12]

We conclude that $\psi^{-1}\eta < 0$ in D. Since any fluid source must be restricted to the region D plus the axis, this establishes the required result concerning the angular momentum density.

Furthermore, in the region $\psi > 0$ outside the velocity of light curve, the same argument implies that $\psi^{-1}\eta > 0$. Consequently, $\eta > 0$ throughout the space—time except on the axis where $\eta = 0$.

Similarly, consider the Killing scalar

$$\nu = \lambda_{00} + \Omega\lambda_{01} = \psi - \Omega\eta.$$

Then $\psi^{-1}\nu$ satisfies Eq. (4.4) when η is replaced everywhere by ν. Repeating the above argument, the Hopf theorem then implies that $\nu < 0$ throughout the space–time.

5. DISCUSSION

The global inequalities for the Killing scalars η and ν obtained in Sec. 4 provide fundamental restrictions on the possible interior and exterior geometries for uniformly rotating fluid stars. In particular, the inequality for η insures a positive angular momentum density for such systems. There are, however, two conditions underlying our derivation of this result which deserve further investigation.

First is the condition of completeness of the space–time as a stationary manifold and the resulting implications for the manifold of trajectories S. This rules out not only the possibility of singularities but also the existence of black holes interior to the fluid region, as described by Bardeen.[13] The existence of black holes would complicate the establishment of the necessary boundary conditions on the Killing scalars needed for application of the Hopf theorem.

Second is the uniform rotation condition $\Omega = \text{const}$. If this were weakened to the condition $\Omega \geq 0$, would our results still hold? In the general case of differential rotation with uniform sense, Eq. (4.2) still applies but the steps leading to Eq. (4.3) would no longer be valid. Consequently, the arguments presented in Sec. 4 are not applicable to this case. One might expect on the basis of the Newtonian limit that the angular momentum density remain positive. But in the Newtonian case this result follows from strictly local arguments whereas even in the case of uniform rotation non-local features play an important role in the general relativistic case. The problem can be restated in terms of the velocity v, introduced by Bardeen,[13] which measures the rotational velocity of the fluid relative to local zero angular momentum observers. The angular momentum density has the same sign as v. It is conceivable for differential rotation with $\Omega \geq 0$ that global inertial effects might cause portions of the fluid with small angular velocities to behave as if they were counterrotating ($v < 0$) with respect to the local observers.

[1] J. Winicour and L. Tamburino, Phys. Rev. Letters **15**, 601 (1965).
[2] A. Komar, Phys. Rev. **113**, 934 (1959).
[3] Because of the surface independence of the Komar integrals, this choice does not limit generality.
[4] R. Geroch, J. Math. Phys. **13**, 394 (1972).
[5] More precisely, we regard the upper-case Latin indices as abstract indices over the Lie algebra of Killing vector fields on M.
[6] B. Carter, J. Math. Phys. **10**, 70 (1969).
[7] We scale s^A so that its component in the Killing direction which is timelike at infinity is unity [cf. (2.7) and (2.8)].
[8] B. Carter, Comm. Math. Phys. **17**, 233 (1970).
[9] It appears that our conditions are equivalent to the usual axis regularity conditions. However, on the axis, h_{ab} becomes a direction-dependent tensor field on M, so that the equivalence is not immediately evident.
[10] See, e.g., S. Bochner and K. Yano, *Curvature and Betti Number* (Princeton U. P., Princeton, N.J., 1953), p. 26.
[11] In the Newtonian limit, this curve is a straight line parallel to the axis. Here, we make no assumptions concerning connectivity.
[12] The boundary conditions rule out the possibility $\psi^{-1}\eta = \text{const}$.
[13] J. M. Bardeen, in *Black Holes*, edited by C. DeWitt and B. S. DeWitt (Gordon and Breach, New York, 1973), p. 241.

Lattice Green's function for the body-centered cubic lattice

Michiko Inoue

RCA Research Laboratories, Inc., P.O. Box 5151, Tokyo International 100-31, Japan
(Received 18 November 1974)

We have shown that the lattice Green's function at an arbitrary site with nearest neighbor interactions for the body-centered cubic lattice is expressed as a finite sum of products of the complete elliptic integrals of the first and the second kinds with real values of moduli for the entire range of energy.

1. INTRODUCTION

A lattice Green' s function at a lattice point (l, m, n) for a body-centered cubic (b. c. c.) lattice with nearest neighbor interactions is given by

$$G(l, m, n) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dx\,dy\,dz\,\frac{\cos lx\cos my\cos nz}{E - i\delta - \cos x\cos y\cos z}, \tag{1.1}$$

where l, m and n are zero or integers, E is a real number, and δ is an infinitesimal number. Maradulin *et al.*[1] proved that the above function at the origin $G(0, 0, 0)$ is reduced to a product of the complete elliptic integral of the first kind. In this paper, we show that $G(l, m, n)$ for an arbitrary point (l, m, n) is expressed as a finite sum of products of complete elliptic integrals of the first and second kind. In proving this, we use the method developed previously for the case of a face-centered cubic lattice,[2] in which the knowledge of a group of the Green' s function $G(2p, 0, 0)$ ($p = 0$ or an integer) is sufficient to determine the rest of $G(l, m, n)$ by successive applications of two recurrence formulas. From (1.1), $G(2p, 0, 0)$ is real for $|E| > 1$ and is complex for $|E| < 1$. However, by extending the procedure of analytical continuation it is shown that $G(2p, 0, 0)$ is expressed in terms of the complete elliptic integrals of the first and the second kind with real values of moduli for $-\infty < E < \infty$.

2. RECURRENCE FORMULAS

For a cubic lattice, nonequivalent lattice sites are in a portion of 1/48 of the entire space, and it is generally possible by successive applications of two recurrence relations for the Green' s function to determine the whole family of $G(l, m, n)$ in terms of $G(2p, 0, 0)$'s for a zero or positive integer p.[2]

For a b. c. c. lattice the first formula holds for $G(l, m, n)$' s connecting the nearest neighbor sites and is given by

$$\begin{aligned}&G(l+1, m+1, n+1) + G(l-1, m-1, n-1)\\ &\quad + G(l+1, m+1, n-1) + G(l-1, m-1, n+1)\\ &\quad + G(l+1, m-1, n+1) + G(l-1, m+1, n-1)\\ &\quad + G(l-1, m+1, n+1) + G(l+1, m-1, n-1)\\ &= 8EG(l, m, n) - 8\delta_{l0}\delta_{m0}\delta_{n0},\end{aligned} \tag{2.1}$$

where δ_{l0} is Kronecker' s delta.

The second formula holds for Eq. (1.1) on nine lattice sites which lie inside and on the edges of a square formed by lines joining the $2p$th and the $2p + 4$th sites along the x and y axis on the (0, 0, 1) plane. This recurrence relation enables one to express any $G(2l, 2m, 0)$ in terms of $G(2p, 0, 0)$'s for $p \le l$, and the derivation is similar to the derivation for the f. c. c. lattice, as described in Ref. 2.

Assume $|E| > 1$, and we integrate (1.1) over z to get

$$\begin{aligned}G(2l, 2m, 0) &= \frac{1}{\pi^2}\int_0^\pi\int_0^\pi dx\,dy\,\frac{\cos 2lx\cos 2my}{(E^2 - \cos^2 x\cos^2 y)^{1/2}}\\ &= \frac{1}{\pi^2}\int_0^\pi dx\cos 2lx F_m(E, x),\end{aligned} \tag{2.2}$$

where

$$F_m(E, x) = \int_0^\pi dy\,\frac{\cos 2my}{(E^2 - \cos^2 x\cos^2 y)^{1/2}}. \tag{2.3}$$

Next, we introduce an integral

$$f_m(E, x) = \int_0^\pi dy\cos 2my[E^2 - \cos^2 x\cos^2 y]^{1/2}, \tag{2.4}$$

which is written in terms of $F_m(E, x)$:

$$\begin{aligned}f_m(E, x) &= E^2F_m(E, x) - \frac{\cos^2 x}{4}[F_{m+1}(E, x) + F_{m-1}(E, x)\\ &\quad + 2F_m(E, x)].\end{aligned} \tag{2.5}$$

For $m \neq 0$ we integrate (2.4) by parts, so that

$$f_m(E, x) = -\frac{\cos^2 x}{2m}\int_0^\pi dy\,\frac{\sin 2my\cos y\sin y}{[E^2 - \cos^2 x\cos^2 y]^{1/2}}. \tag{2.6}$$

After combining (2.2), (2.5), and (2.6) and rearranging terms, we get

$$\begin{aligned}&2(4E^2 - 1)G(2l, 2m, 0) - G(2l+2, 2m, 0) - G(2l-2, 2m, 0)\\ &\quad - \tfrac{1}{2}(1 + 1/2m)[G(2l+2, 2m+2, 0) + G(2l-2, 2m+2, 0)\\ &\quad + 2G(2l, 2m+2, 0)] - \tfrac{1}{2}(1 - 1/2m)[G(2l+2, 2m-2, 0)\\ &\quad + G(2l-2, 2m-2, 0) + 2G(2l, 2m-2, 0)]\\ &\quad = 0.\end{aligned} \tag{2.7}$$

For $m = 0$, we calculate directly from (1.1):

$$\begin{aligned}G(2, 2, 0) &= -\frac{4}{\pi^2}\int_0^\pi\int_0^\pi dx\,dy[E^2 - \cos^2 x\cos^2 y]^{1/2}\\ &\quad + (4E^2 - 1)G(0, 0, 0) - 2G(2, 0, 0).\end{aligned} \tag{2.8}$$

The integral on the right-hand side of (2.5) is expressed in terms of the generalized hypergeometric series,

$$I = \int_0^\pi\int_0^\pi dx\,dy[E^2 - \cos^2 x\cos^2 y]^{1/2}$$

$$= E\pi^2 \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{2})_n (\frac{1}{2})_n}{(1)_n (1)_n (1)_n} \frac{1}{E^{2n}}$$

$$= \frac{E\pi^2}{2} \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n}{(1)_n (1)_n (1)_n} [(\tfrac{3}{2})_n (-\tfrac{1}{2})_n + (\tfrac{1}{2})_n (\tfrac{1}{2})_n] \frac{1}{E^{2n}}$$

$$= \frac{E\pi^2}{2} \left[{}_3F_2\left(\tfrac{1}{2}, \tfrac{3}{2}, -\tfrac{1}{2}; 1, 1; \frac{1}{E^2}\right) + {}_3F_2\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; \frac{1}{E^2}\right) \right]. \tag{2.9}$$

By use of the formula[3]

$${}_3F_2(a, c-a, \tfrac{1}{2}c; c, \tfrac{1}{2}c + \tfrac{1}{2}; z)$$
$$= [{}_2F_1(a, c-a, \tfrac{1}{2}c + \tfrac{1}{2}; \tfrac{1}{2} - \tfrac{1}{2}\sqrt{1-z})]^2, \tag{2.10}$$

and the Gauss' transformation for ${}_2F_1(a, b, c; x)$, we get for I

$$I = 2^2 E\{[K(k_0)]^2 - 2K(k_0)E(k_0) + 2[E(k_0)]^2\}, \tag{2.11}$$

with

$$k_0{}^2 = \tfrac{1}{2} - \tfrac{1}{2}(1 - 1/E^2)^{1/2}. \tag{2.11'}$$

Then, $G(2, 2, 0)$ is given by

$$G(2, 2, 0) = (4E^2 - 1)G(0, 0, 0) - 2G(2, 0, 0)$$
$$- \frac{2^4 E}{\pi^2}\{[K(k_0)]^2 - 2K(k_0)E(k_0) + 2[E(k_0)]^2\}. \tag{2.12}$$

3. CALCULATIONS OF $G(2p,0,0)$ for $|E| > 1$

From (1.1), we have

$$G(2p, 0, 0) = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} dx\, dy \frac{\cos 2px}{(E^2 - \cos^2 x \cos^2 y)^{1/2}}. \tag{3.1}$$

Integration of (3.1) over y leads to

$$G(2p, 0, 0) = \frac{1}{\pi E} \int_0^{\pi} dx \cos 2px\, {}_2F_1\left(\tfrac{1}{2}, \tfrac{1}{2}, 1; \frac{\cos^2 x}{E^2}\right). \tag{3.1'}$$

By expanding ${}_2F_1(\frac{1}{2}, \frac{1}{2}, 1; \cos^2 x/E^2)$ in a power series and integrating over x term by term, we get

$$G(2p, 0, 0) = \frac{1}{\pi E} \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{2})_n}{(1)_n (1)_n E^{2n}} \int_0^{\pi} dx \cos 2px \cos^{2n} x$$
$$= \frac{1}{E} \sum_{r=0}^{p} \frac{(-1)^r p}{(2p-r)} \binom{2p-r}{r} 2^{2p-2r} \frac{(\frac{1}{2})_{p-r}}{(1)_{p-r}} {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, p-r+\tfrac{1}{2};$$
$$1, p-r+1; 1/E^2). \tag{3.2}$$

Next, we show that ${}_3F_2(\frac{1}{2}, \frac{1}{2}, p-r+\frac{1}{2}; 1, p-r+1; z)$ ($p - r = 0$ or a positive integer) can always be expanded in a finite sum of products of simple hypergeometric functions ${}_2F_1(a+\frac{1}{2}, b+\frac{1}{2}, c; \frac{1}{2} - \frac{1}{2}\sqrt{1-z})$ with integers a, b, and c. We start with an identity which holds for ${}_3F_2(\frac{1}{2}, \frac{1}{2}, p+\frac{1}{2}; 1, p+1; z)$ with p a postive integer,

$${}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, p+\tfrac{1}{2}; 1, p+1; z)$$
$$= \sum_{s=0}^{q} D^p_{s,q}\, {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, p-s-\tfrac{1}{2}; 1, p-s; z)$$
$$+ \frac{\Gamma(p+1)\Gamma(q+\frac{3}{2})\Gamma(p-q-\frac{1}{2})}{[\Gamma(\frac{1}{2})]^3[\Gamma(p+\frac{1}{2})]^2}$$
$$\times \sum_{n=0}^{\infty} \frac{[\Gamma(n+\frac{1}{2})]^2 \Gamma(n+p-q-\frac{1}{2})}{[\Gamma(n+1)]^2 \Gamma(n+p+1)} z^n \prod_{s=0}^{q} (n+s+\tfrac{1}{2}), \tag{3.3}$$

where $q < p$ and

$$D^p_{s,q} = \frac{(-1)^s \Gamma(p+1)[\Gamma(p-s-\frac{1}{2})]^2}{\Gamma(p-s)[\Gamma(p+\frac{1}{2})]^2}$$
$$\times \sum_{r=0}^{q-s} \binom{r+s}{s} (p-2r-2s-1) \frac{\Gamma(p-r-s)}{\Gamma(p-r-2s)}. \tag{3.4}$$

Validity of (3.3) and (3.4) is readily proved by induction. Now, if we put $p = 2m$ and $q = m-1$ in (3.3), we get after some calculations

$${}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, 2m+\tfrac{1}{2}; 1, 2m+1; z)$$
$$= \sum_{s=0}^{m-1} D^{2m}_{s,m-1}\, {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, 2m-s-\tfrac{1}{2}; 1, 2m-s; z)$$
$$+ \left(\frac{\Gamma(m+\frac{1}{2})}{\Gamma(\frac{1}{2})}\right)^3 \frac{1}{[\Gamma(2m+\frac{1}{2})]^2 \Gamma(m+1) 2^{2m}}$$
$$\times \sum_{a=0}^{2m} \binom{2m}{a} \Gamma(a+\tfrac{1}{2}) \Gamma(2m-a+\tfrac{1}{2})$$
$$\times {}_3F_2(a+\tfrac{1}{2}, 2m-a+\tfrac{1}{2}, m+\tfrac{1}{2}; 2m+1, m+1; z). \tag{3.5}$$

Similarly, for $p = 2m+1$, and $q = m$, Eq. (3.3) is written as

$${}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, 2m+\tfrac{3}{2}; 1, 2m+2; z)$$
$$= \sum_{s=0}^{m} D^{2m+1}_{s,m}\, {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, 2m-s+\tfrac{1}{2}; 1, 2m-s+1; z)$$
$$+ \left[\frac{\Gamma(m+\frac{1}{2})}{\Gamma(2m+\frac{3}{2})}\right]^2 \frac{\Gamma(m+\frac{3}{2})}{[\Gamma(\frac{1}{2})]^3 \Gamma(m+1) 2^{2m+1}}$$
$$\times \sum_{a=0}^{2m+1} \binom{2m+1}{a} \Gamma(a+\tfrac{1}{2}) \Gamma(2m-a+\tfrac{3}{2})$$
$$\times {}_3F_2(a+\tfrac{1}{2}, 2m-a+\tfrac{3}{2}, m+\tfrac{1}{2}; 2m+2, m+1; z). \tag{3.6}$$

Then, by successive use of (3.5) and (3.6), we can reduce ${}_3F_2(\frac{1}{2}, \frac{1}{2}, p+\frac{1}{2}; 1, p+1; z)$ to a linear combination of ${}_3F_2(r+\frac{1}{2}, 2q-r+\frac{1}{2}, q+\frac{1}{2}; 2q+1, q+1; z)$ and ${}_3F_2(r+\frac{1}{2}, 2q-r+\frac{3}{2}, q+\frac{1}{2}; 2q+2, q+1; z)$, where q and r are zero or positive integers satisfying $2q - r + \frac{1}{2} > 0$. Furthermore, those generalized hypergeometric functions are reduced to a sum of products of a simple hypergeometric functions. By use of (2.10), we get

$${}_3F_2(r+\tfrac{1}{2}, 2q-r+\tfrac{1}{2}, q+\tfrac{1}{2}; 2q+1, q+1; z)$$
$$= [{}_2F_1(r+\tfrac{1}{2}, 2q-r+\tfrac{1}{2}, q+1; \tfrac{1}{2} - \tfrac{1}{2}\sqrt{1-z})]^2, \tag{3.7}$$

and we also have

$${}_3F_2(r+\tfrac{1}{2}, 2q-r+\tfrac{3}{2}, q+\tfrac{1}{2}; 2q+2, q+1; z)$$
$$= [{}_2F_1(r+\tfrac{1}{2}, 2q-r+\tfrac{1}{2}, q+1; \tfrac{1}{2} - \tfrac{1}{2}\sqrt{1-z})]^2$$
$$+ \left(\frac{r+\frac{1}{2}}{2q+2}\right)^2 z[{}_2F_1(r+\tfrac{3}{2}, 2q-r+\tfrac{3}{2}, q+2; \tfrac{1}{2} - \tfrac{1}{2}\sqrt{1-z})]^2. \tag{3.8}$$

The relation (3.8) is easily obtained by applying Gauss' transformation of the simple hypergeometric series to the formula derived by Burchnall and Chaundy.[4] Finally, we note that $F(a+\frac{1}{2}, b+\frac{1}{2}, c; k_0{}^2)$ for integers a, b, and c is reduced to a linear combination of $K(k_0)$ and $E(k_0)$.

To illustrate, we give below the explicit expressions for $G(2p, 0, 0)$ for $p = 0, 1, 2, 3$ calculated by our method

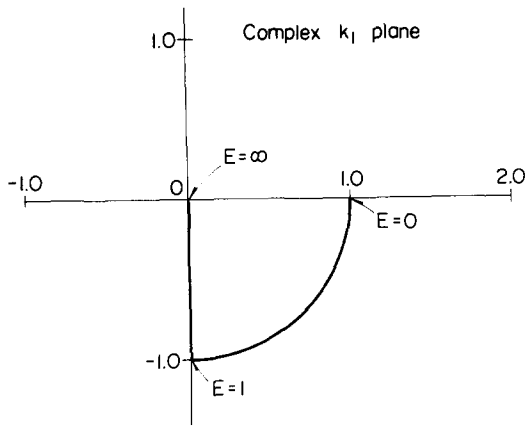

FIG. 1. The values of k_1 in the complex plane.

described above:

$$G(0,0,0)=(4/\pi^2 E)[K(k_0)]^2, \tag{3.9}$$

$$G(2,0,0)=\frac{4(1-k_0^2)}{\pi^2 E k_0^2}\left(K(k_0)-\frac{1}{1-k_0^2}E(k_0)\right)^2, \tag{3.10}$$

$$G(4,0,0)=\frac{4}{9\pi^2 E k_0^4}\left((2-3k_0^2)K(k_0)-\frac{2(1-2k_0^2)}{1-k_0^2}E(k_0)\right)^2, \tag{3.11}$$

$$G(6,0,0)=\frac{4}{\pi^2 E k_0^2(1-k_0^2)}\left[\left(1-k_0^2+\frac{4(k_0^2-2)}{15k_0^2}\right)K(k_0)+\left(\frac{8(k_0^4-k_0^2+1)}{15k_0^2(1-k_0^2)}-1\right)E(k_0)\right]^2, \tag{3.12}$$

where k_0 is given by (2.11′).

4. ANALYTICAL CONTINUATION OF $G(2p,0,0)$ FOR $|E|<1$

The Green' s function $G(l,m,n)$ represented by (1.1) has a nonvanishing imaginary part for $|E|<1$. Notice that the real and the imaginary parts of $G(l,m,n)$ satisfy the following relations with respect to the change in sign of E, namely,

$$\mathrm{Re}G(l,m,n,E)=\mathrm{Re}G(l,m,n,-E)(-1)^{l+m+n+1}$$

and (4.1)

$$\mathrm{Im}G(l,m,n,E)=\mathrm{Im}G(l,m,n,-E)(-1)^{l+m+n},$$

so that it is sufficient to evaluate $G(l,m,n)$ for $0\leq E<+\infty$. The two recurrence relations in Sec. 2 are valid for all values of E, applying analytical continuation to $G(l,m,n)$' s.

The expressions for $G(2p,0,0)$ derived in the preceding section are valid for $1<E<+\infty$. In order to obtain $G(2p,0,0)$ for $0\leq E\leq 1$, we extend the procedure of analytical continuation[5,6] to transform $K(k_0)$ and $E(k_0)$ having real modulus k_0 for $E>1$ given by (2.11′) into $K(q)$ and $E(q)$ with real modulus q for $0\leq E\leq 1$. By applying a transformation,

$${}_2F_1(\tfrac{1}{2},\pm\tfrac{1}{2},1;k_0^2)=(1-k_0^2)^{\mp 1/2}\,{}_2F_1(\tfrac{1}{2},\pm\tfrac{1}{2},1;k_0^2/(k_0^2-1)), \tag{4.2}$$

we get $K(k_1)$ and $E(k_1)$ for which the modulus $k_1=k_0/\sqrt{k_0^2-1}$ is on a line along the negative imaginary axis for $E>1$ and on a circle of unit radius for $0\leq E\leq 1$ in the complex k_1 plane, as shown in Fig. 1. When k_1 is a complex number with $|k_1|=1$, it is possible to map k_1 into a line along the real axis starting from the point greater than unity in the complex q plane by the transformation

$$q=2\sqrt{k_1}/(1+k_1). \tag{4.3}$$

The functions $K(k_1)$ and $E(k_1)$ are accordingly transformed to

$$K(k_1)=[1/(1+k_1)]K(q)$$

and

$$E(k_1)=\tfrac{1}{2}[(1+k_1)E(q)+(1-k_1)K(q)]. \tag{4.4}$$

In applying the above transformations, care is to be taken to put

$$(E-c)^{1/2}=(E-c)^{1/2} \quad \text{for } E-c\geq 0,$$

and (4.5)

$$(E-c)^{1/2}=-i(c-E)^{1/2} \quad \text{for } E-c<0,$$

when we take the limiting values $E-i\delta$ as $\delta\to 0$ for $\delta>0$. Furthermore, $K(q)$ and $E(q)$ with $q>1$ are expressed in terms of $K(1/q)$, $E(1/q)$ and those with the complementary modulus $1/q'=(1-1/q^2)^{1/2}$ as

$$K(q)=(1/q)[K(1/q)-iK'(1/q)]$$

and

$$E(q)=q\left[E\left(\frac{1}{q}\right)+iE'\left(\frac{1}{q}\right)-\left(1-\frac{1}{q^2}\right)K\left(\frac{1}{q}\right)-i\frac{1}{q^2}K'\left(\frac{1}{q}\right)\right]. \tag{4.6}$$

Finally, by combining (4.2), (4.4), and (4.6), we write $K(k_0)$ and $E(k_0)$ in terms of $K(1/q)$, $K'(1/q)$, $E(1/q)$, and $E'(1/q)$ as

$$K(k_0)=\frac{E^{1/2}}{2}(1+i)\left[K\left(\frac{1}{q}\right)-iK'\left(\frac{1}{q}\right)\right]$$

and

$$E(k_0)=\frac{1}{2E^{1/2}}\left\{(1-i)\left[E\left(\frac{1}{q}\right)+iE'\left(\frac{1}{q}\right)\right]+\tfrac{1}{2}[(1-E)^{1/2}+i(1+E)^{1/2}]\{[(1+E)^{1/2}-(1-E)^{1/2}]K(\tfrac{1}{2})-[(1+E)^{1/2}+(1-E)^{1/2}]K'(1/q)\}\right\}, \tag{4.7}$$

where

$$1/q=\tfrac{1}{2}[(1+E)^{1/2}+(1-E)^{1/2}]. \tag{4.7′}$$

Clearly, $1/q$ is real and smaller than unity for $0\leq E\leq 1$. Therefore, by simply replacing $K(k_0)$ and $E(k_0)$ by the expression, (4.7) and (4.7′) together with Eq. (4.5) in the relevant coefficients involved in $G(l,m,n)$ in the preceding section, we can evaluate $G(l,m,n)$ in terms of the complete elliptic integrals of the first and the second kinds with real moduli for $0\leq E<1$.

5. SUMMARY

We have developed a general method to express the lattice Green's function (l,m,n) at an arbitrary site

(l, m, n) for b.c.c. lattice as a finite sum of products of the complete elliptic integrals of the first and the second kind with real moduli for the entire range of values of energy. The present method is particularly useful for high-accuracy numerical evaluations of $G(l, m, n)$ and can be extended to evaluation of the lattice Green's functions for non-cubic symmetry.

Note added in proof: Since this paper was written, the author has learned that G.S. Joyce had already shown that $G(l, m, n)$ given by our Eq. (1.1) was expressed in terms of the complete elliptic integrals of the first and second kind for $|E| > 1$, and that he also derived the analytical continuation of $G(0, 0, 0)$ for $|E| < 1$ [J. Phys, C1, 1510(1971); J. Math. Phys. 12, 1390 (1971)]. The author is grateful to Professor S. Katsura for pointing out the papers of Joyce.

ACKNOWLEDGMENT

The author acknowledges Dr. S. Tosima's critical reading of the manuscript.

[1]A.A. Maradudin *et al.*, Acad. Roy. Belg. Classe Sci. **9**, No. 7 (1960).
[2]M. Inoue, J. Math. Phys. **15**, 704 (1974).
[3]*Higher Transcendental Functions*, edited by A. Erdèly *et al.* (McGraw-Hill, New York, 1953) Vols. I—III.
[4]J. L. Burchnall and T.W. Chaundy, Q. J. Math. Oxford Ser. **11**, 249 (1940); **12**, 112 (1941).
[5]M. Inoue, to be published in J. Math. Phys.
[6]A different approach to express $G(0,0,0)$ for $0 \leq E \leq 1$ in terms of ${}_2F_1(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}; 1 - E^2)$ and ${}_2F_1(\frac{3}{4}, \frac{3}{4}, \frac{3}{2}; 1 - E^2)$ was given by S. Katsura and T. Horiguchi, J. Math. Phys. **12**, 230 (1971).

Convergence of Padé approximants using the solution of linear functional equations *

George A. Baker, Jr.

Applied Mathematics Department, Brookhaven National Laboratory, Upton, New York 11973
(Received 20 December 1973; final revised manuscript received 20 March 1974)

We prove that a projection of the solutions to a linear functional equation of the Fredholm type with a compact kernel, projected into the Cini-Fubini subspaces, converge strongly to the solution in the whole space. Here either the whole sequence converges for all nonsingular points of the functional equation with at most one exceptional point, or by selecting at most two infinite subsequences we can obtain convergence for all nonsingular points. We then prove that the diagonal Padé approximants to the inner product of the solution with another element converge. For certain kernels of trace class, the numerator and denominator separately converge. As applications of these results, we prove the pointwise convergence of the Padé approximants to a wide class of meromorphic functions. We also prove the convergence, for decent potentials, of the Padé approximants to the scattering amplitudes for nonrelativistic quantum mechanical scattering problems. The numerators and denominators of the Padé approximants to the partial wave scattering amplitudes for single signed potentials converge separately to entire functions of the coupling constant.

1. INTRODUCTION AND SUMMARY

In this paper we discuss the relation between Padé approximants and the solutions of linear functional equations. Our discussion is substantially different in approach than the classical matrix theory of continued functions[1] and different in results as well. Our study had its genesis in an effort to remove a number of unnecessary restrictions in the work of Garibotti and Villani[2] on the convergence of Padé approximants in nonrelativistic quantum mechanical scattering theory.

Since Chisholm[3] first considered the solution of integral equations by Padé approximants, the field has developed in two directions. On one hand, there has been considerable study of the definition and properties of Padé approximants to matrix formal power series, as Chisholm originally had considered. For a recent review, see Bessis.[4] The alternative approach was to consider the Padé approximants to the matrix elements separately. It is this latter approach that we shall take. Tani[5] and Nuttall[6] soon realized that the matrix element of the solution to an integral (or more generally a linear functional) equation when properly projected is exactly a Padé approximant to the solution to the equation in the whole space. In the scattering theory context, the proper projection is the Cini—Fubini one.[7]

In the second section of this paper we review, in a more general setting, the relationship between Padé approximation and projection in Hilbert space as it relates to the solution of linear, functional equations of the Fredholm type.

In the third section we review some of the known properties of the trace class of compact operators. In the fourth section we prove that the solutions to properly truncated Fredholm equations with a certain subclass of the trace class of kernels converge strongly to the correct solution. Furthermore, the numerator and denominator to the $[M-1/M]$ Padé approximants separately converge to entire functions as $M \to \infty$.

In the fifth section we consider general Fredholm-type equations whose kernels are only assumed to be compact. We again prove strong convergence of a projection of the solutions to properly projected equations. Either the whole sequence converges everywhere not a singular point of the functional equation with at most one exceptional point, or by selecting at most two infinite subsequences we can obtain convergence for all nonsingular points. The convergence of the Padé approximants, to the matrix elements is then immediate, but the numerators and denominators do not necessarily separately converge. This result proves a modification of a theorem conjectured by Chisholm.[3]

In the sixth section we consider a wide class of meromorphic functions which can be associated with functional equations with compact kernels. We prove convergence for the Padé approximants in the same pointwise sense as in the fifth section. This result proves a modification of a theorem conjectured by Baker and Gammel.[8] It also improves (for a narrower class of functions) Nuttall's results[9] which proved convergence in measure (or capacity, Pommerenke[10]) for the whole class of meromorphic functions. For a more restricted class we prove numerator and denominator converge as well.

Finally in the last section we treat nonrelativistic scattering theory. For decent potentials we prove convergence of the Padé approximants to the scattering amplitude for all real, physical momentum plus for short-range potentials for a strip about the real axis. In addition, we prove for single-signed potentials convergence for the partial wave scattering amplitude in the same region, where the numerator converges and the denominator converges to the Jost function. This last result extends the results of Garibotti and Villani[2] for real momentum.

2. THE PADÉ APPROXIMANT AS THE EXACT SOLUTION IN THE CINI-FUBINI SUBSPACE

We are concerned with the solution of the functional equation

$$\mathbf{f} = \mathbf{g} + \lambda \mathbf{A}\mathbf{f}, \tag{2.1}$$

where $\mathbf{f}$ is an element of a Hilbert space $\mathcal{H}$ and $\mathbf{A}$ is a linear operator whose properties we shall detail latter. It has been known for some time, Tani[5] and Nuttall,[6] in the context of scattering theory that the Padé approximants[3] in λ to $(\mathbf{h},\mathbf{f})$ are the exact solution to the truncation of Eq. (2.1) in the Cini–Fubini[7] subspace where $\mathbf{h}\in\mathcal{H}$. We repeat these arguments here in a more abstract setting to free them from a number of unnecessary restrictions.

Let us introduce the elements

$$\varphi_i=\mathbf{A}^{i-1}\mathbf{g},\quad \varphi_i'=(\mathbf{A}^\dagger)^{i-1}\mathbf{h}, \tag{2.2}$$

where $\mathbf{A}^\dagger$ is the Hermitian conjugate of $\mathbf{A}$.

Let us further define the $N\times N$ matrix

$$\begin{aligned}R_{ij}&=(\varphi_i',\varphi_j)=((\mathbf{A}^\dagger)^{i-1}\mathbf{h},\mathbf{A}^{j-1}\mathbf{g})\\&=(\mathbf{h},\mathbf{A}^{i+j-2}\mathbf{g})\equiv\omega_{i+j-2}.\end{aligned} \tag{2.3}$$

If $\det|R_{ij}|\neq 0$, we can define the operator

$$\mathbf{P}_N=\sum_{i,j=1}^{N}\varphi_i(R^{-1})_{ij}(\varphi_j'\ ). \tag{2.4}$$

We can verify easily by direct computation that $\mathbf{P}_N^2=\mathbf{P}_N$, that is, $\mathbf{P}_N$ is an idempotent. Further, since $\mathbf{P}_N\varphi_i=\varphi_i$, the range of $\mathbf{P}_N$ is the space spanned by the φ_i and no larger than (2.4). Hence, by known results,[11] $\mathbf{P}_N$ is a projection operator on the space $\mathcal{S}_N$ spanned by the φ_i. It may happen that $\mathbf{P}_N$ is an oblique, rather than an orthogonal, projection. Then $\|\mathbf{P}_N\|>1$. The operators $\mathbf{P}_N$ define a nesting sequence of spaces as $\mathbf{P}_N\mathbf{P}_M=\mathbf{P}_M\mathbf{P}_N=\mathbf{P}_M$, if $M\leq N$.

Let us now consider the truncated equation

$$\mathbf{f}_N=\mathbf{g}+\lambda\mathbf{P}_N\mathbf{A}\mathbf{P}_N\mathbf{f}_N. \tag{2.5}$$

By construction, the solution of (2.5) must be of the form

$$\mathbf{f}_N=\sum_{j=1}^{N}a_j\varphi_j. \tag{2.6}$$

By direct substitution we get

$$\sum_{j=1}^{N}a_j\varphi_j=\mathbf{g}+\lambda\mathbf{P}_N\sum_{j=1}^{N}a_j\mathbf{A}\varphi_j; \tag{2.7}$$

to obtain a convenient set of equations, we may take the inner product of these equations with the elements φ_i'. If we use the definitions (2.3) and (2.4), we obtain the equations

$$\sum_{j=1}^{N}a_j(\omega_{i+j-2}-\lambda\omega_{i+j-1})=\omega_{i-1}. \tag{2.8}$$

If we introduce the $N\times N$ matrix

$$U_{ij}=\omega_{i+j-2}-\lambda\omega_{i+j-1} \tag{2.9}$$

and the adjoint matrix V_{ij} composed of the first order minors of U, then we may write the solution of (2.8) as

$$\mathbf{f}_N=\left(\sum_{i=1}^{N}\sum_{j=1}^{N}\varphi_iV_{ij}\omega_{j-1}\right)\Big/(\det|U_{ij}|). \tag{2.10}$$

Now, it follows directly from Eq. (2.9) that, as a function of λ, the coefficient of each φ_i is a rational fraction whose numerator is of degree at most $N-1$ and whose denominator is of degree at most N. This solution is possible as, for $\lambda=0$, $\det|U_{ij}|=\det|R_{ij}|\neq 0$ by hypothesis.

Of particular interest in the rest of this section is the inner product

$$(\mathbf{h},\mathbf{f}_N)=\left(\sum_{i=1}^{N}\sum_{j=1}^{N}\omega_{i-1}V_{ij}\omega_{j-1}\right)\Big/(\det|U_{ij}|). \tag{2.11}$$

Next let us consider forming the $[N-1/N]$ Padé approximants to the Liouville–Neumann series to the solution of (2.1). The Liouville–Neumann series is

$$\mathbf{f}=\mathbf{g}+\lambda\mathbf{A}\mathbf{g}+\lambda^2\mathbf{A}^2\mathbf{g}+\lambda^3\mathbf{A}^3\mathbf{g}+\cdots. \tag{2.12}$$

If we take the inner product of $\mathbf{f}$ given by Eq. (2.12) with some element $\mathbf{h}$, we define a formal power series

$$(\mathbf{h},\mathbf{f})=h(\lambda)=\omega_0+\lambda\omega_1+\lambda^2\omega_2+\lambda^3\omega_3+\cdots, \tag{2.13}$$

where we have used the definition (2.3). The defining equations for the $[L/M]$ Padé approximants[12] to a formal power series, $s(z)$, are

$$\begin{aligned}&s(z)\,Q_M(z)-P_L(z)=O(z^{L+M+1}),\\&Q_M(0)=1.0,\end{aligned} \tag{2.14}$$

where Q_M is a polynomial of degree at most M and P_L is a polynomial of degree at most L. If we apply these equations to the calculation of the $[N-1/N]$ Padé approximant to $h(\lambda)$, we obtain, after a little manipulation of the Cramer's rule solution of the linear equations (2.14), the Nuttall compact form[6,12] result

$$\begin{aligned}[N-1/N]&=\left(\sum_{i=1}^{N}\sum_{j=1}^{N}\omega_{i-1}V_{ij}\omega_{j-1}\right)\Big/(\det|U_{ij}|)\\&=(\mathbf{h},\mathbf{f}_N).\end{aligned} \tag{2.15}$$

Thus, provided $\det|\omega_{i+j-2}|\neq 0$, we have shown that the $[N-1/N]$ Padé approximant to $(\mathbf{h},\mathbf{f})$, where $\mathbf{f}$ satisfies (2.1), is identically equal to $(\mathbf{h},\mathbf{f}_N)$, where $\mathbf{f}_N$ satisfies the truncated equation (2.5), of finite rank. Hence, in order to study the convergence of the Padé approximants, we may replace the difficult procedure of Padé approximation by the more easily controllable procedure of projection.

Now, with regard to the restriction $\det|\omega_{i+j-2}|\neq 0$. If this determinant for a given N vanishes, then the set of N elements φ_i is not linearly independent in the space $\mathcal{S}_N'$ spanned by the elements φ_i'. Since this determinant is also the determinant for the Padé equations, the possibilities have been extensively studied.[13] The case must be that either $(\mathbf{h},\mathbf{f})$ is a rational fraction of finite degree (zero is specifically included in this case), or there exists an infinite number of N's for which that determinant is different from zero. When the determinant vanishes, the Padé approximant equations are either consistent or inconsistent. When they are consistent, the Padé approximant is unique,[13] though not the numerator nor denominator separately, and it is equal to a Padé approximant of lower degree. We will not treat this problem further here since we are assured that either a finite order Padé approximant is the exact function $h(\lambda)$ or that there exists at least an infinite subsequence of $[M-1/M]$ to which we can, without loss, confine our attention.

The results given above can be extended to any sequence $[M+J/M]$, $J\geq -1$, of Padé approximants as a nesting family of subspaces can be defined for it and a modified equation

$$\mathbf{f} = \mathbf{A}^{J+1}\mathbf{g} + \lambda \mathbf{A}\mathbf{f} \tag{2.16}$$

associated with it, by the elementary properties of the Padé approximant.[12]

3. TRACE-CLASS OPERATORS

Since the properties of trace-class operators (see, Kato[11]) are not generally well known among physicists, we will review some of those that we need here. First suppose that the operator **A** is compact. That is to say, for every sequence of elements $\{\mathbf{f}_n\}$ with the property that $\|\mathbf{f}_n\| \leq C$, then the sequence of elements $\{\mathbf{A}\mathbf{f}_n\}$ contains a convergent subsequence of elements $\{\mathbf{g}_m\}$. The convergence is in the sense $\|\mathbf{g}_j - \mathbf{g}_k\| \to 0$ as j and k go to infinity.

It follows by well-known theory[14] that the operator $\mathbf{A}^\dagger\mathbf{A} = \mathbf{T}$ is compact, self-adjoint, and nonnegative definite. Furthermore, it has at most a denumerably infinite number of eigenvalues. Thus we may write

$$\mathbf{T}\psi_i = \alpha_i^2\psi_i, \tag{3.1}$$

where the ψ_i are the orthonormal eigenvectors and we take $\alpha_i \geq \alpha_{i+1} \geq 0$. The trace norm of the operator **A** is defined as

$$\|A\|_1 = \sum_{i=1}^{\infty} \alpha_i. \tag{3.2}$$

The trace class is all those operators of finite trace norm. It follows easily that $\|\alpha\mathbf{A}\|_1 = |\alpha|\|\mathbf{A}\|_1$ and that $\|A\|_1 \geq 0$ and equals zero only if $\mathbf{A}\mathbf{f} = 0$ for all $\mathbf{f}$ in $\mathcal{H}$. In the study of the properties of this norm, it is convenient to introduce the canonical expansion of **A**. First define

$$\psi_i' = \mathbf{A}\psi_i/\alpha_i. \tag{3.3}$$

The ψ_i' can easily be shown to form an orthonormal set of elements. Then, we have the canonical expansion

$$\mathbf{A} = \sum_i \psi_i'\alpha_i(\psi_i, \ ). \tag{3.4}$$

Since the trace norm is sometimes difficult to evaluate, it is convenient to bound it. Let us consider $\|\mathbf{AB}\|_1$, where **A** and **B** belong to the Hilbert–Schmidt subclass of compact operators, defined by

$$\|\mathbf{A}\|_2 = \sum_{i=1}^{\infty} \alpha_i^2 < \infty. \tag{3.5}$$

Then by using the canonical expansion

$$\mathbf{AB} = \sum_i \varphi_i'\gamma_i(\varphi_i, \ ), \tag{3.6}$$

we have by (3.6)

$$\begin{aligned}
&\|\mathbf{AB}\|_1 \\
&= \sum_i \gamma_i = \sum_i (\varphi_i', \mathbf{AB}\varphi_i) = \sum_i (\mathbf{A}^\dagger\varphi_i', \mathbf{B}\varphi_i) \\
&\leq \sum_i \|A^\dagger\varphi_i\| \, \|B\varphi_i\| \\
&\leq \Big(\sum_i \|A^\dagger\varphi_i\|^2\Big)^{1/2} \Big(\sum_i \|B\varphi_i\|^2\Big)^{1/2} \\
&\leq \|A^\dagger\|_2 \, \|B\|_2 = \|A\|_2 \, \|B\|_2,
\end{aligned} \tag{3.7}$$

where the properties of the inner product, the Cauchy–Schwarz inequality, and the basis independence of the Hilbert–Schmidt norm have been used. Clearly any operator of trace class is also in the Hilbert–Schmidt class. It is also true that any operator of trace class can be factored into two operators of Hilbert–Schmidt class. To see this result, introduce the operator

$$|\mathbf{A}| = \sum_i \psi_i\alpha_i(\psi_i, \ ), \tag{3.8}$$

which has the property $|\mathbf{A}|^2 = \mathbf{T}$. As the $\alpha_i > 0$, we may take the square root of $|\mathbf{A}|$ in an obvious way. Further

$$\mathbf{A} = \sum_{i,j} \psi_i'(\psi_i', \psi_j), \quad \alpha_j(\psi_j, \ ) = \mathbf{U}|\mathbf{A}|, \tag{3.9}$$

where as ψ_i' and ψ_i are orthonormal sets, **U** is unitary. By factoring $\mathbf{A} = (\mathbf{U}|\mathbf{A}|^{1/2})(|\mathbf{A}|^{1/2})$, we then have both factors of Hilbert–Schmidt class, if **A** is of trace class. Finally, we note that it can be shown[11] that

$$\|\mathbf{A} + \mathbf{B}\|_1 \leq \|\mathbf{A}\|_1 + \|\mathbf{B}\|_1. \tag{3.10}$$

There is one further inequality which we will need. It is

$$\|\mathbf{AB}\|_1 \leq \alpha_1(\mathbf{A})\|\mathbf{B}\|_1 \leq \|\mathbf{A}\|_1 \, \|\mathbf{B}\|_1, \tag{3.11}$$

which can be proved by use of (3.7) and factoring $\mathbf{AB} = \mathbf{AU}|\mathbf{B}|^{1/2}|\mathbf{B}|^{1/2}$ so that

$$\begin{aligned}
\|\mathbf{AB}\|_1 &\leq \|\mathbf{AU}|\mathbf{B}|^{1/2}\|_2 \, \|\,|\mathbf{B}|^{1/2}\|_2 \\
&\leq \alpha_1(\mathbf{AU})\|\,|\mathbf{B}|^{1/2}\|_2^2 = \alpha_1(\mathbf{AU})\|\mathbf{B}\|_1,
\end{aligned} \tag{3.12}$$

but as $\alpha_1(\mathbf{AU}) = \alpha_1(\mathbf{A})$ we have (3.11). If we apply (3.11) to $\mathbf{A}^k$, we have

$$\|\mathbf{A}^k\|_1 \leq (\|\mathbf{A}\|_1)^k. \tag{3.13}$$

Next we see that for **A** of trace class that the trace is a well-defined function of **A**. We define

$$\mathrm{tr}(\mathbf{A}) = \sum_i (\varphi_i, \mathbf{A}\varphi_i) \tag{3.14}$$

where φ_i is any complete orthonormal set of elements in $\mathcal{H}$. Using the ψ_i defined in (3.1), we can now show that the sum in (3.14) is absolutely convergent, for

$$\begin{aligned}
\sum_i |(\varphi_i, \mathbf{A}\varphi_i)| &= \sum_i |(\varphi_i, \mathbf{A}^\dagger\varphi_i)| \\
&= \sum_i \Big|\sum_j (\varphi_i, \psi_j)(\psi_j, \mathbf{A}^\dagger\varphi_i)\Big| \\
&\leq \sum_i \sum_j |(\varphi_i, \psi_j)| \, |(\psi_j, \mathbf{A}^\dagger\varphi_i)| \\
&\leq \sum_j \Big(\sum_i |(\varphi_i, \psi_j)|^2\Big)^{1/2} \Big(\sum_i |(\psi_j, \mathbf{A}^\dagger\varphi_i)|^2\Big)^{1/2} \\
&= \sum_j \alpha_j(\mathbf{A}) = \|\mathbf{A}\|_1
\end{aligned} \tag{3.15}$$

or

$$|\mathrm{tr}(\mathbf{A})| \leq \sum_i |(\varphi_i, \mathbf{A}\varphi_i)| \leq \|\mathbf{A}\|_1 \tag{3.16}$$

for any operator of trace class and any orthonormal family. Since the sum in (3.16) is absolutely convergent, the usual arguments can be applied and we conclude that $\mathrm{tr}(\mathbf{A})$ is independent of the basis set.

We conclude this section by defining the determinant

$$D(\lambda) = \det|\mathbf{I} + \lambda\mathbf{A}| = \lim_{N\to\infty} D_N(\lambda), \tag{3.17}$$

where **I** is the identity and **A** is of trace class, and by showing that $D(\lambda)$ is an entire function of λ.

We may write the definition

$$D_N(\lambda) \equiv \exp\{\mathrm{tr}_N[\ln(\mathbf{I}+\lambda\mathbf{A})]\}, \tag{3.18}$$

which is an identity for small enough λ, where $\mathrm{tr}_N(\mathbf{X})$ is a partial trace over the first N elements of an arbitrary orthonormal set. To give meaning to this definition, we expand the logarithm in a power series in λ. By use of inequalities (3.13) and (3.16) we may bound this series term by term by

$$|\mathrm{tr}_N[\ln(\mathbf{I}+\lambda\mathbf{A})]| \leq \sum_{j=1}^{\infty} \frac{1}{j} (|\lambda|\,\|\mathbf{A}\|_1)^j, \tag{3.19}$$

which converges absolutely for $|\lambda| < \|\mathbf{A}\|_1^{-1}$. Thus at least for small λ, the function $D_N(\lambda)$ is an analytic function of λ, uniformly in N. We will now show that in fact $D_N(\lambda)$ is uniformly bounded in N for all λ.

Following Dunford and Schwartz[15] we may write, at least for $|\lambda| < \|\mathbf{A}\|_1^{-1}$ where the relations hold term by term in λ,

$$\begin{aligned} |D_N(\lambda)|^2 &= |\det_N|\mathbf{I}-\lambda\mathbf{A}||^2 \\ &= \det_N|(\mathbf{I}-\lambda^*\mathbf{A}^\dagger)(\mathbf{I}-\lambda\mathbf{A})| \\ &= \exp[|\lambda|^2\,\mathrm{tr}_N(\mathbf{A}^\dagger\mathbf{A}) - \mathrm{tr}_N(\lambda^*\mathbf{A}^\dagger + \lambda\mathbf{A})] \\ &\quad \times \det{}'_N|(1-\lambda^*\mathbf{A}^\dagger)(1-\lambda\mathbf{A})|, \end{aligned} \tag{3.20}$$

where we have used the definition

$$\det{}'_N|\mathbf{I}+\mathbf{B}| = \exp\{\mathrm{tr}_N[-\mathbf{B}+\ln(\mathbf{I}+\mathbf{B})]\}. \tag{3.21}$$

In the case $(\mathbf{I}+\mathbf{B}) = |\mathbf{I}-\lambda\mathbf{A}|^2$, $\ln(\mathbf{I}+\mathbf{B})$ is well defined for all λ since as $\mathbf{A}$ is of trace class it is also bounded. As noted above, we can evaluate the trace using any convenient complete orthonormal basis. If $\mathbf{B}$ is Hermitian and nonnegative definite, then we choose the eigenvectors of the truncation of $\mathbf{B}$ as our basis set. Then, if $B_i > 0$ are the corresponding eigenvalues,

$$\begin{aligned} &\mathrm{tr}[-\mathbf{B}+\ln(\mathbf{I}+\lambda\mathbf{B})] \\ &= \sum_i [-B_i + \ln(1+B_i)] \leq 0 \end{aligned} \tag{3.22}$$

since $\ln(1+x)-x$ is monotonically decreasing for $x \geq 0$ with a maximum at $x=0$.

Thus we obtain the inequality from (3.20) and (3.22)

$$|D_N(\lambda)| \leq \exp(\tfrac{1}{2}|\lambda|^2\,\|\mathbf{A}\|_1^2 + |\lambda|\,\|\mathbf{A}\|_1) \tag{3.23}$$

uniformly in N. From inequality (3.23) it is a simple matter to derive from Cauchy's integral formula for the coefficients

$$D_N(\lambda) = \sum_{j=1}^{N} d_{N,j}\lambda^j \tag{3.24}$$

the term by term bounds

$$|d_{N,j}| \leq [j^{-1/2}\exp(\tfrac{1}{2}\|\mathbf{A}\|_1^2 + j^{-1/2}\,\|\mathbf{A}\|_1)]^j. \tag{3.25}$$

We can now see that

$$\lim_{N\to\infty} D_N(\lambda) = D(\lambda) \tag{3.26}$$

exists and is an entire function of λ. The argument is that for any fixed λ we can, by Eq. (3.25), given any $\epsilon > 0$ find an $M(\epsilon)$ such that

$$|D_N(\lambda) - \sum_{j=1}^{M} d_{N,j}\lambda^j| < \epsilon. \tag{3.27}$$

However, by Eq. (3.18) every $d_{N,j}$ is a polynomial function of $\mathrm{Tr}_N(\mathbf{A}^k)$, $1 \leq k \leq j$, which by (3.16) must converge to a limit as $N\to\infty$. Thus as M is independent of N we deduce that (3.26) holds for any finite λ and that, as the limiting coefficients must obey (3.25), the limit is an entire function of λ. It is plainly sufficient that the basis set used in the definition spans the range of $\mathbf{A}$ for the result to be unique.

4. CONVERGENCE OF THE SOLUTION OF THE TRUNCATED PROBLEM FOR TRACE CLASS OPERATORS

In this section we examine by Fredholm methods for trace-class operators (Sec. 3) the strong convergence of the solutions $\mathbf{f}_N$ to the truncated equation (2.5) in the Cini—Fubini subspace to a limit $\mathbf{f}_\infty$ and show that this limit satisfies Eq. (2.1). This result will then imply the convergence of the Padé approximants. In this section we will need the condition that $\|\mathbf{P}_N\mathbf{A}\mathbf{P}_N\|_1$ be uniformly bounded for any sequence of N's that we consider. We do not know a convenient way to express this condition, and so we will actually treat a less general case in which it must hold. We shall assume in this section that the spaces defined in Sec. 2 are equal, i.e., $\mathcal{S}_N = \mathcal{S}'_N$. This assumption implies that $\mathbf{P}_N$ is an orthogonal projection, and $\mathbf{P}_N = \mathbf{P}'_N$, $\|\mathbf{P}_N\| = 1$. If $\mathbf{A} = \mathbf{A}^\dagger$ and $\mathbf{h} = \mathbf{g}$ (of Sec. 2), then $\mathcal{S}_N = \mathcal{S}'_N$ directly from the definition (2.2). A more general condition which will assure the equality $\mathcal{S}_N = \mathcal{S}'_N$ is that if $\mathbf{A}$ is expressed in terms of the infinite set of orthonormal basis vectors $\mathbf{e}_j$, the first N of which span $\mathcal{S}_N$ for all N, then $\mathbf{A}$ is represented by a tridiagonal matrix. In other words, given $\mathbf{g} = \mathbf{h}$ as the starting vector, the upper Hessenberg form of $\mathbf{A}$ is tridiagonal.

In order to make this investigation, let us introduce the orthonormal basis χ_i for the Cini—Fubini subspace $\mathcal{S}_N = \mathcal{S}'_N$ introduced in Sec. 2 (it is the space spanned by the elements $\mathbf{A}^{i-1}\mathbf{g}$, $i = 1, \ldots, N$). We then resolve the operator $\mathbf{P}_N\mathbf{A}\mathbf{P}_N$ in this space as an $N\times N$ matrix (it may be a smaller space, as pointed out in Sec. 2, but we may restrict our attention to the $N\times N$ case):

$$A_{ij} = (\chi_i, \mathbf{A}\chi_j), \quad i,j = 1, \ldots, N. \tag{4.1}$$

Then Eq. (2.5) becomes

$$\begin{aligned} \mathbf{f}_N &= \sum_{j=1}^{N} b_j \chi_j, \\ b_j &= (\chi_j, \mathbf{g}) + \lambda \sum_{k=1}^{N} A_{jk} b_k. \end{aligned} \tag{4.2}$$

The Fredholm solution of these equations is directly given,[14] provided

$$D_N(\lambda) = \det_N|\delta_{ij} - \lambda A_{ij}| \neq 0 \tag{4.3}$$

by the formula

$$\mathbf{f}_N = \mathbf{g} + \lambda \sum_{j,k=1}^{N} \chi_j D_{N,jk}(\lambda)(\chi_k, \mathbf{g})/D_N(\lambda) \tag{4.4}$$

as $\mathbf{g}$ lies in $\mathcal{S}_N$ by construction, where

$$D_{N,jk}(\lambda) = A_{jk} - \frac{\lambda}{1!}\sum_{l=1}^{N} \begin{vmatrix} A_{jk} & A_{jl} \\ A_{lk} & A_{ll} \end{vmatrix}$$

$$+\frac{\lambda^2}{2!}\sum_{l,m=1}^{N}\begin{vmatrix} A_{jk} & A_{jl} & A_{jm} \\ A_{lk} & A_{ll} & A_{lm} \\ A_{mk} & A_{ml} & A_{mm} \end{vmatrix} - \cdots . \tag{4.5}$$

Naturally the terms in λ^n, $n \geq N$, vanish identically, in conformity with Eq. (2.10). The definition (4.3) agrees with that of Eq. (3.18). That (4.4) is a solution of Eq. (2.5) may be verified by direct substitution through the usual arguments. We next wish to show that the operators $D_{N,jk}(\lambda)$ are uniformly bounded in N.

We have not yet specified which basis set we wish to choose for the χ_j. We can select this set as we wish without loss of generality. We choose to define the χ_j by

$$\mathbf{T}_N \chi_j = (\alpha_j^{(N)})^2 \chi_j \quad \mathbf{T}_N = (\mathbf{P}_N^\dagger \mathbf{A}^\dagger \mathbf{P}_N^\dagger)(\mathbf{P}_N \mathbf{A} \mathbf{P}_N), \tag{4.6}$$

the eigenfunctions of the analog $\mathbf{T}$ of Eq. (3.1) in the Cini–Fubini subspace. Analogously to (3.3) and (3.4) we have the canonical expansion

$$\mathbf{P}_N \mathbf{A} \mathbf{P}_N = \sum_i \chi_i' \alpha_i^{(N)} (\chi_i, \ ) \tag{4.7}$$

where χ_i' is also an orthonormal set. Then we have the inequality for the matrix elements A_{jk}

$$|A_{jk}| \leq \left(\sum_{i=1}^{N} |A_{ji}|^2\right)^{1/2} = \left(\sum_{i=1}^{n} |(\chi_i, \chi_j')|^2 (\alpha_j^{(N)})^2\right)^{1/2} = \alpha_j^{(N)}. \tag{4.8}$$

To establish that $D_{N,jk}(\lambda)$ is a bounded operator, we need the result of the Cauchy–Schwartz inequality

$$\left|\sum_{k=1}^{N} A_{jk} h_k\right|^2 \leq \sum_{k=1}^{N} |h_k|^2 \sum_{k=1}^{N} |A_{jk}|^2 = \|\mathbf{h}\|^2 (\alpha_j^{(N)})^2 \tag{4.9}$$

by (4.8). We are now in a position to apply Hadamard's determinant inequality

$$|\det \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & 2_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix}| \leq \prod_{i=1}^{n} \left(\sum_{j=1}^{n} |a_{ij}|^2\right)^{1/2} \tag{4.10}$$

to Eq. (4.5), acting on an arbitrary $\mathbf{h}$ of unit norm in $\mathcal{S}_N$. Thus, using (4.9), we have

$$\begin{aligned} &\left|\sum_{k=1}^{N} D_{N,jk}(\lambda) h_k\right| \\ &\leq \alpha_j^{(N)} + \frac{|\lambda|}{1!}\sum_{l=1}^{N}[(\alpha_j^{(N)})^2 + |A_{jl}|^2]^{1/2} \\ &\quad \times [(\alpha_l^{(N)})^2 + |A_{ll}|^2]^{1/2} \\ &\quad + \frac{|\lambda|^2}{2!}\sum_{l=1}^{N}\sum_{k=1}^{N}[(\alpha_j^{(N)})^2 + |A_{jl}|^2 + |A_{jm}|^2]^{1/2} \\ &\quad \times [(\alpha_l^{(N)})^2 + |A_{ll}|^2 + |A_{lm}|^2]^{1/2} \\ &\quad \times [(\alpha_m^{(N)})^2 + |A_{ml}|^2 + |A_{mm}|^2]^{1/2} + \cdots . \end{aligned} \tag{4.11}$$

If we now apply (4.8) to the remaining matrix elements, we obtain

$$\begin{aligned} &\left|\sum_{k=1}^{N} D_{N,jk}(\lambda) h_k\right| \\ &\leq \alpha_j^{(N)}\left[1 + \frac{|\lambda|}{1!} 2^{2/2} \sum_{l=1}^{N} \alpha_l^{(N)} \right. \\ &\quad \left. + \frac{|\lambda|^2}{2!} 3^{3/2} \left(\sum_{l=1}^{N} \alpha_l^{(N)}\right)\left(\sum_{m=1}^{N} \alpha_m^{(N)}\right) + \cdots\right] \\ &\leq \alpha_j \left(1 + \frac{|\lambda|}{1!} 2^{2/2} \|\mathbf{A}\|_1 + \frac{|\lambda|^2}{2!} 3^{3/2} \|\mathbf{A}\|_1^2 + \cdots\right) \end{aligned} \tag{4.12}$$

as the characteristic values α_j are monotonically increasing as functions of the subspace size. Thus the square norm implied by (4.12) is

$$\|\mathbf{D}_N(\lambda)\mathbf{h}\| \leq \|\mathbf{A}\|_2 \left(1 + \frac{|\lambda|}{1!} 2^{2/2} \|\mathbf{A}\|_1 + \frac{|\lambda|}{2!} 3^{3/2} \|\mathbf{A}\|_1^2 + \cdots\right) \tag{4.13}$$

and thus $\mathbf{D}_N(\lambda)$ are a sequence of uniformly bounded operators in N for any λ, provided the series (4.13) converges. But as $\|\mathbf{A}\|_1$ is finite (which makes $\|\mathbf{A}\|_2$ finite also), this convergence follows immediately by the ratio test. That the operators $\mathbf{D}_N(\lambda)$ converge in the norm follows directly, as we can show by standard arguments that for $j < J$ the coefficients of λ^j tend uniformly to limits ($N \to \infty$); by selecting J large enough we can make $\sum_{j=J}^{\infty} \alpha_j^2$ as small as we like, which suffices to prove that $\|[\mathbf{D}_N(\lambda) - \mathbf{D}_M(\lambda)]\mathbf{h}\| \to 0$ as $M, N \to \infty$, for all $\mathbf{h}$, $\|\mathbf{h}\| = 1$.

It is then easy to show $[D(\lambda) \neq 0]$ that the $\mathbf{f}_N$ converge strongly to a limit $\mathbf{f}_\infty$, as we have already shown in the previous section that the determinant $D_N(\lambda)$ converges to a limit $D(\lambda)$. That the limiting function satisfies the original equation (2.1) follows $[D(\lambda) \neq 0]$ directly as it does term by term in λ, and the square norm of the remainder can be made arbitrarily small by taking enough powers of λ since the bounding series in (4.13) converges absolutely for all λ.

Thus it follows immediately from Sec. 2 and this result that the sequence of $[N-1/N]$ Padé approximant to $g(\lambda) = (\mathbf{g}, \mathbf{f}) = (\mathbf{g}, \mathbf{f}_\infty)$ converges for all λ, $D(\lambda) \neq 0$, and furthermore the numerator and denominators converge separately to entire functions of λ. When $D(\lambda)$ vanishes, we expect a pole in the Padé approximant. Since $D(\lambda)$ is entire, it has only a finite or denumerably infinite number of zeros with no limit point in the finite λ plane. In the context of scattering theory which we discuss in a latter section, $D(\lambda)$ is the Jost function, as Garibotti and Villani[2] had previously shown.

5. CONVERGENCE OF THE SOLUTION OF THE TRUNCATED PROBLEM FOR COMPACT OPERATORS

In this section we assume only that $\mathbf{A}$ of Eq. (2.1) is compact, rather than restricted to a portion of the trace class as we did in the previous section. We also assume (5.11). In the previous section we showed that the solution $\mathbf{f}_N$ of the truncated problem (2.5) converged strongly to the solution and the Padé numerator and denominator converged separately to entire functions. Here we will prove that either the projection P_N' of the $\mathbf{f}_N$ converges strongly to the solution of (2.1) for all finite λ not a singular point of (2.1) with at most one exceptional value of λ, or there exist two infinite subse-

quences, for one or the other of which the projection of $\mathbf{f}_N$ converges strongly to the solution of (2.1) for all finite λ not a singular point of (2.1).

From the general theory[14] of Eq. (2.1) for a compact operator we know that there are only a finite or denumerably infinite number of singular values of λ for which Eq. (2.1) fails to have a unique, bounded solution. These singular values do not have a limit point in the finite λ plane. Suppose λ is not a singular value of Eq. (2.1). Let us first suppose, with at most a finite number of exceptions, that all of the solutions of the truncated Eq. (2.5) are uniformly bounded. Then, recalling (2.1) and (2.5), we have

$$\mathbf{f}=\mathbf{g}+\lambda\mathbf{A}\mathbf{f},\quad \mathbf{f}_N=\mathbf{g}+\lambda\mathbf{P}_N\mathbf{A}\mathbf{P}_N\mathbf{f}_N. \tag{5.1}$$

Let us introduce the orthogonal projection operators $\mathcal{P}_N$ and $\mathcal{P}'_N$ which project onto the spaces $\mathcal{S}_N$ and $\mathcal{S}'_N$. One may verify directly the properties

$$\mathcal{P}'_N\mathbf{P}_N=\mathcal{P}'_N,\quad \mathbf{P}_N\mathcal{P}_N=\mathcal{P}_N \tag{5.2}$$

from the definition (2.4) of $\mathbf{P}_N$, as long as $\det|R_{ij}|\neq 0$. By multiplication and subtraction we derive from (5.1) and (5.2), by use of $\mathcal{P}'_\infty\mathbf{A}=\mathcal{P}'_\infty\mathbf{A}\mathcal{P}'_\infty$,

$$\begin{aligned}\mathcal{P}'_\infty\mathbf{f}-\mathcal{P}'_N\mathbf{f}_N=&(\mathcal{P}'_\infty\mathbf{g}-\mathcal{P}'_N\mathbf{g})+\lambda\mathcal{P}'_\infty\mathbf{A}(\mathcal{P}'_\infty\mathbf{f}-\mathcal{P}'_N\mathbf{f}_N)\\&+\lambda\mathcal{P}'_\infty(\mathbf{I}-\mathcal{P}'_\infty)\mathbf{A}\mathbf{f}_N-\lambda\mathcal{P}'_\infty\mathbf{A}\mathcal{P}'_\infty(\mathbf{I}-\mathcal{P}'_\infty)\mathbf{f}_N\\&+\lambda(\mathcal{P}'_\infty-\mathcal{P}'_N)\mathbf{A}\mathbf{f}_N-\lambda\mathcal{P}'_\infty\mathbf{A}(\mathcal{P}'_\infty-\mathcal{P}'_N)\mathbf{f}_N.\end{aligned} \tag{5.3}$$

If $\|\mathbf{f}_N\|$ is uniformly bounded for all, then we have: (i) The first term on the right-hand side of (5.3) tends to zero as $N\to\infty$. (ii) The third and fourth terms are zero identically. (iii) The last two terms tend to zero as $\mathbf{A}$ is compact by standard arguments.[16] Thus under this assumption (5.3) reduces to

$$\lim_{N\to\infty}\lambda[(\mathcal{P}'_\infty\mathbf{f}-\mathcal{P}'_N\mathbf{f}_N)-\lambda\mathbf{A}(\mathcal{P}'_\infty\mathbf{f}-\mathcal{P}'_N\mathbf{f})]=0, \tag{5.4}$$

and thus, as λ is not a singular value of (2.1), we conclude by the uniqueness of the solution to

$$\mathbf{d}=0+\lambda\mathbf{A}\mathbf{d} \tag{5.5}$$

that

$$\lim_{N\to\infty}\|\mathcal{P}'_N\mathbf{f}_N-\mathcal{P}'_\infty\mathbf{f}\|=0,$$

$$\lim_{N\to\infty}(\mathbf{h},\mathcal{P}'_N\mathbf{f}_N)=\lim_{N\to\infty}(\mathcal{P}'_N\mathbf{h},\mathbf{f}_N) \tag{5.6}$$

$$=\lim_{N\to\infty}(\mathbf{h},\mathbf{f}_N)=\lim_{N\to\infty}[N-1/N]=(\mathbf{h},\mathbf{f})$$

as $\mathcal{P}'_N\mathbf{h}=\mathbf{h}$, for any sequence of N's for which $\|\mathbf{f}_N\|$ is uniformly bounded.

Next we must consider the question of the existence of a sequence of N's for which $\|\mathbf{f}_N\|$ is uniformly bounded. In order to do so, it is helpful to discuss the structure of $\mathbf{P}_N\mathbf{A}\mathbf{P}_N$ acting on $\mathcal{S}_N$. First, by definition (2.2), $\mathbf{A}\mathbf{P}_N\varphi_i$ is in $\mathcal{S}_N$ when $i\leq N-1$, and so for these elements the left-hand $\mathbf{P}_N$ acts like $\mathcal{P}_N$. Thus if we introduce the orthonormal set of elements $\mathbf{e}_j$ defined by the requirement that $\{\mathbf{e}_j, j=1,\ldots,N\}$ span $\mathcal{S}_N$, any effect of the possible obliqueness of the projection $\mathbf{P}_N$ in this situation is felt only on elements in the direction $\mathbf{e}_N$. Thus we may write

$$\mathbf{P}_N\mathbf{A}\mathbf{P}_N\psi=\mathcal{P}_N\mathbf{A}\mathcal{P}_N\psi+\varkappa_N\rho_N(\mathbf{e}_N,\psi) \tag{5.7}$$

for any ψ in $\mathcal{S}_N$. The element, $\varkappa_N$, is necessarily in $\mathcal{S}_N$ and is taken to be of unit norm. The magnitude of the last term is given by $\rho_N\geq 0$. It is to be noted that there may only be a finite number of $\mathbf{e}_j$. This case corresponds to the case where a finite order Padé approximant is the exact solution, and, as the convergence question does not then arise, we shall assume we are not treating this case.

Now, suppose there is an infinite sequence of $\mathbf{f}_N$ such that $\|\mathbf{f}_N\|\to\infty$. For this sequence define $\mathbf{d}_N=\mathbf{f}_N/\|\mathbf{f}_N\|$ of unit norm. For these elements, (5.1) becomes, by using (5.7),

$$\mathbf{d}_N=\mathbf{g}/\|\mathbf{f}_N\|+\lambda\mathcal{P}_N\mathbf{A}\mathcal{P}_N\mathbf{d}_N+\lambda\varkappa_N\rho_N(\mathbf{e}_N,\mathbf{d}_N), \tag{5.8}$$

which, as $\mathcal{P}_N\mathbf{A}\mathcal{P}_N$ is a compact operator and λ is explicitly assumed not to be a singular value of (2.1), may be rewritten as

$$\mathbf{d}_N=[\mathbf{I}-\lambda\mathcal{P}_N\mathbf{A}\mathcal{P}_N]^{-1}[\mathbf{g}/\|\mathbf{f}_N\|+\lambda\varkappa_N\rho_N(\mathbf{e}_N,\mathbf{d}_N)]. \tag{5.9}$$

Now as $\|\mathbf{d}_N\|=1$ and $\|\mathbf{g}\|/\|\mathbf{f}_N\|\to 0$ by assumption, we must turn our attention to the second term. By (5.2) and (5.7), we have

$$\lim_{N\to\infty}\|\mathcal{P}'_N\varkappa_N\rho_N\|=0, \tag{5.10}$$

where ψ was selected as $\mathbf{e}_N$. To see this result, we multiply Eq. (5.7) on the left by $\mathcal{P}'_N$ and use (5.2) to eliminate $\mathbf{P}_N$. Then by taking the inner product with $\mathbf{e}_N$ we get Eq. (5.10) from the compactness of $\mathbf{A}$ and the fact that the $\mathbf{e}_j$ are an orthonormal set. As we need not consider at this point the possibility $\rho_N\to 0$, as that would immediately preclude, by (5.9), $\|\mathbf{d}_N\|=1$, we conclude from (5.10) that

$$\lim_{N\to\infty}\|\mathcal{P}'_N\varkappa_N\|=0$$

also. Thus, as $\|\varkappa_N\|=1$, it must be that the projection of $\varkappa_N$ into $\mathcal{S}'_N\to 0$ in norm. We now assume that

$$\liminf_{N\to\infty}\|\mathcal{P}_N\mathbf{A}\mathcal{P}_N\mathbf{A}\mathbf{e}_N\|=0. \tag{5.11}$$

Thus, in the limit as $N\to\infty$ there is a subsequence for which we may set $\mathbf{A}=0$ and $\mathbf{g}=0$ in (5.9) and conclude, from the normalization condition on $\mathbf{d}_N$ and $\varkappa_N$, that

$$\lim_{N\to\infty}\|\mathbf{d}_N-\varkappa_N\|=0, \tag{5.12}$$

$$\lim_{N\to\infty}\lambda\rho_N(\mathbf{e}_N,\varkappa_N)=1. \tag{5.13}$$

An explicit calculation in terms of $\mathbf{d}_N=a\varkappa_N+b\mathbf{c}_N$, $(\varkappa_N,c_N)\equiv 0$, and condition (5.11) forces the error in (5.13) to zero, even in the case $\rho_N\to\infty$.

Since the only dependence of (5.13) on λ is that explicitly exhibited, for the particular sequence considered Eq. (5.13) can hold only for a particular value of λ and is a contradiction to the assumption that $\|\mathbf{f}_N\|\to\infty$ for all other values. For those other values which are not singular values of (2.1), the arguments of (5.1)—(5.6) imply convergence. Of course, there may be other sequences of N's which correspond to other values of λ.

We may now summarize our results in the following theorem.

Theorem: Let Λ be any closed, bounded region in the complex λ plane not containing a singular point of Eq.

(2.1). If $\mathbf{f}_N$ is the solution of Eq. (2.5), P'_N is the orthogonal projection onto the space S'_N spanned by the elements φ'_i, $i=1,\ldots,N$, of Eq. (2.2), and (5.11) holds, then *either* a finite order $\mathbf{f}_N$ is exact, *or*

$$\lim_{N\to\infty} \| P'_N \mathbf{f} - P'_N \mathbf{f}_N \| = 0, \tag{5.14}$$

where the limit is over all of the infinite number of N's for which $\mathbf{P}_N$ exists,[13] *or* for each λ in Λ for which (5.14) fails, there exists an infinite subsequence of N's for which (5.14) holds for every other λ in Λ.

By Eqs. (2.15) and (5.6), Eq. (5.14) directly implies the convergence of the $[N-1/N]$ Padé approximants. The two cases allowed by this theorem are: (a) The entire sequence of $\mathbf{f}_N$ satisfy (5.14) everywhere in Λ with at most one exception, or (b) by selecting at most two infinite subsequences of $\mathbf{f}_N$, we may obtain convergence at every point of Λ.

If we make a stronger assumption, then we can prove convergence of the entire sequence, $\mathbf{f}_N$. Let us assume, instead of (5.11) that

$$\lim_{N\to\infty} \| (\mathbf{I} - P'_N) P'_N \| = 0. \tag{5.15}$$

This condition holds automatically if for example $\mathbf{A}$ is Hermitian, or the upper Hessenberg form of $\mathbf{A}$ is tridiagonal, as discussed at the beginning of Sec. 4. Assume that $\| \mathbf{f}_N \|$ are not uniformly bounded; then there must exist a subsequence $\mathbf{d}_n = \mathbf{f}_{N(n)} / \| \mathbf{f}_{N(n)} \|$ for which, as $\| \mathbf{f}_{N(n)} \| \to \infty$, we have

$$\mathbf{d}_n - \lambda \mathbf{P}_{N(n)} \mathbf{A} \mathbf{d}_n \to 0. \tag{5.16}$$

Now since $\mathbf{A}$ is compact, there is a subsequence of the $\mathbf{d}_n$, $\mathbf{d}_m$ such that

$$\lim_{m\to\infty} \lambda \mathbf{A} \mathbf{d}_m = \mathbf{d}. \tag{5.17}$$

By Eq. (5.2), (5.16), and (5.17)

$$\lim_{m\to\infty} P'_{N(m)} \mathbf{d}_m = \lim_{m\to\infty} P'_{N(m)} \mathbf{d} = P'_\infty \mathbf{d} = \mathbf{d} \tag{5.18}$$

as condition (5.15) implies $S'_\infty \supset S_\infty$. Now

$$\lim_{m\to\infty} \| \mathbf{d}_m - P'_{N(m)} \mathbf{d}_m \| \le \lim_{m\to\infty} \| (\mathbf{I} - P'_{N(m)}) P_{N(m)} \| \tag{5.19}$$

as $\|\mathbf{d}_m\| = 1$. Thus by (5.15), (5.18), and (5.19) for the subsequence $\mathbf{d}_m$, we have

$$\lim_{m\to\infty} \mathbf{d}_m = \mathbf{d} \tag{5.20}$$

or by (5.17)

$$\mathbf{d} = 0 + \lambda \mathbf{A} \mathbf{d}, \tag{5.21}$$

which implies, as λ is not a singular value of (2.1), that $\mathbf{d} = 0$, but $\|\mathbf{d}\| = 1$ which is a contradiction. Therefore, it must be that (5.15) implies that $\| \mathbf{f}_N \|$ is uniformly bounded and we obtain convergence by the argument (5.1) to (5.6).

If we only assume (5.15) to hold for a subsequence, then, for that subsequence, the $\|\mathbf{f}_N\|$ is uniformly bounded and convergence is again obtained.

The results of this section prove a modified version of a theorem conjectured by Chisholm[3] a decade ago.

Note added in proof: An intermediate assumption between (5.11) and (5.15) would be that $\mathbf{A}$ is compact and

$$\liminf_{N\to\infty} \| (\mathbf{I} - P'_N) P_N \| = \sigma < 1. \tag{5.22}$$

As arguments (5.2) through (5.6) are valid for these assumptions, we need further analyze only the case where $\| \mathbf{f}_N \| \to \infty$ for all N for which the $\mathbf{f}_N$ are defined; otherwise we could find a bounded, and hence convergent, subsequence in the sense of (5.14). Thus we may consider a subsequence for which both (5.16) and (5.22) hold. By multiplication by $P'_{N(n)}$, we may rewrite (5.16) as

$$P'_{N(n)} \mathbf{d}_n - \lambda P'_{N(n)} P_{N(n)} \mathbf{A} \mathbf{d}_n \to \lambda P'_{N(n)} (P_{N(n)+1} - P_{N(n)}) \mathbf{A} \mathbf{d}_n \tag{5.23}$$

where use was made of the fact that as $\mathbf{d}_n \in S_{N(n)}$, then $\mathbf{A}\mathbf{d}_n \in S_{N(n)+1}$. The right-hand side of Eq. (5.23) tends to zero, by the compactness of $\mathbf{A}$ and $\| \mathbf{d}_n \| = 1$. Now, by the triangle inequality and (5.22) we have

$$\begin{aligned} \| P'_N P_N \mathbf{k} \| &\ge \| P_N \mathbf{k} \| - \| (\mathbf{I} - P'_N) P_N \mathbf{k} \| \\ &\ge \| P_N \mathbf{k} \| - \| (\mathbf{I} - P'_N) P_N \| \cdot \| P_N \| \ge (1 - \sigma) \| P_N \mathbf{k} \|. \end{aligned} \tag{5.24}$$

By the compactness of $\mathbf{A}$, we may select a subsubsequence $\mathbf{d}_m$ of the $\mathbf{d}_n$ with property (5.17), where $\mathbf{d} \in S_\infty$ necessarily. Consider now by (5.23), (5.24), and the compactness of $\mathbf{A}$

$$\begin{aligned} 0 &= \lim_{m\to\infty} \| P'_{N(m)} P_{N(m)} (\mathbf{d}_m - \lambda \mathbf{A} \mathbf{d}_m) \| \\ &\ge (1 - \sigma) \lim_{m\to\infty} \| P_{N(m)} (\mathbf{d}_m - \lambda \mathbf{A} \mathbf{d}_m) \| \\ &= (1 - \sigma) \lim_{m\to\infty} \| \mathbf{d}_m - \lambda \mathbf{A} \mathbf{d}_m \| \\ &\ge \frac{(1 - \sigma) \| \mathbf{d}_m \|}{\| (\mathbf{I} - \lambda \mathbf{A})^{-1} \|} > 0 \end{aligned} \tag{5.25}$$

since λ is not a singular value of $\mathbf{A}$, $\sigma < 1$, and $\| \mathbf{d}_m \| = 1$. But this is a contradiction. Therefore (5.22) implies that there exists at least a subsequence of $\mathbf{f}_N$ which are uniformly bounded; hence by (5.6) those $[N-1/N]$ Padé approximants converge.

6. CERTAIN MEROMORPHIC FUNCTIONS AS SPECIAL CASES

In this section we apply the results of the previous sections to prove the convergence of the Padé approximants to a certain class of meromorphic functions. Consider any function, regular at the origin and meromorphic with only simple poles in the whole complex plane, which is bounded on a series of contours C_n which tend to infinity. Then[17] there exists a representation of it of the form

$$\begin{aligned} f(z) &= f(0) + \sum_{n=1}^{\infty} \left(\frac{b_n}{a_n - z} - \frac{b_n}{a_n} \right) \\ &= f(0) + \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} b_n a_n^{-1-m} \right) z^m, \end{aligned} \tag{6.1}$$

where we suppose that the a_n are ordered, $|a_{n+1}| \ge |a_n|$, and that $\sum b_n a_n^{-2}$ converges by the existence of $f'(0)$. In terms of the vector $\mathbf{g}$ and matrix $\mathbf{A}$

$$\mathbf{A}_{ij} = \delta_{ij} / a_i, \quad \mathbf{g}_i = (b_i)^{1/2} a_i^{-1}, \quad \mathbf{h}_i = g_i^*, \tag{6.2}$$

we may write the equation

$$\mathbf{f} = \mathbf{g} + z \mathbf{A} \mathbf{f} \tag{6.3}$$

and verify directly that

$$f(z) = f(0) + z(\mathbf{h}, \mathbf{f}). \tag{6.4}$$

Since as $f(z)$ is meromorphic, there can be no point of accumulation of the a_n in the finite complex plane; therefore, $1/|a_n| \to 0$ and hence **A** is a compact operator. Here when we have (5.11), then, by the results of the previous section that if R is any finite, closed, bounded region in the complex z plane not containing a pole of $f(z)$, then *either* a finite order $[N-1/N]$ Padé approximant is $f(z)$ exactly, *or* the entire sequence of $[N-1/N]$ Padé approximants (those which exist) converges everywhere in R, *or* for any point in R for which $[N-1/N]$ fails to converge there exists a subsequence of the $[N-1/N]$ Padé approximants which converges at every other point of R. Therefore, either the entire sequence of $[N-1/N]$ Padé approximants converges everywhere in R with at most one exception, or by selecting at most two infinite subsequences we may obtain convergence at every point in R. This result proves a modification of a theorem conjectured by Baker and Gammel[8] over a decade ago. If the a_i are real and $b_i > 0$, then $\mathbf{A} = \mathbf{A}^\dagger$, $\mathbf{g} = \mathbf{h}$, and we have $\zeta_N = \zeta_N'$ so that the entire sequence must converge. This case is the Hamburger moment problem.

The case where multiple poles occur is dealt with by a variant of the above method. First note that the $N \times N$ matrix identity

$$\mathbf{U}^{n+1} \equiv \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}^{n+1}$$

$$= \begin{pmatrix} 1 & \binom{-2}{n} & \binom{-3}{n} & \cdots & \binom{-N}{n} \\ 0 & 1 & \binom{-2}{n} & \cdots & \binom{-N+2}{n} \\ 0 & 0 & 1 & \cdots & \binom{-N+2}{n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \tag{6.5}$$

where $\binom{a}{b}$ is the usual binomial expansion coefficient. The power series expansion for

$$\sum_{j=1}^{N} A_j/(1-z)^j \tag{6.6}$$

is formally generated by the expression

$$(\mathbf{h}, \sum_{n=0}^{\infty} z^n \mathbf{U}^{n+1}\mathbf{g}), \mathbf{h} = (\alpha, 0, 0 \cdots 0), \quad \mathbf{g}_j = A_j/\alpha. \tag{6.7}$$

By including such $N \times N$ blocks $\mathbf{U}/a_j$ for Nth order poles in place of $1/a_j$ in the definition of **A**, we may reproduce the higher order poles without destroying the compactness of **A**.

One may either, as $e^x = \lim_{N\to\infty}(1 - x/N)^{-N}$, work out the application of the theory of the relationship of compact operators to the convergence of Padé approximants by a limiting form of (6.5), or directly as

$$f(x) = 1 + \lambda \int_0^x f(y)\, dy \tag{6.8}$$

has the solution $f(x) = e^{\lambda x}$. The operator $\int_0^x dy$ is compact, as it has $\| \int_0^x dx \|_2 = \frac{1}{2}$ over the range $0 \le x, y \le 1$. Thus, the Padé approximants to e^x converge, as is well known from the work of Padé.[18] Since the sum of two compact operators acting on disjoint spaces is again compact, we can deduce that in addition the sum of any meromorphic function plus a finite number of exponentials is again represented by a compact operator and hence if (5.11) holds has convergent $[N/N]$ Padé approximants. Since, by the invariance theorem[12] Padé approximation is invariant under linear fractional transformation, any function which is representable as $(A + Bf)/(C + Df)$ $(AD - BC \neq 0)$ with f of class (6.1) plus a finite number of exponentials again has convergent $[N/N]$ Padé approximants. It seems likely that the class of functions to which these results can be applied can be greatly extended. The entire-function examples of Gammel and Wallin[13,19] show that we cannot prove convergence of the entire sequence of Padé approximants for the whole class of entire functions.

If we restrict the class of meromorphic functions given by (6.1) by the further requirements that $\sum_n 1/|a_n|$ converges, the poles are simple, the a_i are real, and the $b_i > 0$, then **A** given by (6.2) is of trace class, and by Sec. 4 the Padé numerators and denominators separately converge in addition to the approximants themselves. Edrei[20] has very recently also shown convergence of the numerator and denominator separately for this same special case, but over a wider set of Padé approximants.

We note in passing the interesting case of e^z. Padé[18] showed that for the $[M/M]$ Padé approximant that as $M \to \infty$

$$P_M \to e^{z/2}, \quad Q_M \to e^{-z/2}. \tag{6.9}$$

Furthermore, since $1/(1+e^z)$ is of the class (6.1) as C_n can be taken as a square contour $(z = x + iy)$, $x, y = \pm 2\pi n$, we have by the results of this section and invariance the convergence of the $[M/M]$ Padé approximants as described above. The convergence of the numerator and denominators separately is not established as the poles are at $z = \pm(2n+1)\pi i$ so that $\sum_{j=1}^{N} 1/|a_j|$ diverges logarithmically as $N \to \infty$ so that **A** of (6.2) is not of trace class, even though $\mathrm{Tr}(\mathbf{A}) = 0$. It may be that the trace-class condition and our other conditions can be somewhat weakened for the convergence of the Padé numerator and denominator.

7. QUANTUM SCATTERING THEORY

In this section we shall consider nonrelativistic, quantum mechanical scattering by a fixed potential source. This scattering is governed by the Schrödinger equation which is

$$-\nabla^2\psi(\mathbf{r}) + \lambda V(\mathbf{r})\,\psi(\mathbf{r}) = k^2\psi(\mathbf{r}), \tag{7.1}$$

where ∇^2 is the Laplacian operator, ψ is the wavefunction, $\mathbf{r}$ is a three-dimensional vector, λ is the coupling constant, $V(\mathbf{r})$ is the potential energy, and k^2 is the energy. To complete the description of the scattering problem, we must specify the boundary conditions for (7.1). The standard ones are that at large distances ψ should look like an incoming plane wave. That is,

$$\psi(\mathbf{r}) \approx \exp(i\mathbf{k}\cdot\mathbf{r}) - (1/4\pi r)\exp(ik'r)\,T(\mathbf{k}', \mathbf{k}), \tag{7.2}$$

where $\mathbf{k}$ is the wave vector of the incoming wave and $\mathbf{k}' = |\mathbf{k}|\mathbf{r}/|\mathbf{r}|$ is thought of as the wave vector describing the outgoing wave. One may derive from the bound-

ary conditions and Eq. (7.1) the Green's function equation. It is

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r}) - \lambda \int \frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|} \times V(\mathbf{r}')\,\psi(\mathbf{r}')\,d\mathbf{r}', \tag{7.3}$$

which we may write symbolically as

$$\psi = \varphi - \lambda \mathbf{G}\mathbf{V}\psi. \tag{7.4}$$

The quantity of physical interest is the scattering amplitude

$$T(\mathbf{k}',\mathbf{k}) = \lambda \int \exp(-i\mathbf{k}'\cdot\mathbf{r})\,V(\mathbf{r})\,\psi(\mathbf{r})\,d\mathbf{r} = \lambda(\mathbf{V}^{\dagger}\chi, \psi). \tag{7.5}$$

In order to use the results of the previous sections to discuss the convergences of the Padé approximants in λ to $T(\mathbf{k}',\mathbf{k})$ we must show the kernel is a compact operator. Instead of concerning ourselves with this general case, we will content ourselves with the well-known conditions for the Hilbert–Schmidt class $\|A\|_2 < \infty$, which implies compactness.

First, let us recast Eq. (7.4) slightly, as the kernel is not Hilbert–Schmidt as it stands, by introducing

$$\mathbf{f} = \mathbf{V}^{1/2}\psi, \quad \mathbf{g} = \mathbf{V}^{1/2}\varphi, \quad \mathbf{h} = (\mathbf{V}^{1/2})^{\dagger}\chi. \tag{7.6}$$

Then we have, multiplying Eq. (7.4) by $\mathbf{V}^{1/2}$,

$$\mathbf{f} = \mathbf{g} - \lambda \mathbf{V}^{1/2}\mathbf{G}\mathbf{V}^{1/2}\mathbf{f}, \quad T(\mathbf{k}',\mathbf{k}) = (\mathbf{h},\mathbf{f}), \tag{7.7}$$

where $\mathbf{V}^{1/2}$ is any square root of V. The Hilbert–Schmidt norm is then

$$\tau = \|\mathbf{V}^{1/2}\mathbf{G}\mathbf{V}^{1/2}\|_2^2 = \frac{1}{16\pi^2}\iint d\mathbf{r}\,d\mathbf{r}'\,|V(r)| \times \frac{\exp(-2\nu|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^2}\,|V(\mathbf{r}')|, \tag{7.8}$$

where $\nu = \mathrm{Im}(k)$. Also $\|g\|_2$ and $\|h\|_2$ are finite if

$$\int d\mathbf{r}\,|V(\mathbf{r})|\exp(2|\nu\mathbf{r}|) < \infty, \tag{7.9}$$

where for $\|h\|_2$, the $\mathrm{Im}(k')$ replaces ν. Following Scadron *et al.*,[21] we may rewrite (7.8) in the momentum representation

$$\tau = 2\pi^2 \int d\mathbf{q}\,\frac{|U(\mathbf{q})|^2 \tan^{-1}(q/2\nu)}{q} \leq \pi^2 \int d\mathbf{q}\,\frac{|U(\mathbf{q})|^2}{q} \tag{7.10}$$

for $\nu \geq 0$, where

$$U(\mathbf{q}) = \int \exp(-i\mathbf{q}\cdot\mathbf{r})\,|V(\mathbf{r})|\,d\mathbf{r}. \tag{7.11}$$

The implication is that for $\nu = 0$ (7.9) and (7.10) are finite for decent potentials where $V(\mathbf{r})$ is less singular than $|\mathbf{r}|^{-2+\epsilon}$, $\epsilon > 0$, as $|\mathbf{r}| \to 0$ and goes to zero faster than $|\mathbf{r}|^{-3-\epsilon}$, $\epsilon > 0$, as $|\mathbf{r}| \to \infty$. For $\nu \neq 0$, it suffices to impose (7.9) and the condition that $V(\mathbf{r})$ be less singular at the origin than $|\mathbf{r}|^{-2+\epsilon}$, $\epsilon > 0$.

Thus we conclude from Sec. 5 that if $V(\mathbf{r})$ satisfies the above conditions of being short ranged and not too singular at the origin and for reasonable choices of φ and χ so that (5.11) or (5.22) hold, that the $[M/M]$ Padé approximants in λ to the scattering amplitude $T(\mathbf{k},\mathbf{k})$ converge for all k, k' in a strip around the real axis determined by (7.9). By converge, we mean here, as in Sec. 5, that *either* the entire sequence converges when λ is not a singular value except for at most one value $\lambda_0(k,k')$, *or* we may obtain convergence everywhere (fixed k, k') by selecting at most two infinite subsequences. In the special case of forward scattering where $k^2 < 0$ and $V(r)$ is of fixed sign, the kernel of Eq. (7.7) can be chosen to be Hermitian. As we have remarked previously, in this special case $S_N = S_N'$ so that we can conclude convergence of the entire sequence.

Next we will treat the partial wave scattering amplitudes. Since the partial wave decomposition reduces the general case to block diagonal form, the partial wave kernels are automatically still compact, and so all the above results still apply. We get in fact, a slight loosening of the restrictions on the potential when we impose spherical symmetry in order to study the partial wave scattering amplitudes. In the case of a single-signed potential we can prove in addition the separate convergence of the numerator and denominator. The denominators converge to the Jost function. This result places the result of Garibotti and Villani[2] within our general framework.

If we expand in partial waves

$$\psi(r) = \sum_l (2l+1)\,P_l(\cos\theta)\,\psi_l(r)/kr, \tag{7.12}$$

then Eq. (7.3) becomes, if V has spherical symmetry, the uncoupled set of equations[22]

$$\psi_l(r) = kr\,j_l(kr) - \lambda \int_0^{\infty} g_l(r,r')\,V(r')\,\psi_l(r')\,dr', \tag{7.13}$$

where

$$g_l(r,r') = krr'\,j_l(kr)\,k_l(kr'), \quad r' \geq r, \qquad = krr'\,j_l(kr')\,k_l(kr), \quad r' < r, \tag{7.14}$$

is the Green's function. By using known inequalities[22] for the spherical Bessel functions we may bound

$$|g_l(r,r')| \leq \frac{C^2 \exp[(|\nu| - \nu)r_>]r_<}{1 + |k|\,r_<} \tag{7.15}$$

through the whole complex k plane, where $r_<$ is the lesser and $r_>$ the greater of r and r'.

We will now proceed to show that, for decent potentials, the kernel of an equation closely related to (7.13) is of trace class and so the lth partial wave scattering amplitude

$$T_l(k) = \lambda k^{-1} \int_0^{\infty} j_l(kr)\,V(r)\,\psi_l(r)\,r\,dr \tag{7.16}$$

has $[M/M]$ Padé approximants in λ whose numerators and denominators converge. First we slightly recast Eq. (7.13) as

$$V(r)^{1/2}\psi_l(r) = V(r)^{1/2}kr\,j_l(kr) - \lambda \int_0^{\infty} [V(r)^{1/2}g_l(r,r')\,V(r')^{1/2}] \times V(r')^{1/2}\psi_l(r')\,dr', \tag{7.17}$$

where we take any square root of $V(r)$ for the present. If $V(r) \geq 0$, we will later mean $V(r)^{1/2} \geq 0$ also, and if $V(r) \leq 0$, we will later mean $iV(r)^{1/2} \leq 0$. Then we factor

the kernel as

$$K(r,r') = (V(r)^{1/2} r^{1-\epsilon} (1+r)^{\epsilon+\delta}) \times [r^{-1+\epsilon} (1+r)^{-\epsilon-\delta} g_l(r,r') \times (1+r')^{-\epsilon-\delta} (r')^{-1+\epsilon}] \times [(r')^{1-\epsilon} (1+r')^{\epsilon+\delta} V(r)^{1/2}]. \quad (7.18)$$

By the first part of inequality (3.11), we have for $\nu = \mathrm{Im}(k) \geq 0$,

$$\| K(r,r') \|_1 \leq \left(\max_{0 \leq r < \infty} (|V(r)|^{1/2} r^{1-\epsilon} (1+r)^{\epsilon+\delta}) \right)^2 \times \| r^{-1+\epsilon} (1+r)^{-\epsilon-\delta} C^2 r_<(r')^{-1+\epsilon} (1+r')^{-\epsilon-\delta} \|_1, \quad (7.19)$$

where bound (7.15) has been used. Now it is elementary to show that the potential independent term in (7.19) is a Hermitian, positive definite operator, so that its trace norm is just its trace. Direct calculation shows this trace to be finite, if ϵ, $\delta > 0$. Thus by considering the other factor in (7.19), we see that if $V(r)$ is better behaved than r^{-2} at 0 and ∞, the kernel of Eq. (7.17) is of trace class. Thus as the kernel is necessarily compact, we have, for $\nu = 0$, again the convergence results obtained above. For ν different from zero, we must impose the normalization condition at infinity

$$\int^{\infty} |V(r)| \exp(2|\nu| r)\, dr < \infty \quad (7.20)$$

in order to prove the convergence.

Now, to apply the results of Sec. 4, we need to show that $\mathcal{S}_N = \mathcal{S}'_N$. Garibotti and Villani[2] have shown the equivalent of this result for a single-signed potential and k real. We retain the restriction to a single-signed potential, but generalize to nonreal k. First, for real k, we write out (7.14) explicitly in terms of its real and imaginary parts as

$$\begin{aligned} g_l(r,r') &= krr'[j_l(kr) n_l(kr') \quad r' \geq r, \\ &\quad + i j_l(kr) j_l(kr')], \\ &= krr'[j_l(kr') n_l(kr) \quad r' < r \\ &\quad + i j_l(kr) j_l(kr')], \end{aligned} \quad (7.21)$$

It is to be noticed that the real part is Hermitian and the imaginary part is purely one-dimensional. In fact we may write, for a single signed potential, the structure of the kernel of Eq. (7.17) as

$$K(r,r') = \mathbf{H} + (i/k)\, \mathbf{g}(\mathbf{g}, \quad) \quad (7.22)$$

where H is Hermitian and g is the inhomogeneous term in (7.17). Then, constructing the φ_i of (2.2), we have

$$\begin{aligned} &\varphi_0 = \mathbf{g}, \quad \varphi_1 = \mathbf{H} g + (i/k)\, \varphi_0 \| \varphi_0 \|^2 \\ &\varphi_2 = \mathbf{H}^2 \mathbf{g} + (i/k)\, \varphi_1 \| \varphi_0 \|^2, \cdots \end{aligned} \quad (7.23)$$

so that the space $\mathcal{S}_N$ is plainly the same as that generated by H alone. An analogous argument shows the same result for $\mathcal{S}'_N$. Thus the upper Hessenberg representation of k in terms of the orthonormal basis $\mathbf{e}_j$ which spans the $\mathcal{S}_N$ is tridiagonal. Since for the study of the analytic continuation scattering amplitude, we may simply analytically continue the kernel in this representation, and as the analytic continuation of zero is zero, we find that the kernel stays tridiagonal. Hence, we conclude that $\mathcal{S}_N = \mathcal{S}'_N$, and so the results of Sec. 4 apply. Thus, under the same restrictions on the potential as given above [near (7.20)] we conclude from Sec. 4 that the entire sequence of numerators and denominators converges. We remark that, for k pure imaginary, it follows directly from (7.21) that $g_l(r,r')$ is real and so Hermitian. As $V(r)$ is of a single sign $\sqrt{V} g_l \sqrt{V}$ may be chosen as Hermitian, and so we verify directly that the upper Hessenberg form is tridiagonal, in agreement with our analytic continuation argument.

That the Padé denominators converge to the Jost function (see Newton[22] or Goldberger and Watson,[23] for example, for a definition of the Jost function) follows from the work of Sec. 3. As the $[M/M]$ Padé are the exact solutions to a sequence of truncated problems, their denominators are given by

$$\lim_{M \to \infty} D_M(\mathbf{I} - \lambda \mathbf{A}) = D(\mathbf{I} - \lambda \mathbf{A}),$$

which is one definition of the Jost function.

ACKNOWLEDGMENTS

The author is happy to acknowledge many helpful discussions with Dr. C. I. Goldstein and P. R. Graves-Morris, and wishes to thank Professor J. Nuttall for pointing out an oversight in a previous version of this work.

*Work performed under the auspices of the U. S. Atomic Energy Commission.

[1] J. S. Wall, *Analytic Theory of Continued Fractions* (Van Nostrand, Princeton, N.J., 1948).
[2] C. R. Garibotti and M. Villani, Nuovo Cimento A **59**, 107 (1969); A **61**, 747 (1969).
[3] J. S. R. Chisholm, J. Math. Phys. **4**, 1506 (1963).
[4] D. Bessis, *Padé Approximents*, P. R. Graves-Morris, Ed. (The Institute of Physics, London, 1973), pp. 19ff.
[5] S. Tani, Phys. Rev. **139**, B1011 (1965); Ann. Phys. (N.Y.) **37**, 411, 451 (1966).
[6] J. Nuttall, Phys. Rev. **157**, 1312 (1967).
[7] M. Cini and S. Fubini, Nuovo Cimento **11**, 142 (1954).
[8] G. A. Baker, Jr. and J. L. Gammel, J. Math. Anal. Appl. **2**, 21 (1961).
[9] J. Nuttall, J. Math. Anal. Appl. **31**, 147 (1970).
[10] Ch. Pommerenke, J. Math. Anal. Appl. **41**, 775 (1973).
[11] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1966).
[12] G. A. Baker, Jr. and J. L. Gammel (Eds.), *The Padé Approximant in Theoretical Physics* (Academic, New York, 1970), pp. 1ff.
[13] G. A. Baker, Jr., J. Math. Anal. Appl. **43**, 498 (1973).
[14] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (translation by L. F. Boron) (Ungar, New York, 1955).
[15] N. Dunford and J. T. Schwartz, *Linear Operators. Part II: Spectral Theory.* (Interscience, New York, 1963), Chap. 11, Sec. 9.
[16] Ref. 14, p. 204.
[17] P. Franklin, *A Treatise on Advanced Calculus* (Wiley, New York, 1949), p. 461.
[18] H. Padé, Ann. Sci. Ecole Norm. Sup. **16**, 395 (1899).
[19] H. Wallin, *Applicable Analysis* (to be published).
[20] A. Edrei, private communication.
[21] M. Scadron, S. Weinberg, and J. Wright, Phys. Rev. **135**, B 202 (1964).
[22] R. Newton, J. Math. Phys. **1**, 319 (1960).
[23] M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

Experimental uncertainties in the problem of the unitarity equation

Michael Tortorella

(Received 2 May 1974)
Department of Mathematics, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201

In this article the question of how experimental uncertainties affect the construction of the scattering amplitude from the differential cross section and unitarity at a fixed energy is examined. It is shown that in most cases in which the solution can be found by the method of Newton and Martin, the problem is "well-posed" in the sense that the solution depends continuously on the data. A new proof is given of the fact that if the differential cross section is nearly constant and small enough, there is a unique solution of the problem. Some estimates for the scattering amplitude and other functions of interest are given.

1. INTRODUCTION

The main objective of this article is to show that the problem of determining the scattering amplitude from the differential cross section and unitarity at a fixed energy is "well-posed" for spin-zero elastic scattering under conditions which allow the integral operator which expresses the unitarity to be inverted.

A well-posed problem in the sense of Hadamard is a functional equation which, in some class of functions, has a unique solution which depends continuously on any given data. Historically, this notion was first introduced in connection with initial-value problems for elliptic partial differential equations. Here we will consider the behavior of solutions of a Hammerstein-like nonlinear integral equation under perturbations of the kernel of the linear part of the integral operator, because in this problem the kernel is obtained directly from the data, namely the differential cross section. For the sake of economy, we will call the problem described in the first paragraph of this introduction the problem of the unitarity equation. Accordingly, the problem of the unitarity equation will be said to be well-posed in the function space X and for the class $\mathcal{G}$ of differential cross sections if:

(1) To each differential cross section G in $\mathcal{G}$ there corresponds a unique scattering amplitude F in X which satisfies the integral equation of unitarity and $|F| = G$;

(2) if G_1 is a differential cross section which is close to G in the topology of $\mathcal{G}$, then there corresponds to G_1 a unique scattering amplitude F_1 in X which satisfies the integral equation of unitarity, $|F_1| = G_1$, and F_1 is close to F in the topology of X.

As always, uniqueness is taken in Newton's sense of "essential uniqueness" as in Ref. 1.

This problem of continuous dependence of the solution of the integral equation of unitarity on the data, i. e., the differential cross section, is an interesting one because the differential cross section is obtained from measurements made with the aid of actual instruments and is therefore known only approximately. In previous treatments of the problem of the unitarity equation (including Refs. 1—4) it has been supposed that the differential cross section is given with "infinite accuracy." We will show that in many cases such a supposition is justified because the problem is well-posed.

Section 2 of the article is preparatory. In it we rewrite the unitarity integral equation in such a way as to eliminate the need for dealing with the inverse sine function, which appears in all previous works on this equation. In this section we also obtain some simple but useful estimates on the imaginary part of the scattering amplitude and on some other related functions. In Sec. 3 we complete the program of showing the well-posedness of the problem of the unitarity equation in cases in which it is possible to invert the integral operator of unitarity by the Banach contraction mapping principle. In Sec. 4 we develop some results about branching of solutions of abstract equations of the form $u - KN(u) = 0$, where N is a nonlinear operator and K is a bounded linear operator. In Sec. 5 this material is applied to the problem of the unitarity equation. Our results are principally for the case in which the scattering body or potential has spherical symmetry, although we will also indicate some results under less restrictive hypotheses. In conclusion, we obtain a new proof that if the differential cross section is nearly constant and small enough, there is a unique scattering amplitude that corresponds to this cross section and satisfies the unitarity integral equation.

We will now give a brief review of the background of the problem of the unitarity equation. This will also serve to exhibit the notation we will use. By the "unitarity equation" we mean the nonlinear integral equation

$$4\pi \operatorname{Im}F(\mathbf{n}_1, \mathbf{n}_2) = \int_S F(\mathbf{n}_1, \mathbf{n})\overline{F(\mathbf{n}_2, \mathbf{n})}\, d\Omega(\mathbf{n}), \tag{1.1}$$

where S is the unit sphere in $\mathbb{R}^3$, $\mathbf{n}_1$, $\mathbf{n}_2$, and $\mathbf{n}$ are unit vectors in S, and F is a complex-valued function on $S\times S$ which is proportional to the scattering amplitude. The scattering body or potential is supposed to possess inversion symmetry, so that $F(\mathbf{n}_2, \mathbf{n}_1) = F(\mathbf{n}_1, \mathbf{n}_2)$.[5] The problem of determining the scattering amplitude from the differential cross section and unitarity is then that of finding those solutions of (1.1) which also satisfy

$$|F| = G, \tag{1.2}$$

where G is a nonnegative function on $S\times S$ which is proportional to the differential cross section.

Equating real and imaginary parts in (1.1), we obtain

$$4\pi \operatorname{Im}F(\mathbf{n}_1, \mathbf{n}_2) = \int_S [\operatorname{Re}F(\mathbf{n}_1, \mathbf{n}) \operatorname{Re}F(\mathbf{n}_2, \mathbf{n}) + \operatorname{Im}F(\mathbf{n}_1, \mathbf{n}) \operatorname{Im}F(\mathbf{n}_2, \mathbf{n})]\, d\Omega \tag{1.1'}$$

$$0 = \int_S [\operatorname{Re}F(\mathbf{n}_1, \mathbf{n}) \operatorname{Im}F(\mathbf{n}_2, \mathbf{n}) - \operatorname{Re}F(\mathbf{n}_2, \mathbf{n}) \operatorname{Im}F(\mathbf{n}_1, \mathbf{n})]\, d\Omega. \tag{1.1''}$$

It is well-known that (1.1″) is identically satisfied by

any integrable complex-valued function of the real variable $\mathbf{n}_1 \cdot \mathbf{n}_2$, and so in the case of a spherically symmetric body or potential, Eqs. (1.1) and (1.1′) are equivalent. We shall concentrate primarily on this case, although we shall also give some results for the case in which the scatterer has only inversion symmetry. In this case, F will depend on $\mathbf{n}_1$ and $\mathbf{n}_2$ independently, and (1.1″) will no longer be identically satisfied. Our results for this case will be confined to those which we can obtain by continuing to take (1.1′) as the unitarity condition; in other words, by supposing that (1.1) and (1.1′) are still equivalent. (1.1″) then represents an additional necessary condition to be satisfied by F if it is to be a solution of (1.1). For some further remarks about this situation, see Ref. 4.

2. THE UNITARITY CONDITION

If we write $F = Ge^{i\varphi}$, then from (1.1′) we obtain

$$\sin\varphi(\mathbf{n}_1, \mathbf{n}_2) = \int_S H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) \cos[\varphi(\mathbf{n}_1, \mathbf{n}) - \varphi(\mathbf{n}_2, \mathbf{n})]\, d\Omega, \tag{2.1}$$

where $H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) = [4\pi G(\mathbf{n}_1, \mathbf{n}_2)]^{-1} G(\mathbf{n}_1, \mathbf{n}) G(\mathbf{n}_2, \mathbf{n})$. One way to attack (2.1) is to look for fixed points of the transformation $\mathcal{H}$, defined on a function space X, by

$$\mathcal{H}(\varphi)(\mathbf{n}_1, \mathbf{n}_2) = \sin^{-1}\{\int_S H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) \times \cos[\varphi(\mathbf{n}_1, \mathbf{n}) - \varphi(\mathbf{n}_2, \mathbf{n})]\, d\Omega\}. \tag{2.2}$$

This has been done, and results were obtained by Newton and others by using the Banach contraction mapping principle. We will show in the next section that, under the most general conditions known which allow (2.1) to be solved in this manner, the problem of the unitarity equation is well-posed in the sense we have indicated in the Introduction.

Before doing this, however, we will rewrite the unitarity equation in a way which will enable us to avoid dealing with the inverse sine function. The advantages of this become more apparent in Sec. 4, but for the sake of consistency we will make the change now and work with one form of the equation throughout the whole article. Assume $|\sin\varphi| < 1$, and write $F = G[(1-u^2)^{1/2} + iu]$, where $u = \sin\varphi$ in the polar form $F = G\exp(i\varphi)$. Then (2.1) becomes

$$u(\mathbf{n}_1, \mathbf{n}_2) = \int_S H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) \Phi(u(\mathbf{n}_1, \mathbf{n}), u(\mathbf{n}_2, \mathbf{n}))\, d\Omega, \tag{2.3}$$

where $\Phi(x, y) = (1-x^2)^{1/2}(1-y^2)^{1/2} + xy$ for $x, y \in [-1, 1]$, and the positive square root is chosen. For $|\sin\varphi| < 1$ the two equations (2.1) and (2.3) are completely equivalent because if φ is a solution of (2.1), then $u = \sin\varphi$ is a solution of (2.3), and if u is a solution of (2.3), then $\varphi = \sin^{-1}u$ is a solution of (2.1).

Temporarily we will denote the right-hand side of (2.3) by $T(u)(\mathbf{n}_1, \mathbf{n}_2)$:

$$T(u)(\mathbf{n}_1, \mathbf{n}_2) = \int_S H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) \Phi(u(\mathbf{n}_1, \mathbf{n}), u(\mathbf{n}_2, \mathbf{n}))\, d\Omega. \tag{2.4}$$

We devote the rest of this section to obtaining some estimates on the imaginary part of the scattering amplitude and on functions of the form $T(u)$.

Proposition 2.1: Let $F: S\times S \to \mathbb{C}$ be square-integrable in the measure $d_2\Omega = d\Omega \times d\Omega$ and satisfy Eq. (1.1). Then $|\mathrm{Im}F(\mathbf{n}_1, \mathbf{n}_2)| \le \max\{\mathrm{Im}F(\mathbf{n}_j, \mathbf{n}_j) : j = 1, 2\}$.

Proof: From (1.1) and the Schwartz inequality,

$$\begin{aligned} 4\pi |\mathrm{Im}F(\mathbf{n}_1, \mathbf{n}_2)| &\le (\int_S |F(\mathbf{n}_1, \mathbf{n})|^2 d\Omega)^{1/2} (\int_S |F(\mathbf{n}_2, \mathbf{n})|^2 d\Omega)^{1/2} \\ &\le \max\{\int_S |F(\mathbf{n}_j, \mathbf{n})|^2 d\Omega : j = 1, 2\} \\ &\le \max\{4\pi\, \mathrm{Im}F(\mathbf{n}_j, \mathbf{n}_j) : j = 1, 2\}. \end{aligned}$$

In the spherically symmetric case this inequality gives us even more information, because then $\mathrm{Im}f(\mathbf{n}_1 \cdot \mathbf{n}_2) \le \max\{\mathrm{Im}f(\mathbf{n}_j \cdot \mathbf{n}_j) : j = 1, 2\} = \mathrm{Im}f(1)$. Thus in this case, if f is a square-integrable solution of (1.1), them $\mathrm{Im}f$ attains its maximum at the point $x = 1$, that is, in the forward direction.

We shall continue the practice of denoting the quantities F, G, and H in the spherically symmetric case by lower-case letters f, g, and h respectively.

Proposition 2.2: Let $u: S\times S \to [-1, 1]$. Then $G(\mathbf{n}_1, \mathbf{n}_2) \times T(u)(\mathbf{n}_1, \mathbf{n}_2) \le \max\{G(\mathbf{n}_j, \mathbf{n}_j) T(u)(\mathbf{n}_j, \mathbf{n}_j) : j = 1, 2\}$.

Proof: To prove this, begin with Eq. (2.4) and use the Schwartz inequality as in the proof of Proposition 2.1.

Again in the spherically symmetric case we obtain the further information $g(\mathbf{n}_1 \cdot \mathbf{n}_2) T(u)(\mathbf{n}_1 \cdot \mathbf{n}_2) \le g(1) T(u)(1)$ for every $\mathbf{n}_1$ and $\mathbf{n}_2$ in S. Thus the product of the differential cross section with a function in the range of T attains its maximum value over $[-1, 1]$ at the point $x = 1$, the forward direction.

3. SUCCESSIVE APPROXIMATION

We will suppose the differential cross section G is continuous. Let $Q(H)(\mathbf{n}_1, \mathbf{n}_2) = \int_S H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n})\, d\Omega$, $m(G) = \min\{Q(H)(\mathbf{n}_1, \mathbf{n}_2) : \mathbf{n}_1, \mathbf{n}_2 \in S\}$, $M(G) = \max\{Q(H)(\mathbf{n}_1, \mathbf{n}_2) : \mathbf{n}_1, \mathbf{n}_2 \in S\}$, and

$$M_2(G) = (1/2\pi) M(M-m)^2 [1 - 2mM + m^2 - M^2 + M^4]^{-1} \times \max\{\int_S G(\mathbf{n}_1, \mathbf{n})\, d\Omega : \mathbf{n}_1 \in S\}.$$

We will continue to write m and M instead of $m(G)$ and $M(G)$ if there is no possibility of confusion. The most general conditions known under which Eq. (1.3) [and therefore also Eq. (2.3)] can be solved by using the Banach contraction mapping principle are given in Sec. 3 of Ref. 4 and in Ref. 6. We will show that under these conditions the problem of the unitarity equation is well-posed, as previously described.

Theorem 3.1: Let $\mu_0 = [\frac{1}{8}(\sqrt{17} - 1)]^{1/2} \approx 0.6248$. Let $X = C(S\times S)$ with $\|x\| = \max\{|x(\mathbf{n}_1, \mathbf{n}_2)| : \mathbf{n}_1, \mathbf{n}_2 \in S\}$ and let G_0 be a positive function in X satisfying $M(G_0) = \mu_0 - \eta$ for some $\eta > 0$. Then there is a unique solution u_0 in X of Eq. (2.3) which corresponds to G_0 by (1.2), and for each $\epsilon > 0$ there is a $\delta = \delta(\epsilon, G_0) > 0$ such that for each G in $B(G_0, \delta) = \{G \in X : \|G - G_0\| < \delta\}$ there is a unique solution u in X of Eq. (2.3) which corresponds to this G by (1.2), and $\|u - u_0\| < \epsilon$.

Proof: Select $\alpha \in]0, 1[$. Since $G_0 > 0$, the map $G \to M(G)$ is continuous at G_0, and so we can choose $\delta_1 > 0$ so that if $G \in B(G_0, \delta_1)$ then $M(G) \le \mu_0 - \alpha\eta$. Then by Theorem 3.2 of Ref. 4, the existence and uniqueness of a solution u of (2.3) corresponding to such G by (1.2) is assured. It remains to show that u is close to u_0. Letting

$$H_0(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) = [4\pi G_0(\mathbf{n}_1, \mathbf{n}_2)]^{-1} G_0(\mathbf{n}_1, \mathbf{n}) G_0(\mathbf{n}_2, \mathbf{n}),$$

we obtain

$$\begin{aligned}
&|u(\mathbf{n}_1, \mathbf{n}_2) - u_0(\mathbf{n}_1, \mathbf{n}_2)| \\
&\quad = \Big| \int_S H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) \Phi(u(\mathbf{n}_1, \mathbf{n}), u(\mathbf{n}_2, \mathbf{n}))\, d\Omega \\
&\qquad - \int_S H_0(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) \Phi(u_0(\mathbf{n}_1, \mathbf{n}), u_0(\mathbf{n}_2, \mathbf{n}))\, d\Omega \Big| \\
&\quad \leq \Big| \int_S H_0(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) [\Phi(u(\mathbf{n}_1, \mathbf{n},), u(\mathbf{n}_2, \mathbf{n})) \\
&\qquad - \Phi(u_0(\mathbf{n}_1, \mathbf{n}), u_0(\mathbf{n}_2, \mathbf{n}))]\, d\Omega \Big| \\
&\qquad + \int_S |H_0(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) - H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n})| \\
&\qquad \times |\Phi(u(\mathbf{n}_1, \mathbf{n}), u(\mathbf{n}_2, \mathbf{n}))|\, d\Omega \\
&\quad \leq \Big\| \int_S H_0(\cdot, *, \mathbf{n}) [\Phi(u(\cdot, \mathbf{n}), u(*, \mathbf{n})) \\
&\qquad - \Phi(u_0(\cdot, \mathbf{n}), u_0(*, \hat{\mathbf{n}}))]\, d\Omega \Big\| \\
&\qquad + \int_S |H_0(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) - H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n})|\, d\Omega \\
&\quad \leq c_0 \|u - u_0\| + \|Q(|H_0 - H|)\|,
\end{aligned}$$

where $c_0 = 2M(G_0)^2[1 - M(G_0)^2]^{-1/2} < 1$ since $M(G_0) < \mu_0$. Now choose $\epsilon > 0$ and $\delta \leq \delta_1$ so that if $\|G - G_0\| < \delta$, then $\|Q(|H_0 - H|)\| < (1 - c_0)\epsilon$. We then have $\|u - u_0\| \leq c_0\|u - u_0\| + (1 - c_0)\epsilon$, so that finally $\|u - u_0\| < \epsilon$, which completes the proof.

This theorem shows that the problem of the unitarity equation is well-posed in the space $C(S\times S)$ and for the class of differential cross-sections $\mathcal{G} = \{G \in C(S\times S) : G > 0$ and $M(G) < \mu_0\}$. It is also possible to show that the problem of the unitarity equation is well-posed in the space $L^2(S\times S, d_2\Omega)$ and for the class of differential cross sections $\mathcal{G}_2 = \{G \in C(S\times S) : G > 0,\ M(G) < 1,$ and $M_2(G) < 1\}$. This is proved using Theorem 2 of Ref. 6. The estimate in Theorem 3.1 above is modified for the use of the $L^2(S\times S, G_0 d_2\Omega)$-norm instead of the maximum norm. However, we cannot obtain the result for the class of differential cross sections $\{G \in L^2(S\times S, d_2\Omega) : G > 0$ a. e., $M(G) < 1,$ and $M_2(G) < 1\}$ because the map $G \to M(G)$ is not continuous in the topology of L^2.

To summarize, what we have shown is the following: If G_0 is a continuous differential cross section for which $M(G_0) < \mu_0$ [or $M(G_0) < 1$ and $M_2(G_0) < 1$], then there is a unique scattering amplitude F_0 which corresponds to G_0 by (1.2) and which satisfies unitarity in the form of Eq. (1.1′). Furthermore, this is true for any continuous differential cross section G which is sufficiently close to G_0 in the uniform topology, and the scattering amplitude F corresponding to G by (1.2) and (1.1′) is close to F_0 in the uniform topology (or the L^2-topology, respectively). So if G_0 is the differential cross section as measured by the instruments, and if the instruments are fine enough, then the true cross section is (uniformly!) near the measured data G_0. If in addition G_0 satisfies either of the above conditions, then the true scattering amplitude is near the scattering amplitude F_0 constructed from G_0 by unitarity via the Banach contraction mapping principle.

4. THE EQUATION $u - KN(u) = 0$

Let X, Y be Banach spaces, let K be a bounded linear operator from Y into X, and let N be a nonlinear map from X into Y. In this section we will obtain some results for equations of the form $u - KN(u) = 0$, principally concerning the branching of solutions of this equation as the infinite-dimensional parameter K is varied. In the next section we will use this material to study the problem of the unitarity equation. In this problem the measured data G enters into the kernel of K in a continuous fashion and so a change in G amounts to a perturbation of K. This is the motivation for considering the above branching problem.

Proposition 4.1: Let X, Y be Banach spaces and U be a subset of X which has nonempty interior. Let N be a bounded not necessarily linear map of U into Y, and suppose N is C^1 on an open subset D of U. Let $K_0 \in \mathcal{L}(Y, X)$, the Banach space of bounded linear maps from Y into X. Suppose there is a solution u_0 in D of the equation $u - K_0N(u) = 0$ for which 1 is a regular value of $K_0N'(u_0)$. Then there are positive numbers ρ_0 and r such that for every K in $B(K_0, \rho_0)$ there is a unique solution u_K in $B(u_0, r)$ of the equation $u - KN(u) = 0$. Also, 1 is a regular value of $KN'(u_K)$, and u_K depends continuously on K in the sense that for each $\epsilon > 0$ there is a $\delta = \delta(\epsilon, K_0) > 0$ such that whenever $\|K - K_0\| < \delta$, then $\|u_K - u_0\| < \epsilon$.

Proof: Define $z: \mathcal{L}(Y, X)\times D \to X$ by $z(K, u) = u - KN(u)$. Then $z(K_0, u_0) = 0$. The Frechet partial derivative of z with respect to the first argument at (K_0, u_0) is the map $z_1(K_0, u_0)H = -HN(u_0)$, and the Frechet partial derivative of z with respect to the second argument at (K_0, u_0) is the map $I - K_0N'(u_0)$. Since 1 is a regular value of $K_0N'(u_0)$, $z_2(K_0, u_0)^{-1}$ is in $\mathcal{L}(X, X)$, and so we may apply the implicit function theorem (Ref. 7, Theorem 4) at (K_0, u_0). We get positive numbers ρ_0 and r, and a map $u: \mathcal{L}(Y, X) \to D$ such that $u(K_0) = u_0$, $z(K, u(K)) = 0$ for each K in $B(K_0, \rho_0)$, and there is no other solution besides $u(K)$ which is contained in $B(u_0, r)$. Put $u_K = u(K)$. Then 1 is a regular value of $KN'(u_K)$ for each K in $B(K_0, \rho_0)$, and since u is C^1 on $B(K_0, \rho_0)$, it follows that u_K depends continuously on K. This completes the proof.

Proposition 4.1 is the main tool used in the next section for investigating questions about continuous dependence of the solution of the unitarity equation (2.3) on the data G. It says that there is no branching of the solution at any of the points (K, u_K) for $K \in B(K_0, \rho_0)$, and hence the solution varies continuously with the data as long as the data is close to the data of K_0. However, it should not be inferred that this theorem precludes the existence of any other solutions of $u - KN(u) = 0$ for K in $B(K_0, \rho_0)$, $K \neq K_0$. For example, for some K_* in $B(K_0, \rho_0)$, $K_* \neq K_0$, there may be a solution u_* in U satisfying $\|u_* - u_0\| \geq r$. If now $E \subset D$ is a closed set containing u_0, we will show that, under certain conditions, u_K is the only solution of $z(K, u) = 0$ in E for K in $B(K_0, \rho_1)$, where $\rho_1 \leq \rho_0$ may depend on E. A modification of this result will have application to the problem of the unitarity equation in the spherically symmetric case.

Definition 4.2: If E is a subset of $U = \text{domain}(N)$, we denote by $n(E, K)$ the number of solutions in E of $z(K, u) = 0$.

Note that $n(E, K)$ is a nonnegative integer, or may be $+\infty$.

Theorem 4.3: Suppose u_0 is the unique solution of $z(K_0, u) = 0$ in $U = \text{domain}(N)$ and that $u_0 \in D$. Suppose

that 1 is a regular value of $z_2(K_0, u_0)$, and that there is an $\eta \in]0, \rho_0]$ for which

$$C_\eta = \{u \in U : z(K, u) = 0 \text{ for } K \in B(K_0, \eta)\} \tag{4.1}$$

is relatively compact. Let $E \subset D$ be a closed set containing u_0. Then there is a positive number ρ_1, which may depend on E, such that if $K \in B(K_0, \rho_1)$, then $n(E, K) = n(E, K_0) = 1$.

Proof: First of all, if $E \subset B(u_0, r)$ (from Proposition 4.1), then $n(E, K) = n(E, K_0) = 1$ for $K \in B(K_0, \rho_0)$, so that $\rho_1 = \rho_0$ works. Suppose E is not a subset of $B(u_0, r)$. Then by Proposition 4.1 there is a positive number $\tau \leq \eta$ such that if $K \in B(K_0, \tau)$, then $n(E, K) \geq n(E, K_0) = 1$. Suppose there is no such ρ_1 as claimed. Then for every $\rho \in]0, \tau[$ there is a $K_\rho \in B(K_0, \rho)$ with $n(E, K_\rho) \geq 2$. In particular, there is a sequence $\{K_j\}_{j=1}^\infty \subset B(K_0, \tau)$ with $K_j \to K_0$ in $\mathcal{L}(Y, X)$ and $n(E, K_j) \geq 2$ for each j. From Proposition 4.1 we have the sequence $\{u_j\}_{j=1}^\infty = \{u(K_j)\}_{j=1}^\infty \subset B(u_0, r)$, with $u_j \to u_0$, accounting for one solution, for each j. Let $\{u_j^*\}_{j=1}^\infty$ be a sequence composed of other solutions of $u = K_j N(u)$ in E. We have $\{u_j^*\}_{j=1}^\infty \subset C_\tau$, and since $\overline{C}_\tau$ is compact, there is a subsequence $\{u_{j_i}^*\}_{i=1}^\infty$ converging to some $u^* \in E$. Since $\|u_j^* - u_0\| \geq r$ for each j we have $u^* \neq u_0$. Since z is continuous and $z(K_j, u_j^*) = 0$ for every j we have $z(K_0, u^*) = 0$, so that $n(E, K_0) \geq 2$. This contradiction completes the proof.

5. APPLICATION TO THE UNITARITY EQUATION

Let $X = C(S \times S)$ and $Y = C(S \times S \times S)$. For $u_1, u_2 \in [-1, 1]$, let $\Phi(u_1, u_2) = (1 - u_1^2)^{1/2}(1 - u_2^2)^{1/2} + u_1 u_2$, choosing the positive square root. Let U be the closed unit ball in X. Define $N : U \to Y$ by

$$N(u)(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) = \Phi(u(\mathbf{n}_1, \mathbf{n}_3), u(\mathbf{n}_2, \mathbf{n}_3)) \tag{5.1}$$

for $u \in U$. Given a positive $G \in X$, define $K \in \mathcal{L}(Y, X)$ by

$$Ky(\mathbf{n}_1, \mathbf{n}_2) = [4\pi G(\mathbf{n}_1, \mathbf{n}_2)]^{-1} \int_S G(\mathbf{n}_1, \mathbf{n}) G(\mathbf{n}_2, \mathbf{n}) y(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n})\, d\Omega \tag{5.2}$$

for $y \in Y$. Then the unitarity equation (2.3) may be expressed as

$$u - KN(u) = 0. \tag{5.3}$$

For any $u \in U$,

$$\begin{aligned}
&\delta N(u;h)(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) \\
&\quad = [u(\mathbf{n}_2, \mathbf{n}_3) - u(\mathbf{n}_1, \mathbf{n}_3)[1 - u(\mathbf{n}_2, \mathbf{n}_3)^2]^{1/2}[1 - u(\mathbf{n}_1, \mathbf{n}_3)^2]^{-1/2}] \\
&\qquad \times h(\mathbf{n}_1, \mathbf{n}_3) + [u(\mathbf{n}_1, \mathbf{n}_3) - u(\mathbf{n}_2, \mathbf{n}_3)[1 - u(\mathbf{n}_1, \mathbf{n}_3)^2]^{1/2} \\
&\qquad \times [1 - u(\mathbf{n}_2, \mathbf{n}_3)^2]^{-1/2}] h(\mathbf{n}_2, \mathbf{n}_3)
\end{aligned}$$

is the Gateaux variation of N at u in the direction h. Select $b_1 < 1$ and let $\Delta = B'(0, b_1) = \{u \in X : |u(\mathbf{n}_1, \mathbf{n}_2)| \leq b_1, \mathbf{n}_1, \mathbf{n}_2 \in S\}$. For $u \in \Delta$, $h \to \delta N(u;h)$ is linear and continuous, so that we have $\delta N(u;h) = DN(u;h)$, the Gateaux derivative. Furthermore, if $u, u' \in \Delta$, we have

$$\begin{aligned}
&|DN(u;h)(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_2) - DN(u';h)(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)| \\
&\quad \leq 2(1 - b_1^2)^{-3/2}[|h(\mathbf{n}_1, \mathbf{n}_3)| + |h(\mathbf{n}_2, \mathbf{n}_3)|] \\
&\qquad \times [|u(\mathbf{n}_1, \mathbf{n}_3) - u'(\mathbf{n}_1, \mathbf{n}_3)| + |u(\mathbf{n}_2, \mathbf{n}_3) - u'(\mathbf{n}_2, \mathbf{n}_3)|],
\end{aligned}$$

and so

$$\|DN(u;\cdot) - DN(u';\cdot)\| \leq 8(1 - b_1^2)^{-3/2}\|u - u'\|,$$

giving $DN(u;\cdot) = N'(u)$, the Frechet derivative of N at u (see Ref. 8, Sec. 1). Thus N is C^1 on any ball $B(0, b)$ where $b < 1$.

We will now state a basic continuous dependence result for Eq. (5.3), and later turn to the more comprehensive results we can obtain by imposing the additional restriction of spherical symmetry.

Theorem 5.1: Suppose $G_0 \in X$ is positive, K_0 arises from G_0 by (5.2), and u_0 is a solution of the unitarity equation $u - K_0 N(u) = 0$ in $B(0, b)$, $b < 1$, for which $I - K_0 N'(u_0)$ is regular. Then there are positive numbers η, r such that if $G \in B(G_0, \eta)$ there is a solution u_G in $B(0, b)$ of Eq. (5.3) with data G, and this solution is unique in $B(u_0, r)$. For each $\epsilon > 0$, there is a $\delta = \delta(\epsilon, G_0) > 0$ such that if $\|G - G_0\| < \delta$, then $\|u_G - u_0\| < \epsilon$.

Proof: This result follows directly from Proposition 4.1, noting that $\|K - K_0\| \leq \|Q(|H - H_0|)\|$, since

$$\begin{aligned}
\|K - K_0\| &= \sup\{\|Ky - K_0 y\| : \|y\| = 1\} \\
&= \sup\{\| \int_S ([4\pi G(\mathbf{n}_1, \mathbf{n}_2)]^{-1} G(\mathbf{n}_1, \mathbf{n}) G(\mathbf{n}_2, \mathbf{n}) \\
&\qquad - [4\pi G_0(\mathbf{n}_1, \mathbf{n}_2)]^{-1} G_0(\mathbf{n}_1, \mathbf{n}) G_0(\mathbf{n}_2, \mathbf{n})) \\
&\qquad \times y(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n})\, d\Omega \| : \|y\| = 1\} \\
&\leq \sup\{\int_S |H(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}) - H_0(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n})|\, d\Omega : \mathbf{n}_1, \mathbf{n}_2 \in S\} \\
&= \|Q(|H - H_0|)\|.
\end{aligned}$$

Since $G \to H$ is continuous at G_0 and $H \to Q(H)$ is continuous at zero, we can choose $\eta > 0$ such that if $\|G - G_0\| < \eta$, then $\|K - K_0\|$ is small enough so that Proposition 4.1 may be applied. This completes the proof.

Remarks: (1) Since G_0 is positive, $\min\{G_0(\mathbf{n}_1, \mathbf{n}_2) : \mathbf{n}_1, \mathbf{n}_2 \in S\} = \gamma_0 > 0$. η is chosen so that $\eta < \gamma_0$.

(2) We can recover part of Theorem 3.1 from this theorem by making the observation that if $\|K_0 N'(u_0)\| < 1$, then $I - K_0 N'(u_0)$ is invertible. This is because if we try to make $\|K_0 N'(u)\| < 1$ for all $u \in B(0, b)$, we are led to impose the condition $M(G_0) < \mu_0$ [or $M(G_0) < 1$, $M_2(G_0) < 1$], which is the condition under which we can solve (5.3) by the Banach contraction mapping principle (see, for example, the end of Sec. 2 of Ref. 1). However, this does not give the full result of Theorem 3.1—the statement about uniqueness in the whole space is unavailable. However, Theorem 5.1 might be more widely applicable because $I - K_0 N'(u_0)$ may well be invertible under conditions other than $\|K_0 N'(u_0)\| < 1$.

We turn now to the spherically symmetric case for continuous functions, where we will get better results by adding some conditions and taking advantage of the spherical symmetry. Recall our practice of using lower-case letters in this case. We will show that if $u_0 \in \text{interior}(\text{domain}(N))$ is the unique solution in $\text{domain}(N)$ corresponding to the data g_0 by (1.2), then, for g from a certain class of functions and sufficiently close to g_0, the solution u_g corresponding to the data g by (1.2) will also be unique in $\text{domain}(N)$. We use the change of variables (5) of Ref. 1. Let $X = C[-1, 1]$ and $Y = C([-1, 1] \times [-1, 1])$. Then for $u \in X$, $|u| \leq 1$, and $v \in Y$,

$$N(u)(y, z) = \Phi(u(y), u(z)), \tag{5.4}$$

$$Kv(x)=\begin{cases}\displaystyle\int_{E(x)} h(x,y,z)v(y,z)\,dy\,dz, & -1<x<1\\ \displaystyle\frac{1}{2g(x)}\int_{-1}^{1} g(y)g(xy)v(y,xy)\,dy, & x=\pm 1\end{cases} \tag{5.5}$$

where

$$h(x,y,z)=g(y)g(z)[2\pi g(x)(1-x^2-y^2-z^2+2xyz)^{1/2}]^{-1}$$

and $E(x)$ is the interior of the ellipse on which $1-x^2-y^2-z^2+2xyz=0$. The unitarity equation is then (5.3) again.

Theorem 5.2: Suppose $g_0\in X$ is positive, $K_0\in \mathcal{L}(Y,X)$ arises from g_0 by (5.5), u_0 is the unique solution in domain$(N)=B'(0,1)$ of $u-K_0N(u)=0$, $\|u_0\|<1$, $I-K_0N'(u_0)$ is regular, and there is a $\beta<1$ for which $\beta g_0(x)\geq \frac{1}{2}\int_{-1}^{1}\times g_0(t)^2\,dt$ for every $x\in[-1,1]$. Then there is a positive number η_s such that if $g\in B(g_0,\eta_s)$, there is a solution u_g of (5.3) corresponding to the data g by (1.2), and $u_g\to u_0$ as $g\to g_0$. Furthermore, u_g is the only solution of (5.3) with data g in all of domain(N).

Proof: We only need to prove the uniqueness part, because from Theorem 5.1 there is an $\eta>0$ such that if $g\in B(g_0,\eta)$, then there is a solution u_g of (5.3) which has all the other required properties.

Let $\beta_1\in\,]\beta,1[$ and choose $\eta_s\leq\eta$ so that for each $x\in[-1,1]$, $\beta_1 g(x)\geq\frac{1}{2}\int_{-1}^{1}g(t)^2\,dt$ for every $g\in B(g_0,\eta_s)$. Now select c_1 and b so that $\|u_0\|<c_1<b<1$ and $\beta_1<c_1<b<1$. We have domain$(N)=B'(0,1)$; put $D=B(0,b)$ and $E=B'(0,c_1)$. We will show first of all that if $g\in B(g_0,\eta_s)$, then u_g is the only solution in E of (5.3) with data g. This proof is modeled on that of Theorem 4.3, but a modification needs to be made since the set (4.1) of Theorem 4.3 is not, in general, relatively compact because $u\to KN(u)$ is not a compact map. However, in compensation we have that, for all $u\in D$ satisfying (5.3) with data g, there is a $C>0$, independent of u, for which

$$\begin{aligned}&|u(x_1)-u(x_2)|\\ &\quad\leq C[|x_1-x_2|^{1/2}|1-x_2^2|^{-1/2}+|g(x_1)-g(x_2)|],\end{aligned} \tag{5.6}$$

for $x_1^2\leq x_2^2<1$. This follows from (4.22) of Ref. 3, the remarks following (2.3), and the mean value theorem.

Suppose that in every ball in X about g_0 there is a g [with corresponding K, by (5.5)] such that $n(E,K)\geq 2$. Then there is a sequence $\{g_j\}_{j=1}^{\infty}$ (with corresponding $\{K_j\}_{j=1}^{\infty}$) with $g_j\to g_0$ and $n(E,K_j)\geq 2$ for every j. Note that $K_j\to K_0$ in $\mathcal{L}(Y,X)$. For $u\in E$, write $u=vw$ where $w(x)=(1-x^2)^{-1/2}$, and write $\tilde{z}(K,v)=vw-KN(vw)$. Note that v solves $\tilde{z}(K,v)=0$ if and only if $u=vw$ solves $z(K,u)=0$. Let $\{u_j\}_{j=1}^{\infty}$ be the sequence of solutions $\{u_{g_j}\}_{j=1}^{\infty}$ from Theorem 5.1, and let $\{u_j^*\}_{j=1}^{\infty}$ be a sequence composed of other solutions of (5.3) in E. Put $v_j^*=(1/w)u_j^*$. Then from (5.6), for $x_1^2\leq x_2^2<1$,

$$\begin{aligned}&|v_j^*(x_1)-v_j^*(x_2)|\\ &=|(1-x_1^2)^{1/2}u_j^*(x_1)-(1-x_2^2)^{1/2}u_j^*(x_2)|\\ &\leq|(1-x_1^2)^{1/2}-(1-x_2^2)^{1/2}|+|1-x_2^2|^{1/2}\,|u_j^*(x_1)-u_j^*(x_2)|\\ &\leq|(1-x_1^2)^{1/2}-(1-x_2^2)^{1/2}|+C[|x_1-x_2|^{1/2}\\ &\quad+|g_j(x_1)-g_j(x_2)|],\end{aligned}$$

and

$$\begin{aligned}|v_j^*(z)-v_j^*(x)|&=|(1-x^2)^{\alpha}u_j^*(x)|\\ &\leq c_1|1-x^2|^{\alpha},\quad z=\pm 1.\end{aligned}$$

Since $g_j\to g_0$ in $C[-1,1]$, the set $\{g_j\}_{j=1}^{\infty}\cup\{g_0\}$ is equicontinuous. Therefore, the set $\{v_j^*\}_{j=1}^{\infty}$ is equicontinuous; being a subset of $E'=\{u\in X:|u(x)|\leq(1-x^2)^{\alpha}c_1\}$ it is uniformly bounded. Thus there is a subsequence $\{v_{j_i}^*\}_{i=1}^{\infty}$ converging uniformly on $[-1,1]$ to some $v^*\in E'$. But $\tilde{z}$ is continuous on $\mathcal{L}(Y,X)\times E'$ (since $w\in L^1[-1,1]$), and so $u^*-K_0N(u^*)=0$, where $u^*=wv^*$. Also $u^*\in E$ and $u^*\neq u_0$ since u_j is bounded away from u_0 independently of j. Thus $n(E,K_0)\geq 2$, a contradiction, so the uniqueness of u_g in E is established.

Now we show that for $g\in B(g_0,\eta_s)$ u_g is the only solution of (5.3) with data g in all of domain(N). Suppose there is another solution u^* (besides u_g) of (5.3) with data g in domain(N). Then since u_g is the only such solution in E, $\max\{|u^*(x)|:x\in[-1,1]\}$ must be strictly larger than β_1. Say this maximum is attained at x_0. Since by the remarks following Proposition 2.2 we have $|u(x)|g(x)\leq u(1)g(1)$ for every u satisfying (5.3) with data g, it follows that $|u^*(x_0)|g(x_0)\leq u^*(1)g(1)$, or $\beta_1 g(x_0)<u^*(1)g(1)=\frac{1}{2}\int_{-1}^{1}g(t)^2\,dt$, a contradiction. This proves the theorem.

This theorem is primarily about continuous dependence. It says that in the spherically symmetric case, the problem of the unitarity equation is well-posed in $C[-1,1]$ for the class of differential cross sections $\{g\in C[-1,1]: g(x)>\frac{1}{2}\int_{-1}^{1}g(t)^2\,dt$ for every $x\in[-1,1]$ and there is a unique solution u_g of (5.3) in $B(0,1)$ with data $g\}$. The next corollary gives a more specific result, and gives another proof of the fact that if the differential cross section is nearly constant and small enough, there is a unique scattering amplitude that corresponds to this cross section by (1.2) and satisfies the unitarity equation.

Corollary 5.3: If g_0 is identically a constant $c<1$, there is a unique solution in domain(N) of the unitarity equation (5.3) with data g_0. Also, if $\|g-c\|<\eta_s$, there is a unique solution u_g in domain(N) of the unitarity equation with data g, and $u_g\to u_0$ as $g\to g_0$.

Proof: In Theorem 5.2, $\beta=c$ works. Put $\beta_1=(1+c)/2$, say, and choose c_1 and b as before. Trying for a constant solution $u_0\equiv d$, we get

$$d=\frac{c}{2\pi}\int_{-1}^{1}dy\int_{xy-(1-x^2)^{1/2}(1-y^2)^{1/2}}^{xy+(1-x^2)^{1/2}(1-y^2)^{1/2}}(1-x^2-y^2-z^2+2xyz)^{-1/2}\,dz$$

$= c,$

so that $u_0 \equiv c$ is a solution of (5.3), and $\mathrm{Im} f_0 = u_0 \cdot c = c^2$. $c \leq 1$ is necessary for solution since $|\mathrm{Im} f_0| \leq g_0 = c$. For $c < 1$, u_0 is the only solution of (5.3) in domain(N) (by Corollary 3 of Ref. 6). Then since $\|u_0\| < c_1 < b < 1$, $n(U, K_0) = 1$, and $I - K_0 N'(u_0) = I - 0 = I$, the result follows from Theorem 5.2.

It is interesting that this corollary gives an existence and uniqueness result, because Theorem 5.2 is basically a statement about continuous dependence. It applies to cross sections which are "slowly varying," or which may oscillate rapidly but with small amplitude. Of course, Theorem 2 of Ref. 6 says the same thing, and even gives hard numerical estimates, which this corollary does not. However, we include it to point out how the regularity of $I - K_0 N'(u_0)$ is exploited: It may be possible to do this for other K_0 and u_0 as well.

[1]R.G. Newton, J. Math. Phys. **9**, 2050 (1968).
[2]A. Martin, Nuovo Cimento A **59**, 131 (1969).
[3]D. Atkinson, P.W. Johnson, and R.L. Warnock, Commun. Math. Phys. **28**, 133 (1972).
[4]M. Tortorella, J. Math. Phys. **15**, 745 (1974).
[5]R. Glauber and V. Schomaker, Phys. Rev. **89**, 667 (1953).
[6]M. Tortorella, J. Math. Phys. **15**, 1153 (1974), Addendum to Ref. 4.
[7]T.H. Hildebrandt, and L.M. Graves, Trans. Amer. Math. Soc. **29**, 150 (1927).
[8]M.Z. Nashed, "Differentiability and Related Properties of Nonlinear Operators," in *Nonlinear Functional Analysis and Applications*, edited by L.B. Rall (Academic, New York, 1971).

Conformally flat solutions of the Einstein–Maxwell equations for null electromagnetic fields

R. G. McLenaghan

Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada

N. Tariq and B. O. J. Tupper

Department of Mathematics, University of New Brunswick, Fredericton, New Brunswick, Canada
(Received 8 August 1974)

The spin coefficient formalism of Newman and Penrose is employed to obtain a direct derivation of the most general conformally flat solution of the source-free Einstein–Maxwell equations for null electromagnetic fields.

1. INTRODUCTION

In a previous article[1] it was shown, using the Newman–Penrose[2] formalism, that the solution of Bertotti[3] and Robinson[4] is the unique conformally flat solution of the Einstein–Maxwell equations for nonnull fields. In this article we treat the case of null fields using the same formalism. We prove that the only conformally flat solutions of the Einstein–Maxwell equations for null fields are the conformally flat members of the exact plane wave family of solutions[5] of the Einstein–Maxwell equations. This result has been stated without proof by Cahen and Leroy[6] who found the above solutions by applying a limiting process to certain type N solutions of the Einstein–Maxwell equations.

2. NOTATION AND EQUATIONS

A tetrad system of null vectors $(l^\mu, n^\mu, m^\mu, \bar{m}^\mu)$, where l^μ, n^μ are real and $m^\mu, \bar{m}^\mu$ are complex vectors, is defined by the relations

$$l_\mu n^\mu = -m_\mu \bar{m}^\mu = 1$$

with all other inner products zero.

If $F_{\mu\nu}$ is the electromagnetic field tensor, then the three Maxwell scalars are defined by

$$\phi_0 = F_{\mu\nu} l^\mu m^\nu, \quad \phi_2 = F_{\mu\nu} \bar{m}^\mu n^\nu,$$
$$\phi_1 = \tfrac{1}{2} F_{\mu\nu} (l^\mu n^\nu + \bar{m}^\mu m^\nu).$$

In the case of a null field the tetrad can be chosen so that $\phi_0 = \phi_1 = 0$, $\phi_2 \equiv \phi \neq 0$. In this case l^μ is a repeated principal null vector of the electromagnetic field.

By a suitable choice of units the Einstein–Maxwell field equations may be written in the form

$$\Phi_{AB} = \phi_A \bar{\phi}_B,$$

where Φ_{AB} are the complex tetrad components of the Ricci tensor and A, B take the values of $0, 1, 2$. In the present case the only nonzero component of Φ_{AB} is $\Phi_{22} = \phi\bar{\phi}$.

The twelve complex spin coefficients are defined by the expressions

$$\begin{aligned} l_{\mu;\nu} &= (\gamma + \bar{\gamma}) l_\mu l_\nu + (\epsilon + \bar{\epsilon}) l_\mu n_\nu - (\alpha + \bar{\beta}) l_\mu m_\nu - (\bar{\alpha} + \beta) l_\mu \bar{m}_\nu \\ &\quad - \bar{\tau} m_\mu l_\nu - \bar{\kappa} m_\mu n_\nu + \bar{\sigma} m_\mu m_\nu + \bar{\rho} m_\mu \bar{m}_\nu - \tau \bar{m}_\mu l_\nu \\ &\quad - \kappa \bar{m}_\mu n_\nu + \sigma \bar{m}_\mu \bar{m}_\nu, \end{aligned}$$

$$\begin{aligned} n_{\mu;\nu} &= -(\gamma + \bar{\gamma}) n_\mu l_\nu - (\epsilon + \bar{\epsilon}) n_\mu n_\nu + (\alpha + \bar{\beta}) n_\mu m_\nu + (\bar{\alpha} + \beta) n_\mu \bar{m}_\nu \\ &\quad + \nu m_\mu l_\nu + \pi m_\mu n_\nu - \lambda m_\mu m_\nu - \mu m_\mu \bar{m}_\nu + \bar{\nu} \bar{m}_\mu l_\nu \\ &\quad + \bar{\pi} \bar{m}_\mu n_\nu - \bar{\mu} \bar{m}_\mu m_\nu - \bar{\lambda} \bar{m}_\tau \bar{m}_\nu, \end{aligned} \tag{2.1}$$

$$\begin{aligned} m_{\mu;\nu} &= \bar{\nu} \bar{l}_\mu l_\nu + \bar{\pi} \bar{l}_\mu n_\nu - \bar{\mu} \bar{l}_\mu m_\nu - \bar{\lambda} \bar{l}_\mu \bar{m}_\nu - \tau n_\mu l_\nu - \kappa n_\mu n_\nu \\ &\quad + \rho n_\mu m_\nu + \sigma n_\mu \bar{m}_\nu + (\gamma - \bar{\gamma}) m_\mu l_\nu + (\epsilon - \bar{\epsilon}) m_\mu n_\nu \\ &\quad + (\bar{\beta} - \alpha) m_\mu m_\nu + (\bar{\alpha} - \beta) m_\mu \bar{m}_\nu. \end{aligned}$$

Using the facts the five complex tetrad components of the Weyl tensor are zero and $\Phi_{22} = \phi\bar{\phi}$ is the only nonzero component of Φ_{AB}, we find from Bianchi's[7] identities that

$$\kappa = \sigma = \rho = 0. \tag{2.2}$$

Four differential operators D, Δ, δ, $\bar{\delta}$ are defined by

$$D\phi = \phi_{;\mu} l^\mu, \quad \delta\phi = \phi_{;\mu} m^\mu, \quad \bar{\delta}\phi = \phi_{;\mu} \bar{m}^\mu, \quad \Delta\phi = \phi_{;\mu} n^\mu.$$

By taking into account the conditions (2.2), the following commutation relations (integrability conditions) hold:

$$\begin{aligned} &(\Delta D - D\Delta)\phi = (\gamma + \bar{\gamma}) D\phi + (\epsilon + \bar{\epsilon}) \Delta\phi - \pi\delta\phi - \bar{\pi}\bar{\delta}\phi, \\ &(\delta D - D\delta)\phi = (\bar{\alpha} + \beta - \bar{\pi}) D\phi - (\epsilon - \bar{\epsilon}) \delta\phi, \\ &(\delta\Delta - \Delta\delta)\phi = -\bar{\nu} D\phi - (\bar{\alpha} + \beta) \Delta\phi + (\mu - \gamma + \bar{\gamma}) \delta\phi + \bar{\lambda}\bar{\delta}\phi, \\ &(\delta\bar{\delta} - \bar{\delta}\delta)\phi = (\mu - \bar{\mu}) D\phi + (\bar{\beta} - \alpha) \delta\phi + (\bar{\alpha} - \beta) \bar{\delta}\phi. \end{aligned} \tag{2.3}$$

Maxwell's equations are

$$D\phi = -2\epsilon\phi, \tag{2.4}$$

$$\delta\phi = (\tau - 2\beta)\phi. \tag{2.5}$$

Combining (2.5) with Bianchi's identities

$$\bar{\delta}(\phi\bar{\phi}) = (\bar{\tau} - 2\bar{\beta} - 2\alpha)\phi\bar{\phi},$$

we obtain

$$\bar{\delta}\phi = -2\alpha\phi. \tag{2.6}$$

If we evaluate the commutator $(\delta\bar{\delta} - \bar{\delta}\delta)\phi$ using (2.3), (2.4), (2.5), (2.6), and the field equations,[7] we obtain

$$\tau = 0. \tag{2.7}$$

The remaining nontrivial field equations are

$$\begin{aligned} &D\alpha - \bar{\delta}\epsilon = (\bar{\epsilon} - 2\epsilon)\alpha - \bar{\beta}\epsilon + \epsilon\pi, \\ &D\beta - \delta\epsilon = -\bar{\epsilon}\beta - (\bar{\alpha} - \pi)\epsilon, \\ &D\gamma - \Delta\epsilon = \bar{\pi}\alpha + \pi\beta - (\epsilon + \bar{\epsilon})\gamma - (\gamma + \bar{\gamma})\epsilon, \\ &D\lambda - \bar{\delta}\pi = \pi^2 + (\alpha - \bar{\beta})\pi - (3\epsilon - \bar{\epsilon})\lambda, \end{aligned}$$

$$
\begin{aligned}
&D\mu - \delta\pi = \pi\bar{\pi} - (\epsilon + \bar{\epsilon})\,\mu - \pi(\bar{\alpha} - \beta),\\
&D\nu - \Delta\pi = \pi\mu + \bar{\pi}\lambda + (\gamma - \bar{\gamma})\,\pi - (3\epsilon + \bar{\epsilon})\,\nu,\\
&\Delta\lambda - \bar{\delta}\nu = -(\mu + \bar{\mu})\,\lambda - (3\gamma - \bar{\gamma})\,\lambda + (3\alpha + \bar{\beta} + \pi)\,\nu,\\
&\delta\alpha - \bar{\delta}\beta = \alpha\bar{\alpha} + \beta\bar{\beta} - 2\alpha\beta + \epsilon(\mu - \bar{\mu}),\\
&\delta\lambda - \bar{\delta}\mu = (\mu - \bar{\mu})\,\pi + \mu(\alpha + \bar{\beta}) + \lambda(\bar{\alpha} - 3\beta),\\
&\delta\nu - \Delta\mu = \mu^2 + \lambda\bar{\lambda} + (\gamma + \bar{\gamma})\,\mu - \bar{\nu}\pi - (3\beta + \bar{\alpha})\,\nu + \phi\bar{\phi},\\
&\delta\gamma - \Delta\beta = -(\bar{\alpha} + \beta)\,\gamma - \epsilon\bar{\nu} - \beta(\gamma - \bar{\gamma} - \mu) + \alpha\bar{\lambda},\\
&\Delta\alpha - \bar{\delta}\gamma = \epsilon\nu - \beta\lambda + (\bar{\gamma} - \bar{\mu})\,\alpha + \bar{\beta}\gamma.
\end{aligned}
\tag{2.8}
$$

3. SIMPLIFICATION OF THE EQUATIONS

The tetrad rotations preserving l^μ as the principal null direction of the electromagnetic field are the spatial rotations

$$
\begin{aligned}
&l^\mu \to Rl^\mu,\\
&n^\mu \to R^{-1}n^\mu,\\
&m^\mu \to e^{iS}m^\mu,
\end{aligned}
\tag{3.1}
$$

where $R > 0$, S are real functions, and the null rotations

$$
\begin{aligned}
&l^\mu \to l^\mu,\\
&n^\mu \to n^\mu + \bar{T}m^\mu + T\bar{m}^\mu + T\bar{T}l^\mu\\
&m^\mu \to m^\mu + Tl^\mu,
\end{aligned}
\tag{3.2}
$$

where T is a complex function.

We now show that by means of a rotation of the form (3.1) we can eliminate the spin coefficients α, β, ϵ, γ. Under this rotation these spin coefficients transform as follows:

$$
\begin{aligned}
&\tilde{\alpha} = e^{-iS}\left(\alpha + \frac{1}{2R}\,\bar{\delta}R + \frac{i}{2}\,\bar{\delta}S\right),\\
&\tilde{\beta} = e^{iS}\left(\beta + \frac{1}{2R}\,\delta R + \frac{i}{2}\,\delta S\right),\\
&\tilde{\epsilon} = R\epsilon + \frac{1}{2}\,DR + \frac{i}{2}\,RDS,\\
&\tilde{\gamma} = R^{-1}\gamma + \frac{1}{2R^2}\,\Delta R + \frac{i}{2}\,\frac{1}{R}\,\Delta S.
\end{aligned}
$$

To set $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\epsilon}$, $\tilde{\gamma}$ to zero we must choose R and S to satisfy

$$
DA = -2\epsilon, \quad \Delta A = -2\gamma, \quad \delta A = -2\beta, \quad \bar{\delta}A = -2\alpha,
$$

where $A = \log R + iS$. By applying the commutation relations (2.3) to these expressions and using equations (2.8), we find that all the integrability conditions are satisfied. Hence we can always choose R and S so that α, β, ϵ, γ vanish. These conditions are preserved by rotations for which A is constant.

Consider a rotation of the form (3.2). Under this rotation the remaining spin coefficients transform as

$$
\begin{aligned}
&\tilde{\pi} = \pi + D\bar{T},\\
&\tilde{\mu} = \mu + T\pi + \delta\bar{T} + TD\bar{T},\\
&\tilde{\lambda} = \lambda + \bar{T}\pi + \bar{\delta}\bar{T} + \bar{T}D\bar{T},\\
&\tilde{\nu} = \nu + T\lambda + \bar{T}\mu + T\bar{T}\pi + \Delta\bar{T} + T\bar{\delta}\bar{T} + \bar{T}\bar{\delta}\bar{T} + \bar{T}\delta\bar{T} + T\bar{T}D\bar{T}.
\end{aligned}
$$

We now show that by a suitable choice of T, the spin coefficients $\tilde{\pi}$, $\tilde{\mu}$, $\tilde{\lambda}$ can be made to vanish. For this to be possible, T must satisfy the differential equations

$$
\begin{aligned}
&0 = \pi + D\bar{T},\\
&0 = \mu + T\pi + \delta\bar{T} + TD\bar{T},\\
&0 = \lambda + \bar{T}\pi + \bar{\delta}\bar{T} + \bar{T}D\bar{T}.
\end{aligned}
$$

These equations may be rewritten in the form

$$
D\bar{T} = -\pi, \quad \delta\bar{T} = -\mu, \quad \bar{\delta}\bar{T} = -\lambda.
$$

By applying the commutation relations to these expressions and using equations (2.8), remembering that now $\alpha = \beta = \epsilon = \gamma = 0$, we find that all the integrability conditions are satisfied. Hence we can always choose T so that π, μ, λ vanish. Under this rotation ν becomes

$$
\tilde{\nu} = \nu + \Delta\bar{T}.
$$

The presence of the $\phi\bar{\phi}$ term in the tenth equation of (2.8) ensures that T cannot be chosen so that $\tilde{\nu} = 0$. The vanishing of π, μ, and λ is preserved by rotations satisfying $DT = \delta T = \bar{\delta}T = 0$.

Thus ν is the only nonzero spin coefficient, and from the expressions (2.1) we find

$$
l_{\mu;\nu} = 0, \quad m_{\mu;\nu} = \bar{\nu}l_\mu l_\nu
$$

which imply that both l_μ and m_μ are gradient vectors, i.e.,

$$
l_\mu = u_{,\mu}, \quad m_\mu = z_{,\mu},
$$

where u is a real function of the four coordinates and z is a complex function of the four coordinates. Labelling the coordinates x^μ ($\mu = 1, 2, 3, 4$), we now choose coordinates such that $u = x^1$, $z = x^3$, $\bar{z} = x^4$ so that the tetrad vectors take the form

$$
\begin{aligned}
&l_\mu = (1, 0, 0, 0), \quad n_\mu = (n_1, n_2, n_3, n_4),\\
&m_\mu = (0, 0, 1, 0), \quad \bar{m}_\mu = (0, 0, 0, 1),
\end{aligned}
$$

where the components of n_μ are each functions of the four coordinates.

Since ν is the only nonzero spin coefficient, the expressions (2.1) also give

$$
n_{\mu;\nu} = \nu m_\mu l_\nu + \bar{\nu}\bar{m}_\mu l_\nu,
\tag{3.3}
$$

which implies

$$
n_{[\mu;\nu}l_{\sigma]} = 0.
\tag{3.4}
$$

Since only the first components of l_μ is nonzero, Eq. (3.4) leads to

$$
n_{a,b} - n_{b,a} = 0,
$$

where $a, b = 2, 3, 4$. This implies that the three components n_a form a three-dimensional gradient vector with u fixed, i.e.,

$$
n_a = r_{,a},
$$

where r is a function of the four coordinates. We can choose the coordinate $x^2 = r$; then n_μ becomes

$$
n_\mu = (F, 1, 0, 0),
\tag{3.5}
$$

where F is a function of the four coordinates. However, by antisymmetrizing equation (3.3) and putting the suf-

fixes $\mu, \nu = 1, 2$ we obtain $n_{1,2} - n_{2,1} = 0$ which implies that $F = F(u, z, \bar{z})$.

4. THE SOLUTION

The metric tensor $g_{\mu\nu}$ is given by the expression

$$g_{\mu\nu} = l_\mu n_\nu + l_\nu n_\mu - m_\mu \bar{m}_\nu - m_\nu \bar{m}_\mu,$$

from which we find that the metric of the space—time solution has the form

$$ds^2 = 2F du^2 + 2du\, dr - 2dz\, d\bar{z}.$$

In view of (3. 3) and (3. 5) the nonzero spin coefficient ν is given by

$$\nu = -F_{,z}. \tag{4.1}$$

The remaining nontrivial Newman—Penrose equations are

$$D\nu = \bar{\delta}\nu = 0, \quad \delta\nu = \phi\bar{\phi} = q^2(u). \tag{4.2}$$

The fact that $\phi\bar{\phi}$ is a function only of u results from the remaining Bianchi identities, which are $D(\phi\bar{\phi}) = \bar{\delta}(\phi\bar{\phi}) = 0$.

Equations (4. 1) and (4. 2) lead to

$$F_{,zz} = 0, \quad F_{,z\bar{z}} = q^2(u)$$

so that F has the form

$$F = q^2(u)\, z\bar{z} + p(u)\, z + \bar{p}(u)\, \bar{z} + h(u). \tag{4.3}$$

By a transformation of the form

$$z' = z - b$$

$$r' = r - z\dot{\bar{b}} - \bar{z}\dot{b} + c,$$

where b and c are functions of u only and the dot denotes differentiation with respect to u, it is possible to transform away the last three terms of expression (4. 3). Thus the metric takes the final form

$$ds^2 = 2q^2(u)\, z\bar{z}\, du^2 + 2du\, dr - 2dz\, d\bar{z}, \tag{4.4}$$

which is precisely the general solution given by Cahen and Leroy.[6] The solutions (4. 4) are the conformally flat members of the exact plane wave family of solutions[5] of Einstein—Maxwell equations.

Note that the Maxwell equations (2. 4) and (2. 5) now take the form $D\phi = \delta\phi = 0$ and, from Eq. (2. 6), we have, in addition, $\bar{\delta}\phi = 0$. These equations imply that ϕ is a function only of u.

ACKNOWLEDGMENTS

This work was supported in part by operating grants from the National Research Council of Canada to the authors (R. G. M. and B. O. J. T.).

[1] N. Tariq and B. O. J. Tupper, J. Math. Phys. **15**, 2232 (1974).
[2] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).
[3] B. Bertotti, Phys. Rev. **116**, 1331 (1959).
[4] I. Robinson, Bull. Acad. Pol. Sci. Ser. Sci. Math. Astr. Phys. **7**, 351 (1959).
[5] See, for example, R. G. McLenaghan and J. Leroy, Proc. R. Soc. London A **327**, 229 (1972).
[6] M. Cahen and J. Leroy, Bull. Acad. Roy. Belg. **51**, 1179 (1965); J. Math. Mech. **16**, 501 (1966).
[7] F. A. E. Pirani, *Introduction to Gravitational Radiation*, Brandeis Institute in Theoretical Physics 1964, Vol. 1 (Prentice-Hall, Englewood Cliffs, N. J., 1965), pp. 350—51.

Algebraic approach of the infrared-problem for external currents

J. P. Provost, F. Rocca, and G. Vallée

*Physique Théorique, Université de Nice,**† *06034 Nice-Cedex, France*
(Received 4 November 1974)

The infrared problem for external currents is shown to be a consequence of the nonexistence of a particle number in the correct representation. A natural procedure for obtaining nondivergent results is then given.

Generalized coherent states have been introduced in the study of the problem of the electromagnetic field interacting with a prescribed c-number current $J_u(\mathbf{r}, t)$. By working in the Heisenberg picture the resolution of the coupled field equation in the radiation gauge leads to the relation[1]

$$a_{out}(k) = a_{in}(k) + i\mathbf{j}(k), \tag{1}$$

where $\mathbf{j}(k)$ is the Fourier transform on the mass shell of the transverse part of the current. Therefore, the in-vacuum Fock state Ω is a coherent vector state for the out-field operator whose mean number of photons at time $t = +\infty$ is equal to $\|J\|^2$:

$$\|J\|^2 = (\mathbf{j}, \mathbf{j}) = \int \frac{d^3k}{2|k|}\, \mathbf{j}^*(k) \cdot \mathbf{j}(k). \tag{2}$$

For accelerated charged particles, $\mathbf{j}(\mathbf{k})$ behaves like $1/|k|$ when $|k|$ goes to zero and the mean number of photons is strictly infinite: Ω does not belong to the Fock representation space of the out field. In this situation a von Neumann's infinite tensor product representation has been introduced and generalized coherent vector states have been rigourously defined.[2,3] We present in this note a simpler algebraic approach of this infrared problem.

Let $\mathcal{A}$ be the subspace of the one photon Hilbert space $\mathcal{L}$ such that the scalar product $(\mathbf{f}, \mathbf{j})$, $\mathbf{f} \in \mathcal{A}$, is finite. $\mathcal{A}$ is dense in[3,4] $\mathcal{L}$, and we can take for the photon field algebra the C^*-algebra $\overline{\Delta(\mathcal{A}, \sigma)}$ constructed as in Ref. 5: $\Delta(\mathcal{A}, \sigma)$ is the $*$-algebra generated by the elements δ_f, $\mathbf{f} \in \mathcal{A}$, which satisfy the Weyl relation

$$\delta_{\mathbf{f}}\, \delta_{\mathbf{g}} = \exp[-i\sigma(\mathbf{f}, \mathbf{g})]\, \delta_{\mathbf{f}+\mathbf{g}}, \tag{3}$$

where σ is the antisymmetric real bilinear form on $\mathcal{A}$:

$$\sigma(\mathbf{f}, \mathbf{g}) = (1/2i)\,[(\mathbf{f}, \mathbf{g}) - (\mathbf{g}, \mathbf{f})]. \tag{4}$$

$\overline{\Delta(\mathcal{A}, \sigma)}$ is the closure with respect to the C^*-algebra norm which exists on $\Delta(\mathcal{A}, \sigma)$.

Now, by starting with the vacuum Fock vector state Ω as initial vector state, all measurements at time $t = +\infty$ can be deduced from the functional $E(\mathbf{f})$ on $\mathcal{A}$:

$$E(\mathbf{f}) = (\Omega, \exp[iA_{out}(\mathbf{f})]\Omega), \quad \mathbf{f} \in \mathcal{A},$$
$$= \exp[-\tfrac{1}{2}(\mathbf{f}, \mathbf{f}) + 2i\,\mathrm{Im}(\mathbf{f}, \mathbf{j})]. \tag{5}$$

This functional $E(\mathbf{f})$ defines the generalized coherent state ω_j on $\overline{\Delta(\mathcal{A}, \sigma)}$ through the relation

$$\omega_{\mathbf{j}}(\delta_{\mathbf{f}}) = E(\mathbf{f}), \quad \delta_{\mathbf{f}} \in \overline{\Delta(\mathcal{A}, \sigma)}. \tag{6}$$

The G—N—S triplet associated with the state ω_j is $(\mathcal{H}_F, \Pi_j, \Omega)$, where $\mathcal{H}_F$ is the Fock representation space and the representation Π_j is given by

$$\Pi_{\mathbf{j}}(\delta_{\mathbf{f}}) = \Pi_F(\delta_{\mathbf{f}}) \exp[2i\,\mathrm{Im}(\mathbf{f}, \mathbf{j})] \tag{7}$$

(Π_F is the usual Fock representation).

As $\mathbf{j}$ does not belong to $\mathcal{L}$ the linear form on $\mathcal{A}$: $\mathbf{f} \to (\mathbf{f}, \mathbf{j})$ is not continuous with respect to the norm in $\mathcal{L}$ and the state ω_j is not quasiequivalent to a Fock state.[6]

Furthermore, the $*$-automorphisms corresponding to gauge transformations of the first kind:

$$\alpha_\theta \delta_{\mathbf{f}} = \delta_{e^{i\theta}\mathbf{f}} \tag{8}$$

cannot be implemented in the representation Π_j, i.e., there does not exist a weakly continuous group of unitaries such that

$$\Pi_{\mathbf{j}}(\alpha_\theta\, \delta_{\mathbf{f}}) = V_\theta \Pi_{\mathbf{j}}(\delta_{\mathbf{f}})\, V_\theta^{-1}. \tag{9}$$

Indeed it is easy to show that the existence of such unitaries would imply that the representations $\Pi_{(1-e^{-i\theta})\mathbf{j}}$ and Π_F are equivalent. Consequently, no infinitestimal generator N of V_θ, i.e., no particle number for the representation Π_j, can be found.[7] All questions concerning measurements connected with the particle number (mean-value, counting probability, etc.) are then meaningless in this representation. This is the ultimate reason why the (incorrect) use of the Fock representation in describing these measurements leads to infrared divergences.

However, it is possible to extract from the state ω_j a noninfrared divergent Fock part. In this way let us define a projector P_Λ such that

$$(P_\Lambda \mathbf{f})(k) = 0 \quad \text{if } |k| < \Lambda$$
$$= \mathbf{f}(k) \text{ if } |k| \geq \Lambda > 0. \tag{10}$$

One can write

$$\omega_{\mathbf{j}}(\delta_{\mathbf{f}}) = \omega_{\mathbf{j}}(\delta_{P_\Lambda \mathbf{f}}) \cdot \omega_{\mathbf{j}}(\delta_{(1-P_\Lambda)\mathbf{f}}). \tag{11}$$

Actually ω_j is the product state $\omega_{\mathbf{j}}^1 \otimes \omega_{\mathbf{j}}^2$, $\omega_{\mathbf{j}}^1$ (resp. $\omega_{\mathbf{j}}^2$) being the restriction of ω_j to $\overline{\Delta(P_\Lambda \mathcal{A}, \sigma)}$ [resp. $\overline{\Delta((1-P_\Lambda)\mathcal{A}, \sigma)}$]. Thus the G—N—S triplet associated with ω_j can be written $(\mathcal{H}_F^1 \otimes \mathcal{H}_F^2, \Pi_{\mathbf{j}}^1 \otimes \Pi_{\mathbf{j}}^2, \Omega^1 \otimes \Omega^2)$, where $(\mathcal{H}_F^i, \Pi_{\mathbf{j}}^i, \Omega^i)$ is the G—N—S triplet associated with $\omega_{\mathbf{j}}^i$ $(i = 1, 2)$. The interesting feature of this decomposition is that the representation $\Pi_{\mathbf{j}}^1$ is a Fock one since the linear form on $P_\Lambda \mathcal{A}$: $P_\Lambda \mathbf{f} \to (P_\Lambda \mathbf{f}, \mathbf{j})$ is now continuous with respect to the norm in $\mathcal{L}$. Thus for any observable A of the form $A_1 \otimes 1_2$, the mean value in the state ω_j: $(\Omega, A\Omega) = (\Omega^1, A_1\Omega^1)$, is simply a

Fock average. Such a situation is in particular encountered in considering the probability p_n^Λ that n photons of arbitrary polarization and momenta greater than Λ ($\Lambda > 0$) and everything with momenta less than Λ is radiated by the current. In this case, the observable to be considered is $A = P_n^\Lambda \otimes 1_2$, where P_n^Λ is the projector onto the subspace of $\mathcal{H}_F^1$ spanned by the n-photons vector states with all momenta greater than Λ. Then

$$p_n^\Lambda = (\Omega^1, P_n^\Lambda \Omega^1) \tag{12}$$

and a standard calculation gives the expected Poisson distribution [1]

$$p_n^\Lambda = \frac{1}{n!}(\bar{n}_\Lambda)^n \exp(-\bar{n}_\Lambda) \tag{13}$$

with

$$\bar{n}_\Lambda = \int_{|\mathbf{k}| \geq \Lambda} \frac{d^3k}{2|\mathbf{k}|} \, \mathbf{j}^*(\mathbf{k}) \cdot \mathbf{j}(\mathbf{k}). \tag{14}$$

This result is evidently not infrared divergent whatever is Λ strictly positive. If Λ is equal to zero, there is no longer a decomposition of ω_j with a Fock component and as already noted the previous calculation is meaningless in the actual representation.

Let us note that the previous analysis and particularly the decomposition (11) is still valid if one starts with an in-Fock vector state different from the vacuum Ω (neither the representation space nor the representation change, only the cyclic vector does); this enables us to construct a scattering operator which admits a product decomposition very similar to the one defined by Reents in his recent paper. [8]

In conclusion, this algebraic approach of the infrared problem for external current is certainly the most natural and economical one. It permits to recover all previous results without introducing a von Neumann's infinite tensor product representation, and, furthermore, it rigourously stresses the fact that the infrared divergence in the Fock representation is nothing but the consequence of the nonexistence of a particle number operator in the actual representation.

*Equipe de Recherche Associée au C.N.R.S.
†Postal Address: Physique Théorique, I.M.S.P., Parc Valrose, 06034 Nice Cedex, France.

[1]See, for example, J.D. Bjorken and S.D. Drell, *Relativistic Quantum Fields* (McGraw-Hill, New York, 1965), p. 202.
[2]V. Chung, Phys. Rev. **140**, B1110 (1965).
[3]T.W.B. Kibble, J. Math. Phys. **9**, 315 (1968).
[4]G. Roepstorff, Comm. Math. Phys. **19**, 301 (1970).
[5]J.P. Provost, F. Rocca, G. Vallée, and M. Sirugue, J. Math. Phys. **15**, 2079 (1974).
[6]J. Manuceau, Ann. Inst. H. Poincaré VIII, 139 (1968).
[7]J.M. Chaiken, Comm. Math. Phys. **8**, 164 (1968).
[8]G. Reents, J. Math. Phys. **15**, 31 (1974).

NUT-like generalization of axisymmetric gravitational fields*

C. Reina and A. Treves

Istituto di Fisica dell'Università di Milano, 20133 Milano, Italy
(Received 5 October 1974)

The complex potential formulation of the axisymmetric problem discussed by Ernst enables us to construct new solutions from a given one, by multiplying the corresponding potential by a unit complex number. This rotation introduces naturally the NUT parameter in the metric. The generalized Kerr, Weyl, and Tomimatsu–Sato solutions are explicity constructed.

I. INTRODUCTION

In 1963 Newman, Tamburino, and Unti[1] found a family of solutions of the Einstein equations, which contains as a special case the Schwarzschild solution. The interest in the NUT fields is mainly mathematical, since the only member of the family which is flat at infinity is the Schwarzschild solution itself.

A generalization of the Kerr field, analogous to that proposed by NUT, was obtained by Demianski and Newman[2] by means of a mathematical trick, involving a complex coordinate transformation.

In this paper it is shown that the complex potential formalism introduced by Ernst[3] leads naturally to the NUT and to the Demianski and Newman solutions, the NUT parameter being related to an arbitrary phase constant in the Ernst potential ξ_0. The generalization can be extended to any axisymmetric solution, and in particular it is given here for the Tomimatsu–Sato field.

II. NUT AND DEMIANSKI-NEWMAN FIELDS

In canonical cylindric coordinates the most general axisymmetric electrovac line element reads[4]

$$ds^2=f^{-1}[e^{2\gamma}(d\rho^2+dz^2)+\rho^2\,d\varphi^2]-f(dt-\omega\,d\varphi)^2, \tag{1}$$

where the potentials f,γ,ω are functions of ρ, z. It was shown by Ernst[3] that the potentials can be derived from a complex function ξ_0, satisfying the equation,

$$(\xi_0\xi_0^*-1)\nabla^2\xi_0=2\xi_0^*\nabla\xi_0\nabla\xi_0, \tag{2}$$

where ∇^2 is the flat space three-dimensional operator. The equations relating f,ω,γ to ξ_0 are

$$f=\mathrm{Re}\frac{\xi_0-1}{\xi_0+1}, \tag{3}$$

$$\nabla\omega=\frac{2\rho}{(\xi_0\xi_0^*-1)^2}\mathrm{Im}[(\xi_0^*-1)^2\hat{n}\times\nabla\xi_0], \tag{4}$$

$$\frac{\partial\gamma}{\partial\rho}=\frac{\rho}{(\xi_0\xi_0^*-1)^2}\left[\frac{\partial\xi_0}{\partial\rho}\frac{\partial\xi_0^*}{\partial\rho}-\frac{\partial\xi_0}{\partial z}\frac{\partial\xi_0^*}{\partial z}\right], \tag{5}$$

$$\frac{\partial\gamma}{\partial z}=\frac{\rho}{(\xi_0\xi_0^*-1)^2}\left[\frac{\partial\xi_0}{\partial\rho}\frac{\partial\xi_0^*}{\partial z}+\frac{\partial\xi_0^*}{\partial\rho}\frac{\partial\xi_0}{\partial z}\right], \tag{6}$$

where $\hat{n}$ is the azimuth direction.

It was noted by Ernst[5] that from a given solution ξ_0 of Eq. (2), one can generate in a number of ways new solutions, which, however, in general are not physically meaningful. In particular we show that the transformation

$$\xi=\exp(i\alpha)\xi_0 \tag{7}$$

yields the NUT and Demianski–Newman fields for ξ_0 corresponding to the Schwarzschild and Kerr solutions respectively.

In prolate spheroidal coordinates (x,y) $[\rho=k(x^2-1)^{1/2}\times(1-y^2)^{1/2}$; $z=kxy$, k being a scale factor] the Kerr solution corresponds to

$$\xi_0=px+iqy,$$

with $p^2+q^2=1$. The transformation (7) together with Eqs. (3) and (4) gives

$$f=1-2\frac{p\cos\alpha x-q\sin\alpha y+1}{(px+1)^2+q^2y^2+2p(\cos\alpha-1)x-2q\sin\alpha y}, \tag{8}$$

$$\omega=-\frac{2k}{p}q\frac{(1-y^2)(q\sin\alpha y-p\cos\alpha x-1)}{p^2x^2+q^2y^2-1}-2\frac{k}{p}\sin\alpha y. \tag{9}$$

Since Eqs. (5) and (6) are independent of α, the potential γ is unchanged by the transformation (7), and therefore,

$$\exp(2\gamma)=(p^2x^2+q^2y^2-1)/p^2(x^2-y^2). \tag{10}$$

By the coordinate transformation

$$x=(r-m)/k,\quad y=\cos\vartheta$$

the metric is mapped into the form

$$\begin{aligned}ds^2=&\frac{r^2+(a\cos\vartheta-l)^2}{r^2-2mr+a^2-l^2}dr^2+[r^2+(a\cos\vartheta-l)^2]\\&\times\left(d\vartheta^2+\frac{r^2-2mr+a^2-l^2}{r^2-2mr+a^2\cos^2\vartheta-l^2}d\varphi^2\right)\\&-\left(1-2\frac{mr+l(l-a\cos\vartheta)}{r^2+(a\cos\vartheta-l)^2}\right)\\&\times\left[dt-\left(\frac{2a\sin^2\vartheta[mr+l(l-a\cos\vartheta)]}{r^2-2mr-l^2+a^2\cos^2\vartheta}-2l\cos\vartheta\right)d\varphi\right]^2,\end{aligned} \tag{11}$$

where m,l, and a are related to p, q, α, and k by

$$k^2=m^2+l^2-a^2,$$

$$p=k/(m^2+l^2)^{1/2},\quad q=a/(m^2+l^2)^{1/2},$$

$$\cos\alpha=m/(m^2+l^2)^{1/2},\quad \sin\alpha=l/(m^2+l^2)^{1/2}.$$

The line element (11) coincides with the Demianski–Newman uncharged metric, which reduces to the usual Boyer and Lindquist form of the Kerr metric for $l=0$ and to the NUT generalization of the Schwarzschild metric for $a=0$.

III. GENERALIZED WEYL AND TOMIMATSU-SATO FIELDS

The transformation (7) can be applied to algebraically general fields as well. We consider the special family of Weyl solutions

$$\xi_0=[(x+1)^\delta+(x-1)^\delta]/[(x+1)^\delta-(x-1)^\delta], \tag{12}$$

which for $\delta=1$ is the Schwarzschild solution and for $\delta=2$, 3, 4 are the static counterparts of the Tomimatsu–Sato solutions.

Applying the transformation (7) and solving for the potentials f, ω, γ, we have

$$f=2(x^2-1)^\delta/[(\cos\alpha+1)(x+1)^{2\delta}+(\cos\alpha-1)(x-1)^{2\delta}], \tag{13}$$

$$\omega=2k\delta\sin\alpha\, y, \tag{14}$$

$$\exp(2\gamma)=(x^2-1)^{\delta^2}/(x^2-y^2)^{\delta^2}. \tag{15}$$

For $\delta=1$ this reduces to the NUT field.

The Tomimatsu–Sato complex potential for $\delta=2$ reads[6]

$$\xi_0=(u+iv)/(m+in),$$

where

$$u=p^2x^4+q^2y^4-1, \quad v=-2pq\times y(x^2-y^2),$$

$$m=2px(x^2-1), \quad n=-2qy(1-y^2).$$

The rotation (7) yields

$$\xi=[\cos\alpha\, u-\sin\alpha\, v+i(\sin\alpha\, u+\cos\alpha\, v)]/(m+in)$$

and therefore

$$f=A_0/B,$$

where

$$A_0=u^2+v^2-m^2-n^2,$$

$$B=B_0+2(\cos\alpha-1)\eta-2\sin\alpha\,\epsilon,$$

$$B_0=(u+m)^2+(v+n)^2,$$

$$\eta=mu+nv, \quad \epsilon=mv-nu.$$

(Hereinafter a subscript 0 indicates the quantities which are unchanged with respect to the Tomimatsu–Sato case.) The potential γ is that given by Tomimatsu–Sato,

$$\exp(2\gamma_0)=A_0/p^4(x^2-y^2)^4.$$

Equations (4) in prolate spheroidal coordinates yield

$$\frac{\partial}{\partial x}(\omega-\cos\alpha\,\omega_0)=-k\frac{(1-y^2)}{A_0^2}\left[2(1-\cos\alpha)\left(\eta\frac{\partial\epsilon}{\partial y}-\epsilon\frac{\partial\eta}{\partial y}\right)+\sin\alpha\left(B_0\frac{\partial\eta}{\partial y}-\eta\frac{\partial B_0}{\partial y}\right)\right], \tag{16}$$

$$\frac{\partial}{\partial y}(\omega-\cos\alpha\,\omega_0)=k\frac{(x^2-1)}{A_0^2}\left[2(1-\cos\alpha)\left(\eta\frac{\partial\epsilon}{\partial x}-\epsilon\frac{\partial\eta}{\partial x}\right)+\sin\alpha\left(B_0\frac{\partial\eta}{\partial x}-\eta\frac{\partial B_0}{\partial x}\right)\right], \tag{17}$$

where ω_0 reads

$$\omega_0=-2mq\frac{(1-y^2)}{A_0}\{p^3x(x^2-1)[2(x^4-1)+(x^3+3)(1-y^2)]+p^2(x^2-1)[4x^2(x^2-1)+(3x^2+1)(1-y^2)]-q^2(px+1)(1-y^2)^3]\}. \tag{18}$$

From Eqs. (16) and (17) it can be easily shown that ω must be of the form,

$$\omega=\cos\alpha\,\omega_0+kq\frac{(1-y^2)}{A_0}[2(\cos\alpha-1)C+\sin\alpha\, D]+h\sin\alpha\, y, \tag{19}$$

where C, D are polynomials of x, y and h is a constant independent of α. The presence of the last term in Eq. (19) and the condition that it must reduce to the form (14) for $q=0$ is sufficient to show that also this metric is not asymptotically flat. It does not seem therefore very interesting to work out the explicit form of ω.

IV. CONCLUSIONS

We have shown that the Ernst formulation of the axisymmetric problem leads directly to the generalizations of Schwarzschild and Kerr fields given originally by NUT and Demianski and Newman. An advantage of this derivation is that it can be extended to algebraically general fields as the Weyl and Tomimatsu–Sato fields.

It is obvious that the method can be applied also to electrovac solutions. In fact, by using the results of Ernst[7] it is clear that, multiplying ξ_0 by a complex number with modulus different from 1, one obtains the charged NUT-like generalization of any given solution.

*Work partially supported by Laboratorio di Fisica Cosmica e Tecnologie Relative del C.N.R., Milano.

[1]E. T. Newman, L. Tamburino, and T. Unti, J. Math. Phys. **4**, 915 (1963).
[2]M. Demanski and E.T. Newman, Bull. Acad. Pol. Sci. **24**, 653 (1966).
[3]F.J. Ernst, Phys. Rev. **167**, 1175 (1968).
[4]A. Papapetrou, Ann. Physik **12**, 309 (1953).
[5]F.J. Ernst, J. Math. Phys. **15**, 1409 (1974).
[6]A. Tomimatsu and H. Sato, Phys. Rev. Lett. **29**, 1344 (1972).
[7]F.J. Ernst, Phys. Rev. **168**, 1415 (1968).

Nonexistence of dissipative structure solutions to Volterra many-species models

Gerald Rosen

Drexel University, Philadelphia, Pennsylvania 19104
(Received 23 September 1974)

Subject to boundary conditions of practical interest, the only temporally periodic solutions that may be admitted by a generic system of Volterra n-species reaction–diffusion equations are spatially uniform solutions, and thus dissipative structures are precluded as solutions to Volterra n-species models.

Considerable interest has been attached to the recent experimental[1] and theoretical[2] studies of "dissipative structures," temporally periodic but spatially nonuniform solutions to certain systems of nonlinear reaction–diffusion equations. The purpose of the present communication is to report a concise proof which shows that a generic Volterra model system,[3] extended in the natural way to include species diffusion, cannot admit a dissipative structure as a solution.

With inclusion of species diffusion, a Volterra n-species model is governed by coupled nonlinear equations of the form

$$\frac{\partial c_i}{\partial t} = D_i \nabla^2 c_i + \left(k_i + \beta_i^{-1} \sum_{j=1}^{n} \alpha_{ij} c_j\right) c_i, \tag{1}$$

where the enumerator index i runs from 1 to n, $c_i = c_i(\mathbf{x}, t)$ denotes the concentration of the ith participating molecular or biological species, D_i is the diffusivity of the ith species, k_i is the (positive or negative) growth rate constant associated with the ith species, $\beta_i^{-1}(>0)$ is the so-called equivalence number of the ith species [the ratio of i's lost (or gained) through encounters per unit time to j's gained (or lost) through encounters being $\beta_i^{-1}/\beta_j^{-1}$], and $\alpha_{ij} \equiv -\alpha_{ji}$ are the (positive, negative, or zero) interaction rate constants which describe how rapidly encounters between the ith and jth species change the local concentration of the ith species. It is assumed that the system (1) admits a constant equilibrium solution with the $c_i = \bar{c}_i \equiv$ (positive constants) satisfying the algebraic equations implied by (1)[4]

$$k_i = -\beta_i^{-1} \sum_{j=1}^{n} \alpha_{ij} \bar{c}_j. \tag{2}$$

For problems of practical interest the Eqs. (1) are required to hold through a spatial region R (one-, two-, or three-dimensional) with either $c_i = \bar{c}_i$ or $\mathbf{n} \cdot \nabla c = 0$ at all points on the boundary of R, where $\mathbf{n}$ denotes a vector normal to the bounding surface; thus, we consider boundary conditions such that

$$(c_i(\mathbf{x}, t) - \bar{c}_i)(\mathbf{n}(\mathbf{x}) \cdot \nabla c_i(\mathbf{x}, t)) = 0 \tag{3}$$

for all $\mathbf{x} \in \partial R$, all $t \geq 0$ and all $i = 1, \ldots, n$.

Suppose that Eqs. (1) subject to (3) admit a temporally periodic solution

$$c_i(\mathbf{x}, t + T) = c_i(\mathbf{x}, t) \tag{4}$$

with the period T a positive constant. Then it follows that the functional

$$\sigma(t) \equiv \int_R \sum_{i=1}^{n} \beta_i [c_i - \bar{c}_i \ln(c_i/\bar{c}_i)]\, d\mathbf{x} \tag{5}$$

must also be a periodic function of t, i.e., $\sigma(t + T) = \sigma(t)$. But Eqs. (1) imply that

$$\frac{d\sigma(t)}{dt} = \int_R \sum_{i=1}^{n} \beta_i (1 - \bar{c}_i c_i^{-1})(\partial c_i/\partial t)\, d\mathbf{x}$$

$$= \int_R \sum_{i=1}^{n} \beta_i (1 - \bar{c}_i c_i^{-1}) D_i \nabla^2 c_i \, d\mathbf{x} \tag{6}$$

in view of the conditions (2) and the antisymmetrical character of the α_{ij}'s.[5] Integrating the final member of (6) by parts and making use of the conditions (3) on the boundary of R, we obtain

$$\frac{d\sigma(t)}{dt} = -\int_R \sum_{i=1}^{n} \beta_i \bar{c}_i D_i c_i^{-2} |\nabla c_i|^2 \, d\mathbf{x} \leq 0, \tag{7}$$

and thus $\sigma(t)$ is monotone-decreasing with time for all t so long as any c_i varies with $\mathbf{x}$. Hence, a Volterra n-species reaction–diffusion system of the form (1) subject to boundary conditions which imply (3) may admit only spatially uniform periodic solutions and cannot admit a dissipative structure.

[1] A. Zaikin and A. Zhabotinsky, Nature **225**, 535 (1970); M. Herschkowitz-Kaufman, Comptes Rendus 270C, 1049 (1970); A.T. Winfree, Science **175**, 634 (1972); A.M. Zhabotinsky and A.N. Zaikin, J. Theor. Biol. **40**, 45 (1973).

[2] P. Glansdorff and I. Prigogine, *Thermodynamic Theory of Structure, Stability and Fluctations* (Wiley, New York, 1971); I. Prigogine and G. Nicolis, Q. Rev. Biophys. **4**, 107 (1971); H.M. Martinez, J. Theor. Biol. **36**, 479 (1972); L.A. Segel and J.L. Jackson, J. Theor. Biol. **37**, 545 (1972); A. Goldbeter and R. Lefever, Biophys. J. **12**, 1302 (1972); G. Rosen, Phys. Lett. **43A**, 349 (1973); **45A**, 263 (1973).

[3] N.S. Goel, S.C. Maitra, and E.W. Montroll, Rev. Mod. Phys. **43**, 231 (1971); F.M. Scudo, Theor. Pop. Biol. **2**, 1 (1971); M.A.B. Deakin, Bull. Math. Biophys. **33**, 571 (1971); E.W. Montroll, Proc. Natl. Acad. Sci. (U.S.A.) **69**, 2532 (1972).

[4] It is well known that the existence of positive $\bar{c}_i$ requires n to be an even integer (Ref. 3).

[5] For the so-called Verhulst modification (Ref. 3) of the Volterra model (characterized by $\alpha_{ij} = -\alpha_{ji}$ for $i \neq j$ and $\alpha_{ii} \leq 0$) the additional nonpositive term $\sum_{i=1}^{n} \alpha_{ii} (c_i - \bar{c}_i)^2$ appears in the integrands in (6) and (7), and therefore dissipative structures are likewise precluded in the case of such a modified Volterra model.

Symmetry of ensembles of maximum entropy

Elihu Lubkin

Department of Physics, The University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201
(Received 9 May 1974; final revised manuscript received 5 September 1974)

There can be only *one* maximally random ensemble in a given convex-closed family of ensembles, because the mixing of several ensembles increases entropy. Hence, if the family is acted on by a group which does not modify randomness (entropy), the thermodynamic ensemble is *invariant*. This is clear only over a finite-dimensional Hilbert space, prior to thermodynamic limits. Hence, in this situation, strictly spontaneous breakdown of symmetry is impossible.

INTRODUCTION

My thesis will be that the literal "spontaneous breakdown of symmetry" is impossible. Nevertheless, a slight bias away from symmetry exogenously imposed may be greatly magnified. My context will be thermodynamic. The single familiar example of ferromagnetism will make the physical point clear, then mathematical argument will make it general and precise.

The ferromagnetic alignment of N spin-$\frac{1}{2}$'s is often cited as an illustration of the spontaneous breakdown of rotational invariance. The aligned "state" has total angular momentum $\frac{1}{2}N$, and hence is $(N+1)$-fold degenerate. [1] The statistical ensemble in which each "z-component" of angular momentum $(-\frac{1}{2}N, -\frac{1}{2}N+1, \ldots, \frac{1}{2}N)$ is equally weighted, a mixed state with entropy $\ln(N+1)$, is however rotationally invariant, and is furthermore the ensemble which has the greatest entropy among all ensembles which can be built from this $(N+1)$-fold degenerate system. [2] A pure state, e.g., the state with z-component of angular momentum $\frac{1}{2}N$, of course has entropy 0. Hence, specifying this rotationally noninvariant oriented state in place of the rotationally invariant mixture involves negentropy [3] or information $\ln(N+1)$, and thus constitutes an exogenous bias. The information *per spin* here is $N^{-1}\ln(N+1)$, which approaches zero as $N \to \infty$: The exogenous bias involved is in this sense slight. In thermodynamic limits, an entropy which like $\ln(N+1)$ is $o(N)$, is dropped or neglected. Hence thermodynamic limits and discussions which set $N=\infty$ tend to obscure the exogeneous source of asymmetry. That is a physical reason why the dimensionality of the system's Hilbert space in the sequel is taken to be finite, and why no attempt is made to battle technical difficulties so as to seek the conclusion in more general cases.

The basic mathematical tool is #4 below: convexity of entropy in quantum statistical mechanics. Inasmuch as the application represents some sort of denial of the very popular notion of broken symmetry, [4] the simple mathematics is set forth in detail. Any correct discussion of breakdown must in some way circumvent this simple mathematics; the "cause" of breakdown is likely to become better understood by examining the point of departure from the present mathematical format.

A second purpose is to show how #4 may be derived from #2, a lemma from measurement theory. The proofs are fortunately so brief that all can be done here. A reader ready to accept #4 may omit #2, #3, and #5.

The usual context for discussions of symmetry breakdown is Lagrangian dynamics. The Lagrangian is invariant under a group G which acts on the dynamical variables, whereas states are discussed which are not G-invariant, most notably a ground or "vacuum" state. (The breakdown of symmetry is often achieved by an explicitly asymmetric "infinitesimal" term added to the Lagrangian; this is of course in line with my comment referring to slight exogenous bias.) The relationship between properties of the Lagrangian and properties of the associated physical system may however be thought too technical to take the symmetry of the Lagranian as a physical symmetry of the system. This philosophical point may be an incidental motivation for studies [5] which seek to find explicitly physical symmetry in solutions at unusual thermodynamic conditions—e.g., high temperature—for systems which show broken symmetry in other conditions, for then the symmetry under G would be more than a merely technical artifact of a Lagrangian.

In my context here there will be no reference to Lagrangians, only to physical states of the system, including mixed states or ensembles. Symmetry under group G is defined by action of G on a set H of ensembles: To each state $P \in H$ and each element $g \in G$, there corresponds a state $gP \in H$. If the orbit $\{gP : g \in G\}$ has more than one element, then P itself is G-asymmetric, which is the context for broken symmetry; otherwise, $gP = P$, $\forall\, g \in G$, and P is G-symmetric.

The specification of a state without exogenous bias I will take to mean the choice of an ensemble with *maximum entropy* consistent with the physical specifications. By the judicious use of reservoirs, this subsumes cases frequently described by minimizing various "free energies." The "physical specifications" of the states will explicitly be barred by assumption from referring to the statistical weights, as follows: Any convex combination (mixture) of states P which meet the physical specifications must also meet the physical specifications. This assumption, introduced as closure of H under convex combination in #8, rules out the dodge of specifying that, e.g., only pure states will be considered, which indeed would find the states (many of them, all of "maximum" entropy zero), asymmetric in the ferromagnetic example. It is also assumed that the group action does not alter entropy. This is most likely to be attained by having G act on pure states, then promoting the action of G to mixtures by requiring it to commute with convex combination.

This argument, already given very briefly in the Abstract, is in essence only this: The homogeneous mixture of all the states in an orbit will at once have maximum entropy and will be G-symmetric. Selecting the other less symmetric states requires accepting less than the maximum entropy, and so constitutes an exogenous introduction of information. The technical development of this idea follows, culminating in the corollary, #8 below.

THE ARGUMENT

#1. *Definition*: Let f be a strongly convex real-valued function on $[0,1]$, i.e., $f((x+y)/2) > \frac{1}{2}f(x) + \frac{1}{2}f(y)$ if $x \neq y$. We will be interested in the f *entropy* of a density matrix P, defined as $\mathrm{Tr}f(P)$.

The case of physical interest is, of course, $f(x) = -x\ln x$. Items #2–5 below are given to establish the basic convexity theorem, #4.

Von Neumann's "process 1" or measurement process increases f entropy[6]:

#2. *Lemma (von Neumann)*: If $(E_1, \ldots, E_n)$ is a list of orthogonal Hermitian projections such that $\sum_i E_i = I$ (the unit matrix) and if $\sum_i E_i P E_i \neq P$, then $\mathrm{Tr}\, f(\sum_i E_i P E_i) > \mathrm{Tr} f(P)$.

#3. *Proof*: Since the $E_i P E_i$ commute, they may be simultaneously diagonalized on an orthonormal basis, $(u_1, u_2, \cdots)$. Let P be diagonal on the orthonormal basis $(v_1, v_2, \cdots)$. The lemma states that the f entropy of the u-basis diagonal part of P exceeds that of P. Indeed, the diagonal element $\langle u_a | P | u_a \rangle = \sum_i \langle u_a | v_i \rangle \rho_i \langle v_i | u_a \rangle = \sum_i |\langle u_a | v_i \rangle|^2 \rho_i$ is a convex combination of the P eigenvalues ρ_i. Hence $f(\langle u_a | P | u_a \rangle) \geqq \sum_i |\langle u_a | v_i \rangle|^2 f(\rho_i)$. Since P is not diagonal on the u basis, it can be shown that at least one $\langle u_a | P | u_a \rangle$ is a nontrivial convex combination of the ρ_i, whence the inequality holds at least once. Hence, $\sum_a f(\langle u_a | P | u_a \rangle) > \sum_i f(\rho_i) \sum_a \langle v_i | u_a \rangle \langle u_a | v_i \rangle = \sum_i f(\rho_i)$. QED

#4 *Theorem (Convexity of entropy)*: If P, Σ are nonnegative Hermitian matrices, $0 \leqq P \leqq 1$, $0 \leqq \Sigma \leqq 1$, and $P \neq \Sigma$, then $\mathrm{Tr}\, f((P+\Sigma)/2) > \frac{1}{2}\mathrm{Tr} f(P) + \frac{1}{2}\mathrm{Tr} f(\Sigma)$.

#5. *Proof*: If $P\Sigma = \Sigma P$, diagonalize: $P = \mathrm{diag}(\rho_1, \rho_2, \cdots)$, $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \cdots)$, with $\rho_i \neq \sigma_i$ for at least one i. Then the result follows by summing $f((\rho_i + \sigma_i)/2) \geqq \frac{1}{2} f(\rho_i) + \frac{1}{2} f(\sigma_i)$, with the inequality holding at least once. This establishes the commutative case.

If $P\Sigma \neq \Sigma P$, let $(E_1, E_2, \cdots)$ be a list of one-dimensional orthogonal Hermitian projections with $\sum_i E_i = I$, which diagonalizes $(P+\Sigma)/2$. Thus

$$\frac{P+\Sigma}{2} = \sum_i \frac{E_i P E_i + E_i \Sigma E_i}{2}.$$

Then

$$\mathrm{Tr}\, f\left(\frac{P+\Sigma}{2}\right)$$

$$= \mathrm{Tr}\, f\left(\tfrac{1}{2}\sum_i E_i P E_i + \tfrac{1}{2}\sum_i E_i \Sigma E_i\right) \geqq \tfrac{1}{2}\mathrm{Tr}\, f\left(\sum E_i P E_i\right) + \tfrac{1}{2}\mathrm{Tr}\, f\left(\sum_i E_i \Sigma E_i\right)$$

follows from the commutative case, since $\sum_i E_i P E_i$ and $\sum_i E_i \Sigma E_i$ commute. Furthermore, $P \to \sum_i E_i P E_i$ is a von Neumann measurement process, and $P \neq \sum_i E_i P E_i$; otherwise, P and $(P+\Sigma)/2$ would commute, contradicting $P\Sigma \neq \Sigma P$. Hence $\mathrm{Tr}\, f(P) < \mathrm{Tr} f(\sum_i E_i P E_i)$. Similarly, $\mathrm{Tr} f(\Sigma) < \mathrm{Tr} f(\sum_i E_i \Sigma E_i)$. Hence $\mathrm{Tr}\, f((P+\Sigma)/2) > \frac{1}{2}\mathrm{Tr} f(P) + \frac{1}{2}\mathrm{Tr} f(\Sigma)$. QED

The physical point related to the impossibility of symmetry breakdown without even slight exogeneous bias is now easily achieved through a series of obvious corollaries.

#6. *Corollary of* #4: P, Σ as before, $P \neq \Sigma$. If $\mathrm{Tr}\, f(P) = \mathrm{Tr}\, f(\Sigma) = S_0$, then $\mathrm{Tr}\, f((P+\Sigma)/2) > S_0$.

#7. *Corollary of* #6: In any set of ensembles closed under convex combination, there can be no more than one of maximum f entropy.

#8. *Corollary of* #7 (*Symmetry of the ensemble of maximum entropy*): Let H be a set of ensembles closed under a "symmetry group" G and under convex combination; i.e., there is a group G whose elements g act on the H ensembles, $gP \subset H$ for every $g \subset G$ and $P \subset H$, and any convex combination of elements of H belongs to H. Furthermore, let the f entropy be preserved by these G transformations. Then the ensemble P_0 of maximum f entropy is G-symmetric, i.e., $gP_0 = P_0$ for all $g \subset G$.

POSSIBLE FUTURE DEVELOPMENTS RELATED TO MEASUREMENT THEORY

The introduction of a small biasing term in the Lagrangian is a generally familiar device for producing breakdown. Here, other devices, which may seem more deserving of the qualification "spontaneous," are suggested.

The most obvious device, but one which may be difficult to use, is to explore all ensembles at a fixed small nonzero negentropy from the equilibrium ensemble. In such an approach information would be acknowledged, yet without specifying the nature of the bias.

The ferromagnetic example suggests a description in terms of easy polarizability or of long-range correlation. More generally, one may explore correlations between two successive measurements. This suggests that appropriate intrinsic "quadratic" matrix elements be related to the breaking of symmetry by an exogenous bias.

The topic of breakdown of symmetry is commonly introduced by noting that in the ferromagnetic example the alignment is automatically evident to an observer

living within the sample, without any imposed bias. Yet discussions of Maxwell's demon show that internal observers may not function without some negentropy. [3]

ACKNOWLEDGMENT

I wish to acknowledge advice of Dale Snider in improving the exposition. The referee has provided further bibliography [7,8,9] on convexity of entropy, and points out that convexity of f entropy is stated without proof in Ref. 6 (see p. 390).

[1] $\hbar = 1$.
[2] Boltzmann's $k = 1$.

[3] Leon Brillouin, *Science and Information Theory* (Academic, New York, 1956).

[4] In order not to spread confusion I should add that the slight biases away from symmetry exogenously introduced which generate breakdowns of symmetry are indeed a feature of the numerous treatments of symmetry breakdown found elsewhere, which are therefore *not* generally in contradiction with the present paper.

[5] Steven Weinberg, Rev. Mod. Phys. 46, 255 (1974), and references there, especially in Sec. 3, p. 274.
[6] John von Neumann, *Mathematical Foundations of Quantum Mechanics*, translated by R. Beyer (Princeton U. P., Princeton, 1955).
[7] I. E. Segal, J. Math. Mech. 9, 623 (1960).
[8] C. Davis, Proc. Japan Acad. 37, 533 (1961).
[9] D. Ruelle, *Statistical Mechanics: Rigorous Results* (Benjamin, New York, 1969), Proposition 2.5.2.

N-variable rational approximants and method of moments*

C. Alabiso† and P. Butera‡

Stanford Linear Accelerator Center, Stanford University, Stanford, California 94306
(Received 19 August 1974; revised manuscript received 4 October 1974)

The method of moments is applied to pairs of linear permutable self-adjoint operators A and B in a Hilbert space $\mathcal{H}$. An approximate expression for the diagonal matrix elements of the operator $(1 - wA - zB)^{-1}$, where w, z are complex numbers, is taken as a guide to the definition of rational approximants from general formal power series in two variables. Starting from an operator convergence theorem in a certain Hilbert space, we prove the convergence of our approximants to analytic functions of two complex variables with the integral representation $G(w,z) = \int\int d\sigma(\alpha,\beta) / (1 - w\alpha - z\beta)$, under suitable restrictions on the positive measure $\sigma(\alpha,\beta)$. The same approximation scheme can also be applied to the diagonal matrix elements of the operator $[(1 - wA)(1 - zB)]^{-1}$, leading to a different rational approximant which we prove to converge to functions with the integral representation $\tilde{G}(w,z) = \int\int d\sigma(\alpha,\beta) / (1 - w\alpha)(1 - z\beta)$. In both cases the convergence is uniform on appropriate compact subsets of $\mathbf{C}^2$. The extension to the n-dimensional case is straightforward for both approximants. The connections with a standard variational principle are also briefly discussed.

I. INTRODUCTION

In the past few years the technique of Padé approximants (PA's)[1-3] for the approximate summation of power series of one complex variable has been looked at with some interest by physicists as an effective tool for many quantum mechanical and field-theoretic models whose solutions are only available in the form of a perturbative series. We recall that, given the formal power series $f(z) \approx \sum_n f_n z^n$, the $[N/M](z)$ PA is the rational function $P_N(z)/Q_M(z)$, where $P_N(z)$ and $Q_M(z)$ are polynomials of degree N and M, respectively, such that $P_N(z)/Q_M(z) = \sum_{n=0}^{N+M} f_n z^n + O(z^{N+M+1})$. A simple closed expression is available for the $[N/M](z)$ PA and it can be shown that the PA's have some significant formal properties, e.g., if $N = M$ they are invariant under homographical transformations both of the variable and of the function. The PA's converge uniformly on compact sets to extended Stieltjes functions, i.e., the functions $g(z)$ of the form $g(z) = \int_{-\infty}^{\infty} d\sigma(t)/1 - zt$ where $\sigma(t)$ is a positive measure with finite moments $\mu_n = \int_{-\infty}^{\infty} t^n d\sigma(t)$ not too fastly increasing with n; moreover, in a suitably generalized sense, they converge to meromorphic functions.[4] Unfortunately, the extension to the multidimensional case is not straightforward. In fact, the simplest generalization of the usual definition of the PA's, even in the case of two variables only, does not, in general, determine uniquely a rational approximant: additional constraints must be provided. To this problem, very interesting alternative solutions have been recently proposed. In one of these[5,6] the constraints are chosen in such a way that the many variable approximants retain the main formal properties of the usual PA's. In spite of this the study of the convergence properties is not easy and, up to now, only generalizations of de Montessus theorem are available.[7] For another kind of approximant[8] the convergence to holomorphic functions has been proved under the stringent assumption of uniform boundedness of the approximants themselves.

In this paper, we would like to indicate a different approach to the construction of many-variable rational approximants starting from the following remarks. Consider a linear self-adjoint operator A and a vector f on a Hilbert space $\mathcal{H}$. Let $\sum_{n=0}^{\infty} z^n (f, A^n f)$ be the Neumann expansion (not necessarily convergent) of the diagonal matrix element $(f, (1 - zA)^{-1} f)$. Then, for every $N \geq 0$, the $[N/N+1](z)$ PA for this series coincides (a) with the matrix element $(f, (1 - zA_N)^{-1} f)$ where A_N is the $(N+1)$-rank operator obtained at the Nth order in the approximation scheme known as the method of moments[9,10]; (b) with the stationary value of an appropriate functional on a certain finite-dimensional subspace of $\mathcal{H}$.[11] Therefore, we suggest generalizing the PA to the multidimensional case by starting from the definition in terms of the method of moments rather than from the usual definition; more precisely, we suggest that the direct extension of the method of moments to the operator $(1 - wA - zB)^{-1}$ with A and B linear self-adjoint permutable operators should be taken as a guide to the definition and justification of two variable rational approximants. As a result, although some formal properties of the usual PA's are lacking, we still have the same connection with the method of moments (and the variational method). This enables us to give, for a relevant class of functions, a convergence proof which is both simple and of practical use since it involves only assumptions about the analytic properties of the functions to be approximated rather than about the behavior of the approximants themselves. Furthermore, our approximants have a simple explicit expression in any order of approximation.

We shall not study here any application of our approximation scheme, but let us just remark that a natural field of application should be the approximate summation of the perturbative solution of quantum mechanical and field-theoretic models with more than one coupling constant. However, whether the physically interesting models fulfill all the requirements of our convergence theorem, is a question which requires further study. It is also worth mentioning that there are classical special functions which, for a particular choice of some of the defining parameters, have the integral representation required in our convergence proofs, i.e., the two-variable Appel hypergeometric functions and their n-

variable generalizations, the Lauricella functions.[12] The numerical computation of such functions is therefore another possible application of our approximation procedure which, in this case, provides a direct generalization of the classical Jacobi continued fraction expansion of the Gauss hypergeometric function ${}_2F_1(1, \beta, \gamma, z)$.

In Sec. II we consider the method of moments for a pair of self-adjoint permutable operators A and B and we give the "approximate" expression for the matrix element $(f, (1 - wA - zB)^{-1}f)$ where f is a suitable vector of the Hilbert space. From this we obtain a rational expression which can be associated with any double power series. In Sec. III we prove a convergence theorem for operators in a Hilbert space and we use this result to state in Sec. IV a convergence theorem of our approximants to functions of two complex variables with a well-defined analytic structure. In Sec. V we present the trivial extension to the n-dimensional case; the connection with a standard variational principle; and another kind of approximant, suggested by the application of the method of moments to the operator $[(1 - wA)(1 - zB)]^{-1}$.

II. THE METHOD OF MOMENTS

Let A and B be two linear self-adjoint permutable operators with domains $\mathcal{D}(A)$ and $\mathcal{D}(B)$ in the Hilbert space $\mathcal{H}$. Then there exists a dense subset $\mathcal{Q}$ of vectors of $\mathcal{H}$ which are quasi-analytic[13,14] for both A and B. Let $f \in \mathcal{Q}$[15] be such that

$$f_{p-q,q} = A^{p-q}B^q f, \quad p = 0, \cdots, N, \quad q = 0, \cdots, p, \tag{1}$$

are linearly independent vectors for any N. Then, the vectors $\{f_{r,s}\}$ generate a sequence of $[(N+1)(N+2)/2]$-dimensional Hilbert spaces $\mathcal{H}_N \subseteq \mathcal{H}$ and the related orthogonal projection operators P_N. Let us consider the equation

$$(1 - wA - zB)\psi = f \tag{2}$$

where w and z are complex numbers. For any $\{w, z\}$ such that the operator $R(w, z) \equiv (1 - wA - zB)^{-1}$ exists and is bounded, the solution of Eq. (2) is

$$\psi = R(w, z)f. \tag{3}$$

In order to obtain an approximate solution of Eq. (2), let us consider the following equation in the finite-dimensional subspace $\mathcal{H}_N$:

$$(1 - wA_N - zB_N)\psi_N = f \tag{4}$$

where

$$A_N \equiv P_N A P_N, \quad B_N \equiv P_N B P_N. \tag{5}$$

The solution of Eq. (4) is

$$\psi_N = (1 - wA_N - zB_N)^{-1}f \equiv R_N(w, z)f \tag{6}$$

for $\{w, z\}$ such that $R_N(w, z)$ exists and is bounded. Since $\psi_N \in \mathcal{H}_N$ we can also solve Eq. (4) explicitly by expanding ψ_N on the complete set $\{f_{r,s}\}$:

$$\psi_N = \sum_{p=0}^{N}\sum_{q=0}^{p} a_{p,q} f_{p-q,q}. \tag{7}$$

By substituting (7) into Eq. (4) and then taking the scalar product of both sides successively with $f_{r-s,s}$ ($r = 0, 1, \cdots N; s = 0, 1, \cdots r$), we arrive at a system of linear equations for the $a_{p,q}$ and finally we obtain

$$\psi_N = \sum_{p=0}^{N}\sum_{q=0}^{p}\sum_{r=0}^{N}\sum_{s=0}^{r} (M_N^{-1})_{p,q;r,s} F_{r-s,s} A^{p-q}B^q f, \tag{8}$$

where

$$F_{r-s,s} \equiv (f, A^{r-s}B^s f), \tag{9}$$

$$(M_N)_{p,q;r,s} \equiv F_{p+r-q-s,q+s} - wF_{p+r+1-q-s,q+s} - zF_{p+r-q-s,q+s+1},$$

$$p, r = 0, \cdots, N, \quad q = 0, \cdots, p, \quad s = 0, \cdots, r.$$

If we project Eq. (8) on the vector f we obtain the simple expression

$$(f, \psi_N) = (f, R_N(w, z)f) = \sum_{p=0}^{N}\sum_{q=0}^{p}\sum_{r=0}^{N}\sum_{s=0}^{r} F_{p-q,q}(M_N^{-1})_{p,q;r,s}F_{r-s,s}$$
$$\equiv F_N^T M_N^{-1} F_N \tag{10}$$

with obvious definitions for the column matrix F_N, its transpose F_N^T, and the matrix M_N. The corresponding matrix element of the operator $R(w, z)$ has the integral representation

$$(f, R(w, z)f) = \iint \frac{d(f, E(\alpha, \beta)f)}{1 - w\alpha - z\beta} \tag{11}$$

where $E(\alpha, \beta)$ is the spectral family associated with the self-adjoint permutable operators A and B.

In Sec. III we prove the strong convergence of $R_N(w, z)$ to $R(w, z)$ in a subspace of $\mathcal{H}$ for $\{w, z\}$ in a suitable domain and, as a consequence, the convergence of ψ_N to ψ and of (f, ψ_N) to (f, ψ). Since in the latter case we have a rational approximation converging to an analytic function of two complex variables, we are naturally led to introduce for any formal double power series

$$G(w, z) = \sum_{m,n} \binom{m+n}{m} G_{m,n} w^m z^n \tag{12}$$

the rational approximant $G_N(w, z)$ by the formula

$$G_N(w, z) \equiv G_N^T Q_N^{-1} G_N \tag{13}$$

where G_N, G_N^T and Q_N are a column matrix, its transpose, and a matrix defined in terms of the coefficients $G_{m,n}$ by

$$(G_N)_{p,q} \equiv G_{p-q,q},$$

$$(Q_N)_{p,q;r,s} \equiv G_{p+r-q-s,q+s} - wG_{p+r+1-q-s,q+s} - zG_{p+r-q-s,q+s+1}, \tag{14}$$

$$p, r = 0, \ldots, N, \quad q = 0, \ldots, p, \quad s = 0, \ldots, r.$$

Let us write explicitly $G_0(w, z)$ and $G_1(w, z)$:

$$G_0(w, z) = \frac{G_{0,0}G_{0,0}}{G_{0,0} - wG_{1,0} - zG_{0,1}},$$

$$G_1(w, z) = \frac{\begin{vmatrix} G_{0,0} & G_{1,0} & G_{0,1} \\ G_{1,0} & G_{2,0} & G_{1,1} \\ G_{0,1} & G_{1,1} & G_{0,2} \end{vmatrix}}{G_{0,0}G_{1,0}G_{0,1}} \begin{vmatrix} G_{0,0} - wG_{1,0} - zG_{0,1} & G_{1,0} - wG_{2,0} - zG_{1,1} & G_{0,1} - wG_{1,1} - zG_{0,2} \\ G_{1,0} - wG_{2,0} - zG_{1,1} & G_{2,0} - wG_{3,0} - zG_{2,1} & G_{1,1} - wG_{2,1} - zG_{1,2} \\ G_{0,1} - wG_{1,1} - zG_{0,2} & G_{1,1} - wG_{2,1} - zG_{1,2} & G_{0,2} - wG_{1,2} - zG_{0,3} \end{vmatrix}^{-1} \begin{vmatrix} G_{0,0} \\ G_{1,0} \\ G_{0,1} \end{vmatrix}. \tag{15}$$

It is convenient to notice that this rational approximant has some obvious formal properties, e.g., $G_N(w, z)$ is real analytic if $G(w, z)$ is a real analytic function of w and z and it is symmetric in w and z if $G(w, z)$ is. One may also notice that the approximant to a factorized function does not in general factorize and that no simple analog of the homographical covariance properties of the Padé approximant seems to hold.

Finally, it remains to be investigated whether the $G_N(w, z)$ might also be defined by matching their power expansion to that of $G(w, z)$ according to some definite prescription.

III. SOME RESULTS ON OPERATOR CONVERGENCE

In this section we shall extend some results of Refs. 9 and 10 where the case of a single self-adjoint operator has been studied. Let $\mathcal{L}_f$ be the linear manifold of all finite linear combinations of the vectors $\{f_{r,s}\}$ defined in Sec. II. The closure of $\mathcal{L}_f$ is a Hilbert space $\mathcal{H}_f \subseteq \mathcal{H}$.[16] Consider now the restrictions A' and B' of the operators A and B to $\mathcal{L}_f$ and their closures $\bar{A}'$ and $\bar{B}'$. Since f is assumed to be a quasi-analytic vector for both A and B then, by the Theorems 4 and 6 of Ref. 13, $\bar{A}'$ and $\bar{B}'$ are still self-adjoint permutable operators on $\mathcal{H}_f$, and from now on we shall simply call them A and B. These operators and the related ones $A_N \equiv P_N A P_N$ and $B_N \equiv P_N B P_N$ define in $\mathcal{H}_f$ the operators $T(w, z) \equiv wA + zB$, $T_N(w, z) \equiv P_N T(w, z) P_N$, $R(w, z) \equiv (1 - T(w, z))^{-1}$, $R_N(w, z) \equiv (1 - T_N(w, z))^{-1}$ where $\{w, z\} \in \mathbb{C}^2$ is a pair of complex numbers. For simplicity we shall occasionally drop the $\{w, z\}$ dependence from our operators. Let us also stress that, throughout the paper, by operator convergence we shall always mean strong operator convergence. T is a normal maximal operator and, since it is closed,[17] it is the closure of the operator $wA' + zB'$. T_N is a bounded operator and, in general, it is not normal.

In order to prove that $R_N(w, z)$ converges to $R(w, z)$ on $\mathcal{H}_f$ we need some information on the behavior of $T_N(w, z)$ as $N \to \infty$, which is given by the following:

Theorem 1: $T_N(w, z) \to T(w, z)$ in $\mathcal{L}_f$, uniformly with respect to $\{w, z\}$.

Proof: Any vector $g \in \mathcal{L}_f$ can be written as $g = \sum_{m=0}^{M} \sum_{n=0}^{m} a_{mn} A^{m-n} B^n f$. If $N \geq M + 1$ then $T_N(w, z) g \equiv P_N (wA + zB) P_N g = (wA + zB) g = T(w, z) g$. Of course the convergence is uniform with respect to $\{w, z\}$.

Let us now recall that $\overline{\Theta(O)}$, the closure of the numerical range[18] of a linear bounded operator O is a convex set containing the spectrum $\sigma(O)$ of O.[19] If O is a normal maximal operator (not necessarily bounded) $\overline{\Theta(O)}$ is the convex hull of $\sigma(O)$, i.e., $\overline{\Theta(O)}$ is the smallest closed convex set containing $\sigma(O)$.[20] Theorem 1 and the following theorem enable us to prove that $R_N(w, z) \to R(w, z)$ in $\mathcal{L}_f$.

Theorem 2: For all $\{w, z\}$ such that the point 1 is at a positive distance d from $\overline{\Theta(T(w, z))}$, $R(w, z)$ and $R_N(w, z)$ exist as bounded operators and satisfy the bounds $\|R(w, z)\| \leq d^{-1}$, $\|R_N(w, z)\| \leq \delta^{-1}$ where $\delta^{-1} \equiv \max\{1, d^{-1}\}$.

Proof: Since $\overline{\Theta(T(w, z))}$ is the closed convex hull of the spectrum of a normal maximal operator, the point 1 is at least at a distance d from the spectrum itself, and therefore the operator $R(w, z)$ exists and is bounded. If $g \neq 0$ then $R(w, z) g \neq 0$ and we can consider the normalized vector $h = R(w, z) g / \|R(w, z) g\|$. By assumption

$$0 < d \leq |(h, T(w, z) h) - 1| = \frac{|(R(w, z) g, g)|}{\|R(w, z) g\|^2} \leq \frac{\|g\|}{\|R(w, z) g\|},$$

Therefore, $\|R(w, z)\| \leq d^{-1}$. A similar result also obtains for $R_N(w, z)$ from the remark that $|(h, R_N(w, z) h)| \leq \|R_N'(w, z)\| \|h_N\|^2 + \|h_\perp\|^2$ where $R_N'(w, z)$ is the restriction of $R_N(w, z)$ to $\mathcal{H}_N$, $\|h\| = 1$, $h_N \equiv P_N h$, and $h_\perp \equiv (1 - P_N) h$. Since $\Theta_N(T_N) \subseteq \Theta(T)$, where $\Theta_N(T_N)$ is the numerical range of T_N in $\mathcal{H}_N$, then $\|R_N'(w, z)\| \leq d^{-1}$. Therefore, $\|R_N(w, z)\| \leq \delta^{-1} = \max\{1, d^{-1}\}$.

Next, a lemma will be used to extend the convergence from $\mathcal{L}_f$ to the whole space $\mathcal{H}_f$.

Lemma 1: Let $O(w, z)$ be a linear bounded operator defined on a Hilbert space $\mathcal{H}$ and depending on the two complex variables $\{w, z\}$. Let $\{O_N(w, z)\}$ be a sequence of such operators, uniformly bounded with respect to N. If, for a given $\{w, z\}$, $O_N(w, z) \to O(w, z)$ on $\mathcal{S}(w, z)$ where $\mathcal{S}(w, z)$ is a dense subset of $\mathcal{H}$, then $O_N(w, z) \to O(w, z)$ also on $\mathcal{H}$. If, for all $\{w, z\}$ in a domain $\Delta \subset \mathbb{C}^2$, (a) $O(w, z)$ and $\{O_N(w, z)\}$ are uniformly bounded, (b) $\mathcal{S} \equiv \mathcal{S}(w, z)$ does not depend on $\{w, z\}$, (c) $O_N(w, z) \to O(w, z)$ on $\mathcal{S}$ uniformly in Δ, then $O_N(w, z) \to O(w, z)$ on $\mathcal{H}$ uniformly in Δ.

Proof: Consider a fixed $\{w, z\}$. Then for all $g \in \mathcal{H}$ there exists a sequence $\{g_n\} \in \mathcal{S}(w, z)$ such that $g_n \to g$. Therefore,

$$\begin{aligned}\|(O_N(w, z) - O(w, z)) g\| &\leq \|O_N(w, z)(g - g_n)\| \\ &+ \|O(w, z)(g - g_n)\| + \|(O_N(w, z) - O(w, z)) g_n\| \\ &\leq 2M(w, z)\|g - g_n\| + \|(O_N(w, z) - O(w, z)) g_n\|,\end{aligned}$$

where $\|O(w, z)\| \leq M(w, z)$, $\|O_N(w, z)\| \leq M(w, z)$ for all N. Let us fix n_ϵ in such a way that $\|g - g_{n_\epsilon}\| \leq \epsilon / 4M(w, z)$. Since $g_{n_\epsilon} \in \mathcal{S}(w, z)$ and $O_N(w, z) \to O(w, z)$ in $\mathcal{S}(w, z)$, we can choose $N_\epsilon(w, z)$ such that $\|(O_N(w, z) - O(w, z)) g_{n_\epsilon}\| < \epsilon/2$ for all $N > N_\epsilon(w, z)$. Then the first part of the theorem follows. If, for $\{w, z\} \subset \Delta$, the operators are uniformly bounded, the set $\mathcal{S} \equiv \mathcal{S}(w, z)$ does not depend on $\{w, z\}$ and the convergence is uniform on $\mathcal{S}$, then M, n_ϵ, and N_ϵ do not depend on $\{w, z\}$ and the convergence is uniform on Δ.

Before applying Lemma 1 to our case we need the following:

Lemma 2: If $1 \in \rho(T(w, z))$, where $\rho(T(w, z))$ is the resolvent set of $T(w, z)$, then $\mathcal{S}_f(w, z) \equiv (1 - T(w, z)) \mathcal{L}_f$ is a dense linear manifold of $\mathcal{H}$. Moreover, for any finite $\{w, z\}$ and $\{w', z'\}$ such that $1 \in \rho(T(w, z))$ and $1 \subset \rho(T(w', z'))$, $\mathcal{S}_f(w, z)$ coincides with $\mathcal{S}_f(w', z')$.

Proof: By assumption $(1 - T(w, z))^{-1}$ exists as a bounded operator on $\mathcal{H}_f$. Therefore, any vector $h \in \mathcal{H}_f$ can be written as $h = (1 - T) g$ with $g = (1 - T)^{-1} h$. Since $\mathcal{L}_f$ is dense in $\mathcal{H}_f$ and T is the closure of an operator with do-

main $\mathcal{L}_f$, there exists a sequence $g_n \to g$ with $g_n \in \mathcal{L}_f$ such that $h_n = (1 - T)g_n \to h$. The second part of the theorem is proved by a direct check that any vector in $\mathcal{S}_f(w, z)$ also belongs to $\mathcal{S}_f(w', z')$ and vice versa.

We can now state the main theorem.

Theorem 3: Let Δ be a domain of C^2 such that the point 1 is at a positive distance d from $\Theta(T(w, z))$. Then, for $\{w, z\} \in \Delta$, $R_N(w, z)$ converges strongly to $R(w, z)$ on $\mathcal{H}_f$, uniformly on any bounded subset $\Gamma \subset \Delta$.

Proof: For a fixed $\{w, z\} \in \Delta$, let $R(w, z)g$ be in $\mathcal{L}_f$:

$$\|(R_N(w, z) - R(w, z))g\| = \|R_N(w, z)(T_N(w, z) - T(w, z))R(w, z)g\|$$
$$\leq \|R_N(w, z)\| \|(T_N(w, z) - T(w, z))R(w, z)g\|.$$

From Theorem 1 we have that $T_N \to T$ in $\mathcal{L}_f$ and from Theorem 2 that $\|R_N(w, z)\| \leq \delta^{-1}$. Therefore, $R_N(w, z) \to R(w, z)$ on $\mathcal{S}_f(w, z) \equiv (1 - T(w, z))\mathcal{L}_f$. Since, by Lemma 2, $\mathcal{S}_f(w, z)$ is dense in $\mathcal{H}_f$, it follows that $R_N(w, z) \to R(w, z)$ on $\mathcal{H}_f$. To prove uniform convergence let us remark that $T_N(w, z) \to T(w, z)$ uniformly with respect to $\{w, z\}$ and that, for $\{w, z\} \in \Gamma$, $\mathcal{S}_f \equiv \mathcal{S}(w, z)$ does not depend on $\{w, z\}$. It follows that $R_N(w, z) \to R(w, z)$ in $\mathcal{S}_f$, uniformly in Γ. By Lemma 1 we conclude that $R_N(w, z) \to R(w, z)$ on the whole $\mathcal{H}_f$, uniformly in Γ.

IV. CONVERGENCE OF APPROXIMANTS FOR DOUBLE POWER SERIES

In Sec. II convergence theorems have been formulated for operators in an abstract Hilbert space. Let us now turn our attention to the approximant $G_N(w, z)$ defined by Eq. (13) starting from the formal double power series (12) associated to a function of two complex variables $G(w, z)$. Under suitable hypotheses we can prove the convergence of $G_N(w, z)$ to $G(w, z)$, by reducing the problem to the Hilbert space problem considered in Sec. III.

For this purpose let us restrict to the class of functions with the following representation in some domain of C^2

$$G(w, z) = \int\int \frac{d\sigma(\alpha, \beta)}{1 - w\alpha - z\beta}, \tag{16}$$

where $\sigma(\alpha, \beta)$ is a bounded positive Radon measure in R^2 and the formal (not necessarily convergent) double power series expansion

$$G(w, z) \approx \sum_{n,n} \binom{m+n}{n} G_{m,n} w^m z^n \tag{17}$$

exists, i.e., the moments $G_{m,n} = \int\int \alpha^m \beta^n d\sigma(\alpha, \beta)$ are finite. The class of functions with the integral representation (16) may be considered as one possible generalization of the extended Stieltjes functions to the case of two variables.

Let us define the subset $\Theta_\sigma(w, z)$ of the complex t-plane

$$\Theta_\sigma(w, z) \equiv \{t \equiv w\alpha + z\beta \,|\, \{\alpha, \beta\} \in \Sigma_\sigma\} \tag{18}$$

where Σ_σ is the convex hull of the support of $\sigma(\alpha, \beta)$ in R^2. We can state now the following convergence theorem for the approximants $G_N(w, z)$ defined by Eq. (13):

Theorem 4: Let Δ be a domain of C^2 such that the point 1 is at positive distance d from $\overline{\Theta_\sigma(w, z)}$. If $\sum_{m=0}^{\infty} (G_{2m,0})^{-1/2m} = \infty$, $\sum_{n=0}^{\infty} (G_{0,2n})^{-1/2n} = \infty$, and $\{w, z\} \in \Delta$, then $G_N(w, z)$ converges to $G(w, z)$ as $N \to \infty$. The convergence is uniform in any bounded subset $\Gamma \subset \Delta$.

Proof: Let $\mathcal{L}_2(R^2, \sigma)$ be the Hilbert space of the functions on R^2, square integrable with the measure $\sigma(\alpha, \beta)$. Consider the multiplication operators $\hat{\alpha}$ and $\hat{\beta}$ defined by $\hat{\alpha}g(\alpha, \beta) \equiv \alpha g(\alpha, \beta)$ and $\hat{\beta}g(\alpha, \beta) \equiv \beta g(\alpha, \beta)$. They are self-adjoint permutable operators in $\mathcal{L}_2(R^2, \sigma)$ and the constant vector $u(\alpha, \beta) \equiv 1$ is quasi-analytic for both $\hat{\alpha}$ and $\hat{\beta}$ by assumption, since $\|\hat{\alpha}^m \hat{\beta}^n u\|_\sigma^2 = \int\int \alpha^{2m} \beta^{2n} d\sigma(\alpha, \beta) = G_{2m,2n}$. Therefore, the operators $\hat{\alpha}$ and $\hat{\beta}$ and the vector $u(\alpha, \beta)$ satisfy the same hypotheses as A, B, and f considered in Sec. III. Clearly, $G(w, z) = (u, (1 - w\hat{\alpha} - z\hat{\beta})^{-1}u)_\sigma$ and $G_N(w, z) = (u, (1 - w\hat{\alpha}_N - z\hat{\beta}_N)^{-1}u)_\sigma$, where $\hat{\alpha}_N$ and $\hat{\beta}_N$ are defined like A_N and B_N by Eq. (5). Furthermore, it is easy to see that $\overline{\Theta_\sigma(w, z)} \equiv \overline{\Theta(w\hat{\alpha} + z\hat{\beta})}$ and the theorem follows from Theorem 3.

Instead of assuming the integral representation (16), we could as well start from the series (17). In this case sufficient conditions for the double sequence $\{G_{m,n}\}$ to be a determined moment double sequence have been given in Theorem 10 of Ref. 13. $\{G_{n,m}\}$ must satisfy a certain positivity condition and both the sequences $\{G_{m,0}\}$ and $\{G_{0,n}\}$ must satisfy the Carleman criterion: $\sum_{m=0}^{\infty} (G_{2m,0})^{-1/2m} = \infty$ and $\sum_{n=0}^{\infty} (G_{0,2n})^{-1/2n} = \infty$. Since the positivity condition is necessary for $\{G_{m,n}\}$ to be a moment sequence, the two starting points are equivalent.

V. GENERALIZATIONS AND FINAL REMARKS

The extension of our results to any number of self-adjoint permutable operators $A_1, A_2, \cdots, A_p$ is straightforward. The operator $T^{(p)} = z_1 A_1 + z_2 A_2 + \cdots + z_p A_p$ is still normal maximal and we can repeat all the considerations of Sec. III, ending up with convergence theorems which generalize Theorem 3. The structure of the matrix element $(f, R_N(z_1, z_2, \cdots, z_p)f)$ still suggests an approximation scheme which can be used for any function of p complex variables given by its formal multiple power series expansion

$$G(z_1, z_2, \cdots, z_p) \approx \sum_{\{n_i\}} \frac{(\sum_{i=1}^{p} n_i)!}{\prod_{i=1}^{p} n_i!} G_{n_1, n_2, \cdots, n_p} z_1^{n_1} z_2^{n_2} \cdots z_p^{n_p}. \tag{19}$$

In fact, we can still write the expression

$$G_N(z_1, z_2, \cdots, z_p) = G_N^T (Q_N)^{-1} G_N, \tag{20}$$

where the vector G_N and the matrix Q_N are now defined by

$$(G_N)_{n_1, \cdots, n_p} \equiv G_{n_1 - n_2, n_2 - n_3, \cdots, n_{p-1} - n_p, n_p},$$

$$(Q_N)_{n_1,\cdots,n_p;m_1,\cdots,m_p} = G_{m_1-n_2+m_1-m_2,n_2-n_3+m_2-m_3,\cdots,n_p+m_p} - \sum_{i=1}^{p} z_i G_{m_1-n_2+m_1-m_2+\delta_{i1},n_2-n_3+m_2-m_3+\delta_{i2},\cdots,n_s-n_{s+1}+m_s-m_{s+1}+\delta_{is},\cdots,n_p+m_p+\delta_{ip}},$$

$$n_1=0,\cdots,N,\quad n_2=0,\cdots,n_1,\quad n_p=0,\cdots,n_{p-1};$$

$$m_1=0,\cdots,N,\quad m_2=0,\cdots,m_1,\quad m_p=0,\cdots,m_{p-1}. \tag{21}$$

As in the $p=2$ case the convergence properties of $G_N(z_1, z_2, \cdots, z_p)$ to $G(z_1, z_2, \cdots, z_p)$ can be obtained from the study of $(f, R_N(z_1, z_2, \cdots, z_p)f)$.

Since $R_N(w, z)$ converges strongly to $R(w, z)$ on the Hilbert space $\mathcal{H}_f$, we can also apply the method of moments to the equation

$$(1 - wA - zB)\psi = g \tag{22}$$

where g is any vector in $\mathcal{H}_f$. Then

$$(g, R_N(w, z)g) = \sum_{r=0}^{N}\sum_{s=0}^{r}\sum_{p=0}^{N}\sum_{q=0}^{p} E^*_{r-s,s}(M_N)^{-1}_{r,s;p,q}E_{p-q,q}$$
$$\equiv E^{T*}M_N^{-1}E \tag{23}$$

where the matrix M is defined as in Eq. (10) in terms of the matrix elements (f, A^mB^nf) only, while the column matrix $E_{m-n,n}$ is

$$E_{m-n,n} \equiv (f, A^{m-n}B^ng). \tag{24}$$

Although Eq. (23) does not seem relevant for the study of approximants to a general power series, the freedom in the choice of the generating vector f can be used to improve the approximation in purely Hilbert space problems. In fact, a simple variational formulation is available for the approximation procedure we have been discussing. More precisely, consider the functional

$$J = (g, \phi) + (\phi', g) - (\phi', (1 - wA - zB)\phi) \tag{25}$$

and choose the following natural ansatz:

$$\phi = \sum_{m=0}^{N}\sum_{n=0}^{m} a_{mn}A^{m-n}B^nf,$$
$$\phi' = \sum_{m=0}^{N}\sum_{n=0}^{m} a'_{mn}A^{m-n}B^nf. \tag{26}$$

Then the stationary value $\bar{J}$ of J with respect to the parameters $\{a_{mn}\}$ and $\{a'_{mn}\}$ coincides with formula (23). $\bar{J}$ can still be made stationary even with respect to the choice of the vector f.[21] The extension of these considerations to the n-dimensional case is immediate.

In Sec. II, instead of starting from Eq. (2), we could as well start from the equation

$$f = (1 - wA)(1 - zB)\psi. \tag{27}$$

All convergence theorems of Sec. III hold with obvious modifications for the normal maximal operator $\tilde{T}_N(w, z) \equiv P_N(wA + zB - wzAB)P_N$ and a simple sufficient condition for $1 \notin \Theta(\tilde{T}(w, z))$ is in this case that both $\mathrm{Im}\, w \neq 0$ and $\mathrm{Im}\, z \neq 0$. Therefore, we are led to consider functions of two complex variables with the following integral representation:

$$\tilde{G}(w, z) = \int\int \frac{d\sigma(\alpha, \beta)}{(1 - w\alpha)(1 - z\beta)} \approx \sum_{m,n=0}^{\infty} G_{m,n}w^mz^n \tag{28}$$

where, again, $\sigma(\alpha, \beta)$ is a positive bounded Radon measure in $\mathbf{R}^2$ and $G_{m,n}$ are its moments. For these functions we introduce the approximants

$$\tilde{G}_N(w, z) \equiv G_N^T\tilde{Q}_N^{-1}G_N \tag{29}$$

which differ from the approximants $G_N(w, z)$ defined in Eq. (13) only for the matrix $\tilde{Q}_N$ which now reads

$$(\tilde{Q}_N)_{p,q;r,s} = G_{p+r-q-s,q+s} - wG_{p+r-q-s+1,q+s}$$
$$- zG_{p+r-q-s,q+s+1} + wzG_{p+r-q-s+1,q+s+1}. \tag{30}$$

If the Carleman condition is satisfied for both the sequences $\{G_{m,0}\}$ and $\{G_{0,n}\}$, we can repeat the proof of Theorem 4 and conclude that $\tilde{G}_N(w, z) \to \tilde{G}(w, z)$ at least for both $\mathrm{Im}\, w \neq 0$ and $\mathrm{Im}\, z \neq 0$. Again the convergence is uniform in compact sets of $\mathbf{C}^2$.

Also for these approximants the extension to the n-dimensional case as well as the variational formulation are straightforward.

ACKNOWLEDGMENTS

One of us (C. A) is indebted to Professor J. L. McGregor for a very useful discussion. P. B. thanks Professor M. L. Goldberger for his hospitality at the Department of Physics of Princeton University where part of this work has been done and both of us thank Professor S. Drell for his hospitality at SLAC.

*Work supported in part by the U. S. Atomic Energy Commission.

†Consiglio Nazionale delle Richerche fellow.

‡On leave of absence from Istituto Nazionale di Fisica Nucleare, sezione di Milano, Consiglio Nazionale delle Ricerche fellow.

[1]G. A. Baker, Jr., in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic, New York, 1965), Vol. 1, p. 1.

[2]G. A. Baker, Jr. and J. L. Gammel, editors, *Padé Approximant in Theoretical Physics* (Academic, New York, 1970).

[3]P. R. Graves Morris, editors, *Padé Approximants and Their Applications* (Academic, London, 1973).

[4]J. Nuttall, J. Math. Anal. Appl. 31, 147 (1970).

[5]J. S. R. Chisholm, Math. Comput. 27, 841 (1973).

[6]A. K. Common and P. R. Graves Morris, "Some properties of Chisholm approximants," University of Canterbury preprint (1973); R. Hughes Jones, "General rational approximants in N variables," University of Canterbury preprint (1973); P. R. Graves Morris, R. Hughes Jones, and G. Makinson, "The calculation of some general approximants in two variables," University of Canterbury preprint (1973).

[7]J. S. R. Chisholm and P. R. Graves Morris, "Generalizations of the theorem of de Montessus to two-variable approximants," University of Canterbury preprint (1974).

[8]C. H. Lutterodt, "A two-dimensional analogue of Pade ap-

proximant theory," University of Birmingham preprint (1973).
[9]Y. V. Vorobyev, *Method of Moments in Applied Mathematics* (Gordon and Breach, New York, 1965). See also J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, New York, 1943) and N. I. Akhiezer, *The Classical Moment Problem, and Some Related Questions in Analysis* (Hafner, New York, 1965).
[10]D. Masson, "Hilbert space and the Pade approximant," *Padé Approximant in Theoretical Physics* (Academic, New York, 1970), Vol. 71, p. 197.
[11]J. Nuttall, "Variational principles and Pade approximants," and references therein, in *Padé Approximants and Their Applications* (Academic, London, 1973).
[12]A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw, New York, 1953), Vol. I.
[13]A. E. Nussbaum, Arkiv Mat. 6, 179 (1965).
[14]A vector $f\in\cap_{n\geq 1}\mathcal{D}(A^n)$ such that $\Sigma_{n=1}^{\infty}\|A^n f\|^{-1/n}=\infty$ is called a quasi-analytic vector for the operator A. Given the spectral family $E(\alpha,\beta)$ associated with the permutable selfadjoint operators A and B, the vectors $g_\Gamma=\int\int_\Gamma dE(\alpha,\beta)g$ where $g\in\mathcal{H}$ and Γ is any compact domain in $\mathbf{R}^2$, are quasi-analytic vectors for both A and B and they are dense in $\mathcal{H}$.
[15]The assumption that f is a quasi-analytic vector is a sufficient condition in the convergence proof we shall give in Sec. III.
[16]Even if the vectors $\{f_{r,s}\}$ are not all linearly independent, all following results will remain valid.
[17]M. Stone, *Linear Transformations in Hilbert Space and Their Applications to Analysis* (American Mathematical Society, New York, 1932), Theorem 8.8.
[18]The set of complex numbers $\Theta(O)=\{(h,Oh)\mid h\in\mathcal{D}(O),\ \|h\|=1\}$ is called the numerical range of the operator O.
[19]Ref. 17, Theorem 4.20.
[20]Ref. 17, Theorem 8.14.
[21]For applications of these ideas in the one-variable case, see C. Alabiso, P. Butera, and G. M. Prosperi, Nucl. Phys. **B42**, 493 (1972); **B46**, 593 (1972).

Uniform asymptotic expansions in transport theory with small mean free paths, and the diffusion approximation*

G. J. Habetler and B. J. Matkowsky

Department of Mathematical Sciences, Rensselaer Polytechnic Institute, Troy, New York 12181
(Received 30 October 1973; revised manuscript received 27 September 1974)

We consider initial-boundary value and boundary value problems for transport equations in inhomogeneous media. We consider the case when the mean free path is small compared to typical lengths in the domain (e.g., the size of a reactor). Employing the boundary layer technique of matched asymptotic expansions, we derive a uniform asymptotic expansion of the solution of the problem. In so doing we find that in the interior of the domain, i.e., away from boundaries and away from the initial line, the leading term of the expansion satisfies a diffusion equation which is the basis of most computational work in reactor design. We also derive boundary conditions appropriate to the diffusion equation. Comparisons with existing results such as the asymptotic and P_1 diffusion theories, the P_N approximation, and the extrapolated end point condition for these approximations are made. Finally the uniform validity of our expansions is proved, thus yielding the desired error estimates.

1. INTRODUCTION

We consider the motion of neutrons traveling through a material medium. In their travels the neutrons may collide with the nuclei of the medium, they may be absorbed by the nuclei, or they may cause fissions thus giving birth to secondary neutrons. The neutron distribution is a solution of the transport equation,[1,2] sometimes referred to as the linear Boltzmann integrodifferential equation, and appropriate initial and boundary conditions.

Though initial boundary value problems for the transport equation are simple in form, their solution poses numerous difficulties. Indeed, solutions for only a very few problems are known. Therefore, one seeks approximate solutions to these problems. Alternatively, one may formulate approximate theories and then seek solutions of the approximating problems. That is, instead of considering the mathematical model consisting of an initial boundary value problem for the transport equation, one considers a new mathematical model, generally simpler, whose solution, it is hoped, is close in some sense to the solution of the transport problem.

One of the most important and widely used such approximate theories is diffusion theory. Its formulation has been based on *ad hoc* physical assumptions such as Fick's law which states that the gradient of the neutron flux is proportional to the neutron current. The resulting model is then an initial boundary value problem for a diffusion type differential equation for the neutron flux. It is found that in practice diffusion theory often, though not always, yields good working results. If one wishes to determine the accuracy of this "approximation," and indeed the relation of diffusion theory to transport theory, it is appropriate to ask the following questions. In what sense is diffusion theory an approximation to transport theory? When is this approximation valid? What are estimates of the error? Finally, how can one improve on the results of diffusion theory?

It should be mentioned that there have been other attempts to derive diffusion theory from transport theory. One such approach involves an expansion in the Legendre polynomials $P_n(\cos\theta)$. When the expansion is truncated at P_N, the result is referred to as the P_N approximation.[1-3] In particular, the P_1 approximation leads to a diffusion equation for the stationary (time independent) problem. This is referred to as the P_1-diffusion approximation. However, the P_1 approximation for the time dependent problem does not lead to the diffusion (parabolic) equation but rather to the telegraphers (hyperbolic) equation. Then it is argued that the velocity approaches infinity and the mean free path and absorption cross section both approach zero in such a way that the diffusion equation results in the limit. It is then hoped that the P_N approximation ($N > 1$), which describes the behavior of the first $N+1$ Fourier coefficients, provides an improvement on diffusion theory, which describes the behavior of the first two Fourier coefficients (the flux and the current). We note that the coefficients in the P_N approximation satisfy a system of coupled equations whose number increases with N. Further, boundary conditions appropriate to the P_N approximation have not been derived. Rather, two different sets of *ad hoc* conditions due to Marshak[3] and to Mark[4] are generally employed, though their validity has not been established and no error estimates for them are known.

Another approach to diffusion theory involves the use of Fourier transforms to obtain integral representations of the flux for constant coefficient stationary problems in infinite domains. An asymptotic expansion of the integral for points arbitrarily far away from the boundary then leads to a diffusion equation.[1,5] However, the diffusion coefficient in this equation, which we call the asymptotic diffusion equation, is different from the coefficient in the P_1-diffusion equation. Under the additional assumption that the average number of secondary neutrons produced per collision is close to one, the two coefficients approach one another. In each of these approaches the questions posed above remain unanswered. Furthermore, we may inquire about the basis for the use of this approximation in finite domains.

Finally, Pomraning,[6] and Pomraning and Clark[7] employing a variational formulation with the Legendre polynomials P_n as trial functions, have also obtained the

diffusion equation. They also derive boundary conditions from the variational formulation.

In this paper we answer the questions posed above by a systematic formal derivation of diffusion theory from transport theory. Specifically, we show that diffusion theory for the distribution function itself, and not merely its first few Fourier coefficients, emerges as the leading term of an asymptotic expansion of transport theory in powers of two small parameters ϵ and δ. Here ϵ is a measure of the ratio of the mean free path (inverse of the scattering cross section) to a typical length, e.g., the size of a reactor, in the problem. The parameter δ is a measure of the ratio of macroscopic to microscopic velocities or alternatively the collision and observation time scales. When these two parameters are related in a definite manner, diffusion theory results. Higher order terms in the expansion then provide correction to diffusion theory, thus yielding the desired improvement.

We then consider boundary value problems for the time independent transport equation, and show how to derive boundary conditions appropriate to the approximating diffusion equations. Among the problems considered are problems in inhomogeneous media, for which exact solutions are not available. We derive uniform asymptotic expansions of the solutions of these problems. In so doing we find that diffusion theory holds in the interior of the domain. The diffusion boundary conditions are obtained by matching the boundary layer expansion to the interior expansion. We establish rigorously the validity of the formal expansions for certain classes of boundary value problems.

Our derivation, in addition to adding unification and clarification, has several advantages over the other schemes mentioned above. The polynomial expansion will arise naturally in that the dependence on the angular variable is derived rather than assumed as in the P_N approximation. Moreover, our derivation is valid for problems in inhomogeneous media with sources. In addition, the higher order terms in the expansion satisfy a system of uncoupled equations, in that they depend only on already computed lower order terms. This yields computational simplification in obtaining corrections to diffusion theory. Furthermore, our method does not appear to be restricted to special geometries. Thus, for example, extensions to higher dimensions follow in a straightforward manner.

Finally, for a specific boundary value problem, we present comparisons with other methods, of the numerical value of a certain constant, called the extrapolated end point, which is a measure of the diffusion boundary condition.

2. THE FORMAL EQUATIONS

To simplify the presentation, we consider the one group transport equation in a homogeneous, isotropic, source free medium with slab symmetry. Other problems may be treated by similar methods. Thus we seek a solution of the initial boundary value problem governed by the integrodifferential equation

$$\frac{1}{v}\psi_\tau(x,\mu,\tau)+\mu\psi_x(x,\mu,\tau)+\sigma(x)\psi(x,\mu,\tau)-\frac{c^*(x)\sigma(x)}{2}\int_{-1}^{1}\psi(x,\mu',\tau)\,d\mu'=0, \tag{2.1}$$

$$0<x<d,\quad -1\le\mu\le 1,$$

subject to the boundary conditions

$$\psi(0,\mu,\tau)=f_1^*(\mu,\tau)\quad\text{for }\mu>0, \tag{2.2}$$

$$\psi(d,\mu,\tau)=f_2^*(\mu,\tau)\quad\text{for }\mu<0 \tag{2.3}$$

and the initial condition

$$\psi(x,\mu,0)=g^*(x,\mu). \tag{2.4}$$

Here $\psi(x,\mu,\tau)$ denotes the neutron distribution function, i.e., the probable number of neutrons at position x at time τ traveling with speed v in direction $\mu=\cos\theta$. σ is the total macroscopic scattering cross section, and the function $c^*(x)$ is the average number of secondary neutrons produced in a collision.

3. ASYMPTOTIC ANALYSIS

We introduce the nondimensional variables η, t, ϵ, and δ by defining

$$\eta\equiv x/d, \tag{3.1}$$

$$t\equiv\bar{v}\tau/d, \tag{3.2}$$

$$\epsilon\equiv 1/\bar{\sigma}d,\quad \delta\equiv\bar{v}/v, \tag{3.3}$$

$$a^*\equiv\sigma(x)/\bar{\sigma}. \tag{3.4}$$

Here $\bar{\sigma}$ is a typical scattering cross section of the problem, and $\bar{v}$ is a typical macroscopic velocity, e.g., $d/(1\text{ unit of }\tau)$. We assume that ϵ and δ are small parameters, i.e., the mean free path is much smaller $[O(\epsilon)]$ than a typical elngth in the problem, and the microscopic time scale $1/\bar{\sigma}v$ of collision is much smaller $[O(\epsilon\delta)]$ than the macroscopic time scale τ of observation. Alternatively, the macroscopic velocity is much smaller $[O(\delta)]$ than the microscopic velocity v. In terms of the nondimensional variables the Eqs. (1.1)—(1.4) become

$$\epsilon\delta\psi_t(\eta,\mu,t;\epsilon,\delta)+\epsilon\mu\psi_\eta(\eta,\mu,t;\epsilon,\delta)+a(\eta)\psi(\eta,\mu,t;\epsilon,\delta)-\frac{a(\eta)c(\eta,\epsilon)}{2}\int_{-1}^{1}\psi(\eta,\mu',t;\epsilon,\delta)\,d\mu'=0\begin{cases}0<\eta<1\\-1\le\mu\le 1\end{cases}, \tag{3.5}$$

$$\psi(0,\mu,t;\epsilon,\delta)=f_1(\mu,t)\quad\text{for }\mu>0, \tag{3.6}$$

$$\psi(1,\mu,t;\epsilon,\delta)=f_2(\mu,t)\quad\text{for }\mu<0, \tag{3.7}$$

$$\psi(\eta,\mu,0,\epsilon,\delta)=g(\eta,\mu). \tag{3.8}$$

Here $a(\eta)=a^*(\eta d)$, $c(\eta)=c^*(\eta d)$, $f_j(\mu,t)=f_j^*(\mu,dt/\bar{v})$ and $g(\eta,\mu)=g^*(\nu d,\mu)$. We assume that $\delta=O(\epsilon)$. Thus we assume that $\delta=K\epsilon$ with K a constant, and that ψ and c are represented asymptotically by

$$\psi\sim\sum_{j=0}\psi^j(\eta,\mu,t)\epsilon^j \tag{3.9}$$

and

$$c\sim\sum_{j=0}c_j(\eta)\epsilon^j. \tag{3.10}$$

Note that we have allowed c to depend on ϵ. We shall show that choosing the coefficients $c_0(\eta)$ and $c_1(\eta)$ appropriately will lead to diffusion theory.

We note that Eq. (3.5) is of singular perturbation form, so that the expansion (3.9) cannot in general satisfy the prescribed boundary conditions (3.6) and (3.7) nor the initial condition (3.8).[8] Thus, there will be boundary layers near $\eta=0$ and $\eta=1$ and an initial layer near $t=0$. The representation (3.9) is to be valid in the interior of the domain and not in the boundary or initial layers. Inserting (3.9) and (3.10) into (3.5) and equating the coefficient of each power of ϵ separately to zero, we obtain a recursive system of equations for the determination of the functions $\psi^j(\eta, \mu, t)$:

$$L\psi^0 \equiv a\left[\psi^0 - \frac{c_0}{2}\int_{-1}^{1}\psi^0\, d\mu'\right] = 0, \tag{3.11}$$

$$L\psi^j = r_j \equiv -\mu\psi_\eta^{j-1} + a\sum_{p=1}^{j}\frac{c_p}{2}\int_{-1}^{1}\psi^{j-p}\, d\mu' - K\psi_t^{j-2}$$

$$(j=1, 2, 3\cdots). \tag{3.12}$$

From (3.11) we see that ψ^0 is independent of μ, i.e.,

$$\psi^0(\eta, \mu, t) = \psi^{00}(\eta, t) \tag{3.13}$$

and that

$$c_0(\eta) = 1. \tag{3.14}$$

Equation (3.12) with $j=1$ implies that

$$\psi^1(\eta, \mu, t) = \psi^{11}(\eta, t)\mu + \psi^{10}(\eta, t) \tag{3.15}$$

where

$$\psi^{11} = (-1/a)\psi_\eta^{00} \tag{3.16}$$

and that

$$c_1(\eta) = 0. \tag{3.17}$$

Equation (3.12) with $j=2$ implies

$$\psi^2(\eta, \mu, t) = \psi^{22}(\eta, t)\mu^2 + \psi^{21}(\eta, t)\mu + \psi^{20}(\eta, t), \tag{3.18}$$

where

$$\psi^{22} = (-1/a)\psi_\eta^{11}, \tag{3.19}$$

$$\psi^{21} = (-1/a)\psi_\eta^{10}, \tag{3.20}$$

$$\psi^{22} + 3c_2\psi^{00} - (3K/a)\psi_t^{00} = 0. \tag{3.21}$$

Employing (3.16) and (3.19) in (3.21) we obtain

$$\frac{1}{a}\left(\frac{1}{a}\psi_\eta^{00}\right)_\eta + 3c_2\psi^{00} - \frac{3K}{a}\psi_t^{00} = 0. \tag{3.22}$$

Equation (3.22) is a diffusion equation. It is homogeneous since (2.1) was homogeneous. Clearly if (2.1) contained an $O(\epsilon)$ source, (3.22) would be inhomogeneous. We note that (3.16) is an asymptotic statement of Fick's law. Thus the leading term in the expansion of the distribution function ψ satisfies the diffusion equation. We note that (3.22) was derived under the conditions (3.14) and (3.17), i.e., that the system must be close to critical. No conditions are put on c_j $(j \geq 2)$. Conditions (3.14) and (3.17) are necessary for a nonzero flux to be maintained in the interior of the domain, in the absence of a source. (With a source present, it is possible to have nonzero flux in the interior even if $c < 1$. This problem has been treated by the authors.)

To obtain improvements on diffusion theory, we can calculate higher order terms in the expansion for ψ. Thus proceeding as above, we find that

$$\frac{1}{a}\left(\frac{1}{a}\psi_\eta^{10}\right)_\eta + 3c_2\psi^{10} - \frac{3K}{a}\psi_t^{10} = -3c_3\psi^{00}. \tag{3.23}$$

Continuing in this manner we find that ψ^j is a jth order polynomial in μ with coefficients ψ^{jk} depending on η and t. The leading term ψ^{00} satisfies the homogeneous diffusion equation. The functions ψ^{j0} satisfy inhomogeneous diffusion equations, whose inhomogeneous terms have been determined at an earlier stage in the recursive scheme. The functions ψ^{jk} $(j \geq k \geq 1)$ are derivatives of the functions ψ^{r0} $(r < j)$. Note that the dependence of ψ on μ is derived rather than assumed and the equations for the functions ψ^{jk} are completely uncoupled.

Now the functions ψ^{jk} are not determined until boundary and initial conditions for them are specified. In the following section we show how to derive boundary conditions for the stationary diffusion equations which are obtained by setting $K=0$ above, by performing boundary layer analyses near $\eta=0$ and $\eta=1$. We shall not consider the initial layer problem since in fact, problems of reactor start-up are much more complicated than the linear problem we consider. Indeed, during start-up the problem is nonlinear in that σ depends on ψ and is further complicated by the fact that c changes in time. Finally, during start-up the power level is sufficiently low that statistical fluctuations must be taken into account.

4. BOUNDARY LAYER ANALYSIS AND THE DIFFUSION BOUNDARY CONDITIONS

To determine boundary conditions for our diffusion equations it is necessary to perform boundary layer analyses in the neighborhood of the boundaries $\eta=0$ and $\eta=1$. Then the required boundary conditions are obtained by matching the boundary layer expansion to the interior (diffusion) expansion. We consider the boundary layer at $\eta=0$. The analysis near $\eta=1$ is obtained in a similar manner.

We introduce

$$\zeta = h(\eta) \equiv \int_0^\eta a(t)\, dt, \tag{4.1}$$

so that the time independent transport equation becomes

$$\epsilon\mu\hat{\psi}_\zeta + \hat{\psi} - \frac{\hat{c}(\zeta;\epsilon)}{2}\int_{-1}^{1}\hat{\psi}\, d\mu' = 0, \tag{4.2}$$

where

$$\hat{\psi}(\zeta, \mu;\epsilon) = \psi(h^{-1}(\zeta), \mu;\epsilon) \tag{4.3}$$

and

$$\hat{c}(\zeta;\epsilon) = c(h^{-1}(\zeta);\epsilon). \tag{4.4}$$

Now we employ the stretching transformation

$$y = \zeta/\epsilon \tag{4.5}$$

{for the boundary layer at $\eta=1$ $[\zeta=\zeta_0\equiv\int_0^1 a(t)\, dt]$, we employ the transformation $z=(\zeta_0-\zeta)/\epsilon$} in (4.2) to ob-

tain the boundary layer equation for $\rho(y, \mu; \epsilon) = \hat{\psi}(\epsilon\zeta, \mu; \epsilon)$ as

$$\mu\rho_y + \rho - \frac{\hat{c}(\epsilon y; \epsilon)}{2}\int_{-1}^{1} \rho(y, \mu'; \epsilon)\, d\mu' = 0,$$

$$0 \leq y < \infty, \quad -1 \leq \mu \leq 1. \tag{4.6}$$

We note that the coefficient $\hat{c}$ in this equation is slowly varying and assume that ρ and $\hat{c}$ are given asymptotically by

$$\rho(y; \mu; \epsilon) \sim \sum_{j=0} \rho^j(y, \mu)\epsilon^j \tag{4.7}$$

and

$$\hat{c}(\epsilon y, \epsilon) \sim 1 + \sum_{j=2} \hat{c}_j(\epsilon y)\epsilon^j = 1 + \hat{c}_2(0)\epsilon^2 + O(\epsilon^3). \tag{4.8}$$

Inserting (4.7) and (4.8) into (4.6) and equating the coefficient of each power of ϵ separately to zero, we obtain the following system of equations for the recursive determination of the functions $\rho^j(y, \mu)$.

$$M\rho^0 \equiv \mu\rho^0_y + \rho^0 - \frac{1}{2}\int_{-1}^{1} \rho^0\, d\mu' = 0,$$

$$0 \leq y < \infty, \quad -1 \leq \mu \leq 1, \tag{4.9}$$

$$M\rho^1 = 0, \tag{4.10}$$

$$M\rho^j = R_j \quad (j \geq 2) \tag{4.11}$$

where R_j depends on $\rho^0 \ldots \rho^{j-1}$ and on the function $\hat{c}$ and its derivatives. The functions ρ^j must also satisfy the boundary conditions at $\eta = 0$, namely,

$$\rho^0(0, \mu) = f(\mu), \quad \mu > 0, \tag{4.12}$$

$$\rho^j(0, \mu) = 0, \qquad \mu > 0 \quad (j \geq 1). \tag{4.13}$$

A similar expansion can be constructed at $\zeta = \zeta_0$ $(\eta = 1)$, which will satisfy the given boundary condition at that end.

We note that the operator M defined in (4.9) has constant coefficients. This fact is the basis for the use of the constant coefficient half plane problem [cf. (4.9)] in asymptotic diffusion theory. The solution of (4.9) is given by (Ref. 9, see Ref. 10 for a proof of the validity of this solution)

$$\rho^0(y, \mu) = a_0 + b_0(y - \mu) + \int_{-1}^{1} A_0(\nu)\phi_\nu(\mu)\exp(-y/\nu)\, d\nu, \tag{4.14}$$

where

$$\phi_\nu(\mu) = \frac{\nu}{2}P\frac{1}{\nu - \mu} + \delta(\nu - \mu)[1 - \nu\tanh^{-1}\nu]. \tag{4.15}$$

The representation (4.14) is an eigenfunction expansion of the solution of (4.9) where P denotes the Cauchy principal value and δ the Dirac delta function. The functions 1 and $(y - \mu)$ are classical solutions of (4.9) and correspond to the discrete spectrum of the transport operator while the functions $\phi_\nu(\mu)\exp(-y/\nu)$ are a one parameter family of singular or distributional solutions, which are the contribution of the continuous spectrum. The constant a_0 and b_0 as well as the function $A(\nu)$ will be determined by the boundary condition at $y = 0$ and the matching condition as $y \to \infty$. Clearly, the diffusion approximation contains no growing exponentials, so that the matching condition implies that

$$A_0(\nu) = 0 \quad \text{for } \nu < 0. \tag{4.16}$$

Employing (4.16) in (4.14) and applying the boundary condition (4.12) at $y = 0$, we have

$$f(\mu) = a_0 - b_0\mu + \int_0^1 A_0(\nu)\phi_\nu(\mu)\, d\nu, \quad \mu > 0. \tag{4.17}$$

We multiply (4.17) respectively by $\gamma(\mu)$ and $\phi_{\nu'}(\mu)\gamma(\mu)$ to obtain

$$\int_0^1 f(\mu)\gamma(\mu)\, d\mu = a_0\gamma^0 - b_0\gamma^1 \tag{4.18}$$

and

$$\int_0^1 f(\mu)\phi_{\nu'}(\mu)\gamma(\mu)\, d\mu = \frac{b_0\nu'\gamma^0}{2} + \frac{A_0(\nu')}{\nu'}\gamma(\nu')N(\nu'). \tag{4.19}$$

Here

$$\gamma(\mu) = \frac{3\mu}{2X(-\mu)} \tag{4.20}$$

with

$$X(z) = \frac{1}{1 - z}\exp\frac{1}{\pi}\int_0^1 \frac{1}{\mu' - z}\tan^{-1}\frac{\pi\mu'}{2(1 - \mu'\tanh^{-1}\mu')}\, d\mu', \tag{4.21}$$

$$\gamma^j = \int_0^1 \mu^j\gamma(\mu)\, d\mu, \tag{4.22}$$

and

$$N(\nu) = \nu\left((1 - \tanh^{-1}\nu)^2 + \frac{\pi^2\nu^2}{4}\right). \tag{4.23}$$

To obtain (4.18) and (4.19) we have made use of the orthogonality relations

$$\int_0^1 \phi_\nu(\mu)\gamma(\mu)\, d\mu = 0 \tag{4.24}$$

and

$$\int_0^1 \phi_\nu(\mu)\phi_{\nu'}(\mu)\gamma(\mu)\, d\mu = \frac{\gamma(\nu)}{\nu}N(\nu)\delta(\nu - \nu'). \tag{4.25}$$

Indeed, it was to enable us to use these orthogonality relations that we showed (4.16) without completing the matching at that point. Equations (4.18) and (4.19) may be solved for a_0 and $A_0(\nu)$ as

$$a_0 = \frac{b_0\gamma^1}{\gamma^0} + \frac{1}{\gamma^0}\int_0^1 f(\mu)\gamma(\mu)\, d\mu \tag{4.26}$$

and

$$A_0(\nu) = \frac{-b_0\nu^2\gamma^0}{2\gamma(\nu)N(\nu)} + \frac{\nu}{\gamma(\nu)N(\nu)}\int_0^1 f(\mu)\phi_\nu(\mu)\gamma(\mu)\, d\mu. \tag{4.27}$$

Thus far the constant b_0 is undetermined. We shall now determine it by completing the matching procedure. To do so we assume the existence of a domain of overlap in which both the boundary layer and interior (diffusion) expansions are valid. Then by comparing the expansions at a fixed value of η (or equivalently ζ) we obtain the matching conditions. We first consider the behavior of $\rho^0(y, \mu)$ as $y \to \infty$ since (4.5) implies that $y \to \infty$ for fixed η as $\epsilon \to 0$. Thys as $y \to \infty$, $\rho^0(y, \mu)$ behaves like

$$\rho^0(y, \mu)\,|_\infty = a_0 + b_0(y - \mu). \tag{4.28}$$

Now we examine the behavior of the interior expansion for ζ fixed in the neighborhood of $\zeta = 0$. We recall that the leading term of the interior expansion is given by

$$\psi^0(\eta, \mu) = \psi^{00}(\eta) \tag{4.29}$$

which is a solution of (3.22) with $K = 0$,

$$\frac{1}{a}\left(\frac{1}{a}\psi^{00}_\eta\right)_\eta + 3c_2\psi^{00} = 0,$$

or, equivalently, using (4.1), as a solution of

$$\psi^{00}_{\xi\xi} + 3c_2\psi^{00} = 0.$$

Near $\zeta = 0$, $\psi^{00}(\zeta)$ behaves like $\psi^{00}(0)$. Thus the matching condition implies that

$$a_0 = \psi^{00}(0) \tag{4.30}$$

and

$$b_0 = 0. \tag{4.31}$$

Equations (4.30) and (4.31) with a_0 given by (4.26) yield the leading term of the diffusion boundary conditions.

We now proceed to the next term $\rho^1(y, \mu)$ in the boundary layer expansion. Since Eq. (4.10) is the same as (4.9), we have that

$$\rho^1(y, \mu) = a_1 + b_1(y - \mu) + \int_0^1 A_1(\nu)\phi_\nu(\mu)\exp(-y/\nu)\,d\nu. \tag{4.32}$$

The boundary condition for ρ^1 is now zero, so that following (4.28) and (4.29) we find that

$$a_1 = b_1\gamma^1/\gamma^0 \tag{4.33}$$

and

$$A_1(\nu) = -b_1\nu^2\gamma^0/2\gamma(\nu)N(\nu). \tag{4.34}$$

The behavior of $\rho^1(y, \mu)$ as $y \to \infty$ is given by

$$\rho^1(y, \mu)\big|_\infty = a_1 + b_1(y - \mu). \tag{4.35}$$

The interior expansion is given by

$$\begin{aligned}\psi(\zeta, \mu; \epsilon) &= \psi^0(\zeta, \mu) + \epsilon\psi^1(\zeta, \mu) + O(\epsilon^2)\\ &= \psi^{00}(\zeta) + \epsilon[\psi^{10}(\zeta) + \psi^{11}(\zeta)\mu] + O(\epsilon^2).\end{aligned} \tag{4.36}$$

Near $\zeta = 0$, it is given by

$$\psi^{00}(0) + \epsilon[\psi^{10}(0) + \psi^{00}_\xi(0)y + \psi^{11}(0)\mu] + O(\epsilon^2). \tag{4.37}$$

Employing (3.16) with $K = 0$ or its equivalent in terms of ζ which states that

$$\psi^{11} = -\psi^{00}_\xi,$$

$$\psi(\zeta, \mu)\big|_{\zeta=0} = \psi^{00}(0) + \epsilon[\psi^{10}(0) + \psi^{00}_\xi(0)(y - \mu)] + O(\epsilon^2). \tag{4.38}$$

Matching the $O(\epsilon)$ term to $\rho^1(y, \mu)\big|_\infty$ implies that

$$a_1 = \psi^{10}(0) \tag{4.39}$$

and

$$b_1 = \psi^{00}_\xi(0). \tag{4.40}$$

Thus the leading terms of the boundary conditions appropriate to diffusion theory are given by

$$\psi^{00}(0) = a_0 = \frac{1}{\gamma^0}\int_0^1 f(\mu)\gamma(\mu)\,d\mu \tag{4.41}$$

and

$$\psi^{10}(0) = a_1 = \frac{b_1\gamma^1}{\gamma^0} = \frac{\gamma'}{\gamma^0}\psi^{00}_\xi(0). \tag{4.42}$$

Using (4.22) and (4.20) and formulas (1), (23), and (16a) in Ref. 9(pp. 125, 138, 171 respectively), we can evaluate γ^0 and γ^1 as

$$\gamma^0 = \int_0^1 \gamma(\mu)\,d\mu = 1 \tag{4.43}$$

and

$$\gamma^1 = \int_0^1 \mu\gamma(\mu)\,d\mu = \frac{3}{2}\int_0^1 \frac{\mu^2}{X(-\mu)}\,d\mu = (0.7104), \tag{4.44}$$

so that (4.41) and (4.42) become

$$\psi^{00}(0) = \int_0^1 f(\mu)\gamma(\mu)\,d\mu = \frac{3}{2}\int_0^1 \frac{\mu f(\mu)}{X(-\mu)}\,d\mu \tag{4.45}$$

and

$$\psi^{10}(0) = \gamma^1\psi^{00}_\xi(0). \tag{4.46}$$

In terms of the original variable x, these boundary conditions are

$$\psi^{00}(0) = \frac{3}{2}\int_0^1 \frac{\mu f(\mu)}{X(-\mu)}\,d\mu \tag{4.47}$$

and

$$\psi^{10}(0) = \frac{\gamma^1 d}{a^*(0)}\psi^{00}_x(0). \tag{4.48}$$

The boundary conditions at the other end point $x = d$, are obtained by symmetry considerations as

$$\psi^{00}(d) = \frac{3}{2}\int_0^1 \frac{\mu g(-\mu)}{X(-\mu)}\,d\mu \tag{4.49}$$

and

$$\psi^{10}(d) = \frac{-\gamma^1 d}{a^*(d)}\psi^{00}_x(d). \tag{4.50}$$

We note that the boundary conditions at each end point involve the local scattering cross section, i.e., $a^*(0)$ and $a^*(d)$. The function $X(-\mu)$ appearing in the boundary conditions is tabulated (see, e.g., Ref. 9). Higher order terms in the boundary layer expansion can be calculated in a similar manner. Then by matching these terms to higher order terms in the interior expansion, higher order terms in the diffusion boundary conditions can be calculated.

5. THE ASYMPTOTIC EIGENVALUES

In the above problem, we have assumed the existence of a unique solution, i.e., that we are not at an eigenvalue [following standard practice, we set $c(\eta; \epsilon) = \lambda(\epsilon)\tilde{c}(\eta)$ with $\tilde{c}(\eta)$ appropriately normalized; then λ is the eigenvalue parameter] of the problem. This implies that, (3.22) with $K = 0$, (4.47), and (4.49) have a unique solution. Equivalently, this means that the matching can be performed. Of course, at an eigenvalue, this is not true. The asymptotic eigenvalues are clearly given by $\lambda = 1 + \lambda_2\epsilon^2 + \lambda_3\epsilon^3 + O(\epsilon^4)$. Then to first order we seek nontrivial solutions of the diffusion equation (3.22) with $K = 0$ subject to the homogeneous boundary conditions, given here in terms of the variable η as

$$\psi^{00}(0) = \psi^{00}(1) = 0. \tag{5.1}$$

Letting $u(\eta)$ and $v(\eta)$ be a basis for the solution space of (3.22) with $K=0$, we see that the eigenvalues are obtained from the conditions

$$\begin{aligned} &\alpha u(0)+\beta v(0)=0,\\ &\alpha u(1)+\beta v(1)=0. \end{aligned} \tag{5.2}$$

This yields a countable number of discrete eigenvalues λ_2 [obtained from $c_2(\eta)$], which we denote by λ_2^n. A similar condition on λ_3 is obtained by considering the next term in the expansion. Thus, given $\lambda_2=\lambda_2^n$, we seek solutions of (3.23) with $K=0$, with boundary conditions

$$\psi^{10}(0)-\frac{\gamma^1}{a(0)}\psi_\eta^{00}(0)=\psi^{10}(1)+\frac{\gamma^1}{a(d)}\psi_\eta^{10}(1)=0. \tag{5.3}$$

Thus $\lambda_3=\lambda_3^n$ are determined in terms of λ_2^n from the conditions

$$\begin{aligned} &\alpha u(0)+\beta v(0)=r(\psi_\eta^{00}(0),\psi_\eta^{00}(1),\ \lambda_2^n,\lambda_3),\\ &\alpha u(1)+\beta v(1)\ =s(\psi_\eta^{00}(0),\psi_\eta^{00}(1),\lambda_2^n,\lambda_3), \end{aligned} \tag{5.4}$$

where the right-hand sides are functions of the variables indicated. From (5.2), it follows that the right-hand side must satisfy an orthogonality relation in order that solutions of (5.4) exist. This condition determines $\lambda_3=\lambda_3^n$ in terms of λ_2^n. For the constant coefficient problem, the asymptotic eigenvalues are given by

$$\lambda^n=c^n=1+\epsilon^2n^2\pi^2/3+O(\epsilon^3). \tag{5.5}$$

6. THE UNIFORM EXPANSION

We have obtained expansions in the interior and boundary layer regions. We now construct a composite expansion which is to be uniformly valid throughout the region. To do so we add together the separate expansions and subtract those terms which the two expansions have in common, so that they are not counted twice. These latter terms are precisely the terms of the boundary layer expansion which were matched in the overlap region, i.e., the terms $\rho|_\infty$ of the boundary layer expansion which did not approach zero as y became infinite. Thus the N term uniform expansion is given by

$$\psi_N^{\mathrm{unif}}=\psi_N+\rho_N-\rho_N|_\infty. \tag{6.1}$$

The leading terms of our uniform expansion are given by

$$\begin{aligned} \psi^{\mathrm{unif}}&=\psi^{00}(\eta)+\rho^0(y)-\rho^0(y)|_\infty+\epsilon[\psi^{10}(\eta)\\ &\quad+\mu\psi^{11}(\eta)+\rho^1(y)-\rho^1(y)|_\infty]+O(\epsilon^2)\\ &=\psi^{00}(\eta)+\int_0^1 A_0(\nu)\phi_\nu(\mu)\exp(-y/\nu)\,d\nu\\ &\quad+\int_0^1 B_0(\nu)\phi_\nu(\mu)\exp(-(1-y)/\nu+\epsilon[\psi^{10}(\eta)\\ &\quad+\mu\psi^{11}(\eta)+\int_0^1 A_1(\nu)\phi_\nu(\mu)\exp(-y/\nu)\,d\nu\\ &\quad+\int_0^1 A_1(\nu)\phi_\nu(\mu)\exp(-(1-y)/\nu)\,d\nu]+O(\epsilon^2), \end{aligned} \tag{6.2}$$

where $\psi^{00}(\eta)$ is a solution of the homogeneous diffusion equation (3.22) with $K=0$ and the boundary conditions (4.47) and (4.49), $\psi^{10}(\eta)$ is a solution of the inhomogeneous diffusion equation (3.23) with $K=0$, and the boundary conditions (4.48) and (4.50), and $\psi^{11}(\eta)$ is given by (3.16). The functions $A_0(\nu)$, $B_0(\nu)$, $A_1(\nu)$, and $B_1(\nu)$ are given by

$$A_0(\nu)=\frac{\nu}{\gamma(\nu)N(\nu)}\int_0^1 f(\mu)\phi_\nu(\mu)\gamma(\mu)\,d\mu, \tag{6.3}$$

$$B_0(\nu)=\frac{\nu}{\gamma(\nu)N(\nu)}\int_0^1 g(-\mu)\phi_\nu(\mu)\gamma(\mu)\,d\mu, \tag{6.4}$$

$$A_1(\nu)=-\frac{\nu^2}{2\gamma(\nu)N(\nu)}\frac{\psi_\eta^{00}(0)}{a(0)}, \tag{6.5}$$

and

$$B_1(\nu)=\frac{\nu^2}{2\gamma(\nu)N(\nu)}\frac{\psi_\eta^{00}(1)}{a(1)}, \tag{6.6}$$

while $\phi_\nu(\mu)$ is given by (4.15).

We shall now prove that the formal expansions obtained are in fact uniformly valid. First, we state a positivity result which will be useful in the analysis of these problems.

7. A POSITIVITY RESULT

Theorem: Let $\psi(x,\mu)$ be a solution of

$$\begin{aligned} &\epsilon\mu\frac{\partial\psi}{\partial x}+a(x)\psi=\frac{c(x;\epsilon)}{2}a(x)\int_{-1}^1\psi(x,\mu')\,d\mu'+S(x,\mu),\\ &x\in(0,1),\quad \mu\in[-1,1],\\ &\psi(0,\mu)=f(\mu),\quad \mu>0,\\ &\psi(d,\mu)=g(\mu),\quad \mu<0, \end{aligned} \tag{7.1}$$

with $0\le c(x)\le c<1$ and $a(x)\ge a>0$. Let S, f, g be continous nonnegative functions. Then ψ is nonnegative. This theorem was essentially stated in Ref. 11 where plausibility arguments for its validity were given. Those arguments can be made rigorous in a straightforward manner and therefore shall not be presented here.

8. PROOF OF VALIDITY OF THE ASYMPTOTIC EXPANSION

We consider the problem

$$\begin{aligned} &L\psi\equiv\epsilon\mu\psi_x+\psi-\frac{[1-\epsilon^2\bar c(x)]}{2}\int_{-1}^1\psi(x,\mu')\,d\mu'=0,\\ &\psi(0,\mu)=f(\mu),\quad \mu>0,\\ &\psi(1,\mu)=g(\mu),\quad \mu<0, \end{aligned} \tag{8.1}$$

with $\bar c(x)\ge c^1>0$ throughout $[0,1]$. [Clearly, the problem with $\bar c=\sum_{j=0}\bar c_j(x)\epsilon^j$ can be treated with no additional difficulty.]

Employing the methods described in the previous sections, we can construct N term interior expansions $\psi_N\sim\sum_{j=0}\psi^j\epsilon^j$ and boundary layer expansions $\rho\sim\sum_{j=0}^N\rho^j\epsilon^j$ for the above problem. Then an N term uniform expansion ψ_N^{unif} can be constructed as described in Sec. 6.

We define the error R_N as

$$R_N=\psi-\psi_N^{\mathrm{unif}}=\psi-[\psi_N+\rho_N-\rho_N|_\infty]. \tag{8.2}$$

The expansions ψ_N and ρ_N have been constructed so that

$$LR_N=O(\epsilon^{N+1}), \tag{8.3}$$

$$R_N=0 \text{ on } \Omega=\{X=0,\ \mu>0\ ;X=1,\ \mu<0\}$$

with all the coefficients in the composite expansion uni-

formly bounded. We wish to show that $R_N = O(\epsilon^{N+1})$. We write (8.3) as

$$\mathcal{L} R_N = \epsilon^{N+1} M(x;\epsilon), \quad R_N = 0 \text{ on } \Omega. \tag{8.4}$$

Next we write (8.4) in terms of the constant coefficient operator $\mathcal{L}_0$.

$$\mathcal{L}_0 R_N \equiv \epsilon\mu (R_N)_x + R_N - \frac{(1-\epsilon^2 c^0)}{2}\int_{-1}^{1} R_N \, d\mu'$$

$$= \epsilon^{N+1} M + \frac{\epsilon^2}{2}(c^0 - \bar{c}(x))\int_{-1}^{1} R_N \, d\mu' \equiv S(x;\epsilon),$$

$$R_N = 0 \text{ on } \Omega. \tag{8.5}$$

where $c^0 = \max_{[0,1]} \bar{c}(x)$. Let $S^0 = \max_{[0,1]} |S|$ and let Γ be the solution of

$$\mathcal{L}_0 \Gamma = S^0, \quad \Gamma = 0 \text{ on } \Omega. \tag{8.6}$$

It then follows from our positivity result that

$$\Gamma \pm R_N \geq 0 \tag{8.7}$$

or

$$|R_N| \leq \Gamma \tag{8.8}$$

pointwise, so that

$$\max_{[0,1]} |R_N| \leq \max_{[0,1]} \Gamma. \tag{8.9}$$

To bound Γ, we consider the function $W \equiv \Gamma - S^0/\epsilon^2 c^0$ and find that

$$\mathcal{L}_0 W = 0, \quad W = -S^0/\epsilon^2 c^0 \leq 0 \text{ on } \Omega. \tag{8.10}$$

The positivity result now implies that

$$W \leq 0 \tag{8.11}$$

or

$$\Gamma \leq S^0/\epsilon^2 c^2, \tag{8.12}$$

so that

$$\max |R_N| \leq \frac{S^0}{\epsilon^2 c^0} \leq \frac{1}{\epsilon^2 c^0} \max_{[0,1]} \left[\epsilon^{N+1} |M| + \frac{\epsilon^2}{2}(c^0 - \bar{c}(x)) \right.$$

$$\left. \times \left| \int_{-1}^{1} R_N \, d\mu' \right| \right] \leq \frac{1}{\epsilon^2 c^0} [\epsilon^{N+1} \bar{M}$$

$$+ \epsilon^2 \max_{[0,1]}(c^0 - \bar{c}(x)) \max_{[0,1]} |R_N|], \tag{8.13}$$

where $\bar{M} = \max_{[0,1]} |M|$. Thus

$$\max |R_N| \leq \frac{\bar{M}\epsilon^{N-1}}{c^0 - \max_{[0,1]} |c^0 - \bar{c}(x)|} = O(\epsilon^{N-1}), \tag{8.14}$$

since $\max_{[0,1]} |c^0 - \bar{c}(x)|$ is $< c^0$ [recall $c^0 = \max \bar{c}(x)$]. Now, the estimate in (8.14) can be improved by noting that

$$R_N = R_{N+2} + \sum_{k=1}^{2} \epsilon^{N+k}(\psi^{N+k} + \rho^{N+k} - \rho^{N+k}|_\infty). \tag{8.15}$$

Thus

$$|R_N| \leq |R_{N+2}| + \sum_{k=1}^{2} \epsilon^{N+k} |\psi^{N+k} + \rho^{N+k} - \rho^{N+k}|_\infty |. \tag{8.16}$$

Now $|R_{N+2}| = O(\epsilon^{N+1})$ by (8.14) and the second term in the right-hand side of (8.16) is also $O(\epsilon^{N+1})$ since the coefficients in the expansion are uniformly bounded. Therefore, there exists a constant K (independent of x and ϵ) such that

$$|R_N| \leq K\epsilon^{N+1}. \tag{8.17}$$

9. THE EXTRAPOLATED END POINT CONDITION

We shall now show how the notion of the extrapolated end point condition is related to the boundary conditions derived above. We recall that the flux $\Phi(\eta)$ is defined as

$$\Phi(\eta;\epsilon) = \tfrac{1}{2}\int_{-1}^{1} \psi(\eta, \mu, \epsilon)\, d\mu$$

$$= \tfrac{1}{2}\int_{-1}^{1} \{\psi^{00}(\eta) + \epsilon[\psi^{10}(\eta) + \mu\psi^{11}(\eta)] + O(\epsilon^2)\}\, d\mu$$

$$= \psi^{00}(\eta) + \epsilon\psi^{10}(\eta) + O(\epsilon^2). \tag{9.1}$$

We note that Φ satisfies a diffusion equation since all the ψ^{jk} do. We would now like to derive boundary conditions for Φ. We expand the right-hand side of (9.1) in a Taylor series about $\eta = 0$ obtaining

$$\Phi(\eta;\epsilon) = \psi^{00}(0) + \psi^{00}_\eta(0)\eta + O(\eta^2) + \epsilon\psi^{10}(0) + O(\epsilon\eta) + O(\epsilon^2). \tag{9.2}$$

Now we employ (5.3) in (9.2) to obtain

$$\Phi(\eta;\epsilon) = \psi^{00}(0) + \psi^{00}(0)\eta + O(\eta^2) + \frac{\epsilon\gamma^1}{a(0)}\psi^{00}_\eta + O(\epsilon\eta) + O(\epsilon^2). \tag{9.3}$$

We set

$$\eta = \epsilon\eta_0, \tag{9.4}$$

so that

$$\Phi(\epsilon\eta_0;\epsilon) = \psi^{00}(0) + \epsilon\psi^{00}_\eta(0)\left[\eta_0 + \frac{\gamma^1}{a(0)}\right] + O(\epsilon^2). \tag{9.5}$$

A condition on $\psi^{00}(0)$ has already been derived in terms of the prescribed function $f(\mu)$, namely

$$\psi^{00}(0) = \tfrac{3}{2}\int_{-1}^{1} \frac{\mu f(\mu)}{x(-\mu)}\, d\mu, \tag{9.6}$$

however, $\psi^{00}_\eta(0)$ is not known. Therefore, choosing

$$\eta_0 = -\gamma^1/a(0), \tag{9.7}$$

we find that

$$\Phi(\epsilon\eta_0;\epsilon) = \tfrac{3}{2}\int_{-1}^{1} \frac{\mu f(\mu)}{x(-\mu)}\, d\mu + O(\epsilon^2). \tag{9.8}$$

Continuing in this manner we can obtain corrections to η_0 by expanding in a series in ϵ, and choosing the coefficients in the series so that Φ satisfies the same boundary conditions as ψ^{00}. The value of η so determined is referred to as the extrapolated end point. Thus to leading order, the extrapolated end point $\eta = \epsilon\eta_0$ is given in terms of x by

$$x_0 = \epsilon\eta_0 d = \frac{-\epsilon\gamma^1 d}{a^*(0)} = \frac{-\epsilon d(0.7104)}{a^*(0)}. \tag{9.9}$$

This defines the usual extrapolated end point condition. We note that this condition involves the local scattering cross section $a^*(0)$. The condition at the other end will be

$$x_d = d + \frac{\epsilon\gamma^1 d}{a^*(d)} = d + \frac{\epsilon d(0.7104)}{a^*(d)} \tag{9.10}$$

Improvements on these conditions can be obtained by retaining more terms in the asymptotic expansion of the solution and employing them in (9.1) and the equations that follow. We note that the above formulas are valid even for inhomogeneous media ($a \neq 1$) with capture ($c \neq 1$). It is clear from the above and from (4.8) and (4.11) that variations in $a(\eta)$ and $c(\eta)$ affect the extrapolated end point at $O(\epsilon^2)$.

We shall now compare our extrapolated end point with that obtained by other methods, for a specific constant coefficient problem, since not all the other methods are capable of treating variable coefficient problems. The problem we consider is the Milne problem, which is the problem for a homogeneous, noncapturing ($c = 1$), source free medium occupying the half space $x \geq 0$, with boundary condition $\psi(0, \mu) = 0$ for $\mu > 0$. The source of neutrons is considered to be at infinity. This problem is exactly our boundary layer problem (4.9) subject to (4.12) with $f(\mu) = 0$. Further, since $c = 1$, all the functions $\rho^j(y, \mu) = 0$ $(j \geq 1)$ so that $\rho(y, \mu\,; \epsilon) = \rho^0(y, \mu)$. Finally, since we are in a homogeneous medium $a^* \equiv 1$. Thus the extrapolated end point is given, to all orders in ϵ, by

$$- x_0 = \epsilon d(0.7104) = 0.7104/\sigma. \tag{9.11}$$

This value of x_0 is exact, i.e., the value determined from the exact solution of the Milne problem obtained by the Wiener—Hopf method. It is to be compared with the following values determined by other methods. These values are taken from Table II in Ref. 6.

TABLE I. The linear extrapolation distance (in units of mean free paths) for the Milne problem.[a]

	Mark	Marshak	Variational
$P-1$	0.5774	0.6667	0.7071
$P-2$	0.7746	0.6667	0.7071
$P-3$	0.6940	0.7051	0.7118
$P-4$	0.7297	0.702	
$P-5$	0.7039	0.7082	
$P-6$	0.7198		
$P-7$	0.7069		
$P-8$	0.7159		

[a]The exact result is 0.7104.

10. ASYMPTOTIC DIFFUSION THEORY

In the special case of the time independent homogeneous problem (i.e., $a = 1$ and c constant), we can cast our diffusion equations into a form which is more amenable to numerical calculations. In so doing, we will find that the resulting asymptotic expansion satisfies the asymptotic diffusion equation mentioned in the introduction. Thus, we consider the boundary value problem for the equation

$$\epsilon \mu \psi_\eta + \psi - \frac{c}{2} \int_{-1}^{1} \psi(\eta, \mu')\, d\mu' = 0. \tag{10.1}$$

We introduce the variable ξ defined by

$$\xi = \eta/\epsilon\nu_0 \tag{10.2}$$

where

$$\frac{1}{\nu_0} \sim \sum_{j=1} d_j \epsilon^j, \tag{10.3}$$

where the constants d_j are chosen so that the resulting diffusion equations for ψ^{j0} are all homogeneous, with diffusion coefficient equal to one. That is, we assume an asymptotic expansion of the form

$$\psi(\xi, \mu, \epsilon) \sim \sum_{j=0} \psi^j(\xi, \mu)\epsilon^j,$$

$$c \sim \sum_{j=0} c_j \epsilon^j \tag{10.4}$$

valid in the interior of the region. Proceeding as above by inserting (10.2), (10.3), and (10.4) into (10.1) and equating the coefficient of each power of ϵ separately to zero, we obtain

$$\mu \sum_{k=0}^{j-1} d_{j-k} \psi^k_\xi + \psi^j - \frac{1}{2} \sum_{k=0}^{j} c_{j-k} \int_{-1}^{1} \psi^k(\xi, \mu')\, d\mu' = 0, \quad j = 0, 1, 2, \cdots \tag{10.5}$$

with $\psi^{-1} \equiv 0$.

In order to have nontrivial solutions, we must have

$$c_0 = 1 \tag{10.6}$$

and

$$c_1 = 0 \tag{10.7}$$

with

$$\psi^j(\xi, \mu) = \sum_{k=0}^{j} \psi^{jk}(\xi)\mu^k. \tag{10.8}$$

Then the constants d_j are chosen so that

$$D\psi^{j0} \equiv \psi^{j0}_{\xi\xi} + \psi^{j0} = 0. \tag{10.9}$$

The first few d_j are given by

$$d_1 = (3c_2)^{1/2}, \tag{10.10}$$

$$d_2 = c_3 d_1 / 2c_2, \tag{10.11}$$

$$d_3 = \frac{-d_1 c_3^2}{(2c_2)^2 4c_2} - \frac{4c_2^2}{5} - c_4. \tag{10.12}$$

The functions ψ^{jk} are then given by

$$\psi^{jk} = - \sum_{n=1}^{j-k+1} d_n \psi^{j-n,k-1}_\xi \quad (k \geq 1). \tag{10.13}$$

Thus all the coefficients ψ^{jk}, and therefore the entire expansion for ψ, satisfies the same diffusion equation given by (10.9); similarly, the flux satisfies

$$\Phi_{\xi\xi} + \Phi = 0. \tag{10.14}$$

In terms of the original variable x, Eq. (10.14) becomes

$$\Phi_{xx} + (\sigma/\nu_0)\Phi = 0 \tag{10.15}$$

which is the usual asymptotic diffusion approximation to transport theory (cf. Ref. 5, where the expansion for ν_0, though derived in a different manner, agrees with ours). Since the diffusion coefficient in (10.15) contains ν_0, i.e., a full series in ϵ, while the P_1 diffusion coefficient contains only the leading term of that series, we may compare the difference between the P_1 and asymptotic diffusion approximations to the difference between the Born and Rytov approximations in wave propagation.[12]

*This work was supported by the National Science Foundation Grant GP 27368. One of the authors (BJM) would like to acknowledge the support of the Applied Mathematics Summer Institute (Dartmouth 1972) and ONR during the final stages of this work.

[1]B. Davison, *Neutron Transport Theory* (Oxford U.P. Oxford, 1957).
[2]A.M. Weinberg and E.P. Wigner, *The Physical Theory of Neutron Chain Reactors* (Chicago U.P., Chicago, 1956).
[3]R. Marshak, Rev. Mod. Phys. **19**, 185 (1947).
[4]J.C. Mark, "The Spherical Harmonics Method," National Research Council Reports MT92, 1944 and MT97, 1945.
[5]J.H. Tait, *Neutron Transport Theory* (American Elsevier, New York, 1964).
[6]G.C. Pomraning, Ann. Phys. **27**, 193 (1964).
[7]G.C. Pomraning and M. Clark, Nucl. Sci. Eng. **16**, 147 (1963).
[8]K.O. Friedrichs, Bull. Am. Math. Soc. **61**, 485 (1955).
[9]K.M. Case and P.F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967).
[10]E.W. Larsen and G.J. Habetler, Commun. Pure Appl. Math. **26**, 525 (1973).
[11]K.M. Case and P.F. Zweifel, J. Math. Phys. **4**, 1376 (1963).
[12]J.B. Keller, J. Opt. Soc. Am. **59**, 1003 (1969).

On the strength of a system of partial differential equations

Bernard F. Schutz

Department of Applied Mathematics and Astronomy, University College, Cardiff, Wales
(Received 4 November 1974)

It is shown that Einstein's concept of the "strength" of a system of differential equations is directly related to the number of dynamical degrees of freedom the equations permit. It may become a useful tool for investigating the structure of the system.

In a recent paper, Mariwalla[1] discussed Einstein's[2] concept of the "strength" of a system of partial differential equations. Although both suggested that the strength was related to the amount of arbitrariness in the solutions to the system, neither Mariwalla nor Einstein made that relationship satisfactorily quantitative, and both were surprised to find that the Maxwell and Einstein equations had the same strength, twice that of the scalar wave equation. The purpose of this paper is to show that the strength is related in a well-defined manner to the number of arbitrary functions of $d-1$ variables (where d is the dimension of the manifold) necessary to determine a solution locally. For hyperbolic systems this is the amount of Cauchy data; it defines the amount of dynamical freedom in the system. The strengths of the scalar, Maxwell, and Einstein systems are then readily understood in terms of the number of polarization states available to the massless particles associated with them. When extended to examine arbitrariness in fewer than $d-1$ variables, the method may become a useful tool in examining the structure of the system of equations.

Suppose we have a system of equations for n unknowns U_A on a d-dimensional manifold. If all the equations can be placed in the normal form

$$\partial^k U_A/\partial x^k = f_A(x, y_\alpha, \partial^{l+m} U_B/\partial^l x\, \partial^m y_\beta) \tag{1}$$

[where $\{x, y_\alpha\ (\alpha = 1, \ldots, d-1)\}$ are the d coordinates, k is fixed, and $l+m \leq k$, $l<k$] in some coordinate system, then a local analytic solution is always uniquely determined by giving analytic functions for U_A and their first $k-1$ derivatives with respect to x in the hypersurface $x=\text{const}$ (Cauchy–Kowalewsky theorem). That is, the sytem allows kn free functions of $k-1$ variables. However, it may not always be possible to choose coordinates $\{x, y_\alpha\}$ such that all the equations of the system take the form (1). In the Maxwell or Einstein equations, for example, some equations represent *constraints*, of the form

$$0 = g_A(x, y_\alpha, \partial^{l+m} U_B/\partial^l x\, \partial^m y_\beta). \tag{2}$$

Associated with the existence of these contraints are gauge functions, whose values are arbitrary everywhere. These gauge functions are physically unmeasurable, but must be eliminated before the Cauchy–Kowalewsky theorem can be brought to bear on the problem. The existence of the constraints, moreover, means that not all the initial data is freely specifiable. We shall show that Einstein's concept of the "strength" of the system provides a direct, if somewhat heuristic, method of discovering just how much real freedom there is in a complicated system of partial differential equations.

Consider the Taylor expansion of an analytic function of d variables about a point. The total number of terms of nth order in the expansion is[1]

$$\left[\begin{matrix} d \\ n \end{matrix}\right] \equiv \frac{(n+d-1)!}{n!(d-1)!} = \binom{n+d-1}{n}. \tag{3}$$

If the function is completely unconstrained, then all of these coefficients in the Taylor series may be given arbitrarily. If for any reason the function can be given arbitrarily on a $(d-1)$-dimensional hypersurface, but its behavior in the remaining dimension is determined, then only $\left[\begin{smallmatrix} d-1 \\ n \end{smallmatrix}\right]$ coefficients of order n are arbitrary. The converse is not necessarily true (the $\left[\begin{smallmatrix} d-1 \\ n \end{smallmatrix}\right]$ free coefficients need not form a $(d-1)$-dimensional Taylor expansion), but in the context in which we shall use it we can suppose it will generally be true. The fraction of free coefficients in such a function is

$$\left[\begin{matrix} d-1 \\ n \end{matrix}\right] \Big/ \left[\begin{matrix} d \\ n \end{matrix}\right] = \frac{d-1}{n+d-1},$$

which goes to zero for large n.

In order to determine the amount of freedom in a system of partial differential equations, Einstein[2] suggested one should expand all the dependent variables in Taylor series and determine the number of relations among the various coefficients of order n that are implied by the differential equations of the system. By subtraction there remains a number Z_n of free coefficients of order n. Einstein[2] and Mariwalla[1] have computed this number for several physically interesting fields. After removing all the gauge freedom in the fields, they found that the ratio $Z_n/\left[\begin{smallmatrix} d \\ n \end{smallmatrix}\right]$ always went to zero as $1/n$ for large n, and they interpreted this to mean that there were no completely free functions of d variables left in the theories. They then *defined* the coefficient of $1/n$ to be the "strength," but did not interpret it satisfactorily. It is clear, however, from the discussion of the previous paragraph, that the limit for large n of $Z_n/\left[\begin{smallmatrix} d-1 \\ n \end{smallmatrix}\right]$, which differs from the Einstein strength by a factor of $(d-1)$, is in fact the number of free functions of $d-1$ variables in the theory. We can

formulate this precisely as follows. It is clear from Eq. (3) that $\left[\begin{smallmatrix} d \\ n \end{smallmatrix}\right]$ is a polynomial in n of order $d-1$. Since Z_n is always a sum of such terms,[1,2] it is also a polynomial in n of maximum order $d-1$. Therefore, it has a unique representation of the form

$$Z_n = \sum_{k=1}^{d} N_k \begin{bmatrix} k \\ n \end{bmatrix} . \tag{4}$$

Then, at least heuristically, the number of free functions of k variables in the solution is N_k. (In the Appendix we show that all N_k are integers, as they must be for this approach to make sense.)

As a concrete example, let us consider the Maxwell field in four dimensions. When the equations are formulated in terms of a vector potential and the gauge freedom is removed from Z_n explicitly, one obtains[1]

$$Z_n{}^{(1)} = 4\begin{bmatrix} 4 \\ n \end{bmatrix} - \begin{bmatrix} 4 \\ n+1 \end{bmatrix} - 4\begin{bmatrix} 4 \\ n-2 \end{bmatrix} + \begin{bmatrix} 4 \\ n-3 \end{bmatrix} .$$

If we were not to subtract the gauge freedom, the second term would not be present. If the vector potential is not introduced at all, one obtains[1,2]

$$Z_n{}^{(2)} = 6\begin{bmatrix} 4 \\ n \end{bmatrix} - 8\begin{bmatrix} 4 \\ n-1 \end{bmatrix} + 2\begin{bmatrix} 4 \\ n-2 \end{bmatrix} .$$

Writing these in the form of Eq. (4) gives

$$Z_n{}^{(1)} = 4\begin{bmatrix} 3 \\ n \end{bmatrix} - 2\begin{bmatrix} 2 \\ n \end{bmatrix} - 2\begin{bmatrix} 1 \\ n \end{bmatrix} ,$$

$$Z_n{}^{(2)} = 4\begin{bmatrix} 3 \\ n \end{bmatrix} + 2\begin{bmatrix} 2 \\ n \end{bmatrix} .$$

Neither Z_n contains any free functions of four variables, and both have four free functions of three variables. These correspond to the two dynamical degrees of freedom in electromagnetism: On a Cauchy hypersurface one can specify two variables and their time derivatives freely. On the other hand, the two versions of Maxwell's equations appear to differ at the two- and one-dimensional level. In fact they do not: Because $Z_n{}^{(1)}$ refers to a potential version of the $Z_n{}^{(2)}$ equations, a term of order n in the latter is of order $n+1$ in the former. To "lower" the order of the former, we rewrite $Z_n^{(1)}$ in terms of $m \equiv n-1$ and find

$$Z_m{}^{(1)} = 4\begin{bmatrix} 3 \\ m \end{bmatrix} + 2\begin{bmatrix} 2 \\ m \end{bmatrix} .$$

So in this sense both versions are equivalent. The interpretation of this two-dimensional term is not at all clear, but in view of its independence of the use of a potential, it appears to contain some real information about Maxwell's equations. We may conjecture that it describes the freedom to set a boundary condition on the elliptical constraint equation in the initial hypersurface, but it should bear a more thorough investigation. There is another tantalizing suggestion in the Einstein equations of general relativity, for which $Z_n{}^{1,2}$ takes the form

$$Z_n{}^{\mathrm{GR}} = 4\begin{bmatrix} 3 \\ n \end{bmatrix} - 2\begin{bmatrix} 2 \\ n \end{bmatrix} - 8\begin{bmatrix} 1 \\ n \end{bmatrix} .$$

This is derived using the metric tensor as the fundamental variable; but the metric may be considered to be a second-order potential for the Riemann tensor, which is physically measureable. Shifting the order by two ($m \equiv n-2$), we get

$$Z_m{}^{\mathrm{GR}} = 4\begin{bmatrix} 3 \\ m \end{bmatrix} + 6\begin{bmatrix} 2 \\ m \end{bmatrix} .$$

The coefficient of $\left[\begin{smallmatrix} 1 \\ m \end{smallmatrix}\right]$ is zero, and the other coefficients are positive, just as for electromagnetism.

Whatever the significance of the lower coefficients may be, it is clearly not surprising that for the Einstein and Maxwell equations, as well as for the Weyl and Dirac equations,[1] one finds $N_3 = 4$, while for the scalar wave equation $N_3 = 2$. All are field theories for spinning particles: for zero spin particles there is only one dynamical degree of freedom, while for massless particles with spin there are two possible helicities and hence two degrees of freedom.

APPENDIX

The expressions given by Einstein[2] and Mariwalla[1] are always of the form

$$Z_n = \sum_{\substack{\text{integer} \\ m}} K_m \begin{bmatrix} d \\ n-m \end{bmatrix} ,$$

where d is the dimension of the manifold and the K_m are always integers. This is in fact the general form for Z_n, because each term results from K_m equations (always in d dimensions) containing m derivatives of the field variables. We wish to reexpress this in the form of Eq. (4). By using the definition of $\left[\begin{smallmatrix} d \\ n \end{smallmatrix}\right]$ it is easy to derive the basic relation

$$\begin{bmatrix} d \\ n+1 \end{bmatrix} = \begin{bmatrix} d \\ n \end{bmatrix} + \begin{bmatrix} d-1 \\ n+1 \end{bmatrix} , \quad d \geq 2. \tag{A1}$$

By iteration of this we find

$$\begin{bmatrix} d \\ n+1 \end{bmatrix} = \begin{bmatrix} d \\ n \end{bmatrix} + \begin{bmatrix} d-1 \\ n \end{bmatrix} + \begin{bmatrix} d-2 \\ n \end{bmatrix} + \cdots + \begin{bmatrix} 1 \\ n \end{bmatrix} .$$

Equation (A1) can be rewritten as

$$\begin{bmatrix} d \\ n-1 \end{bmatrix} = \begin{bmatrix} d \\ n \end{bmatrix} - \begin{bmatrix} d-1 \\ n \end{bmatrix} ,$$

from which follows by iteration

$$\begin{bmatrix} d \\ n-m \end{bmatrix} = \sum_{p=0}^{m} (-1)^p \binom{m}{p} \begin{bmatrix} d-p \\ n \end{bmatrix} .$$

Since all the coefficients are integers, the coefficients N_k in Eq. (4) are also integers.

[1] K. H. Mariwalla, J. Math. Phys. **15**, 468 (1974). Note the error in Eq. (23), where $\binom{d}{2}$ should everywhere be replaced by $\binom{d+1}{2}$.

[2] A. Einstein, *Meaning of Relativity* (Methuen, London, 1956), 6th ed., Appendix II; also (Princeton U. P., Princeton, N. J., 1955), 5th ed.

Nonspreading solutions of the inhomogeneous scalar wave equation*

W. E. Couch and R. J. Torrence

Department of Mathematics, University of Calgary, Calgary, Alberta, Canada T2N IN4
(Received 25 November 1974)

A simple condition that is necessary and sufficient for the solution of the inhomogeneous wave equation to be a nonspreading wave is derived for a class of driving terms that arise in certain physical problems. The condition is applied to the analysis of the self-scattering of gravitational multipole radiation at second perturbative order. It is proved that there is no scattering at the multipole component of highest order in the second-order gravitational field. It is conjectured that there is no scattering for every component of the second-order field. A mathematical expression of this conjecture, derived from the condition for nonspreading, is given and it implies conjectured identities on Clebsch–Gordan coefficients.

1. INTRODUCTION

The homogeneous wave equation

$$\Box\psi=0, \tag{1.1}$$

has what has been called the characteristic propagation property, or, equivalently, its solution can be described as nonspreading.[1] In physical terms this means that a field satisfying Eq. (1.1) can, with the appropriate boundary conditions, be nonvanishing for only a finite time for a fixed observer. This property is of such obvious physical interest that Kundt and Newman[1] looked for more general linear homogeneous hyperbolic equations for which it holds, and found that there are others which, however, are comparatively rare.

In this paper we consider a related problem for the *inhomogeneous wave equation*

$$\Box\psi=\delta. \tag{1.2}$$

More specifically, we shall consider Eq. (1.2) where δ satisfies[2]

$$\delta(u,r,\theta,\varphi)\neq 0 \Rightarrow u_1\leq u\leq u_2. \tag{1.3}$$

This condition is pictured in Fig. 1 where δ is nonvanishing only in the region labeled B. Equation (1.3) might seem an unnatural assumption to make about δ; however, important quasilinear hyperbolic equations, or systems of equations, such as Einstein's equations or Maxwell's equations in a nonlinear medium, can lead to Eqs. (1.2) and (1.3) if a weak field perturbative approach is used. The retarded linearized solutions will satisfy equations like Eq. (1.1) and may be assumed to have the support pictured in Fig. 1. The second-order corrections will satisfy equations like Eq. (1.2), where δ will be bilinear in, and thus have the same support as, those linearized solutions. Such a δ, and the solutions of Eq. (1.2) which it generates, will be called *nonspreading* if one can choose boundary data in such a way that ψ also has the support pictured in Fig. 1.[3] Physically, we are looking for a class of driving terms for which a fixed observer can, depending on boundary conditions, observe a nonvanishing ψ for only a finite time. We, also, shall find that they exist but are comparatively rare.

For simplicity we assume that δ and ψ are axially symmetric and expand them in spherical harmonics. Equation (1.2) becomes

$$2\frac{\partial^2\psi}{\partial u\partial r}-\frac{\partial^2\psi}{\partial r^2}+\frac{2}{r}\left(\frac{\partial\psi}{\partial u}-\frac{\partial\psi}{\partial r}\right)+\frac{L(L+1)}{r^2}\psi=\delta, \tag{1.4}$$

where L denotes the Lth multipole and L subscripts on ψ_L and δ_L are suppressed in this and the next section. We note that if $\delta=0$, Eq. (1.4) is solved by the retarded and advanced multipole fields

$$\psi_{\rm ret}=\sum_{\alpha=0}^{L}\frac{C_{L\alpha}}{r^{\alpha+1}}\frac{d^{L-\alpha}}{du^{L-\alpha}}a(u)Y_{L0} \tag{1.5}$$

and

$$\psi_{\rm adv}=\sum_{\alpha=0}^{L}\frac{(-1)^\alpha C_{L\alpha}}{r^{\alpha+1}}\frac{d^{L-\alpha}}{dv^{L-\alpha}}b(v)Y_{L0},\quad v\equiv u+2r, \tag{1.6}$$

where $a(u)$ and $b(v)$ are arbitrary profile functions, the $C_{L\alpha}$ are given by

$$C_{L\alpha}=K_\alpha^2(L)/2^\alpha\alpha!,\quad K_\alpha(L)\equiv[(L+\alpha)!/(L-\alpha)!]^{1/2},$$

and the Y_{Ls} denote spherical harmonics. Because the retarded solutions are series in $1/r$, and the corresponding solutions for higher spin equations are too, the quasilinear problems described above would lead to δ's which are also series in $1/r$. Therefore, we now restrict ourselves to[4]

$$\delta=\sum_{n=3}^{\infty}\frac{d_n(u)}{r^n}, \tag{1.7}$$

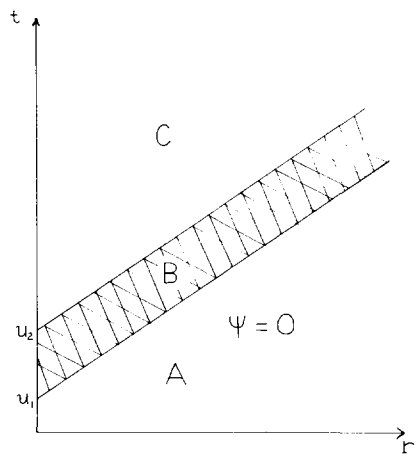

FIG. 1. The support of δ.

where the $d_n(u)$ satisfy Eq. (1.3). We see from Eq. (1.4) that the corresponding ψ will be of the form

$$\psi=\sum_{n=1}^{\infty}\frac{f_n(u)}{r^n}. \tag{1.8}$$

We now argue that ψ is nonspreading if and only if, expressed as in Eq. (1.8), it is a *finite* series in $1/r$, that is, if there is an integer T such that $n\geq T\Rightarrow f_n(u)=0$.

The argument has two parts. First, since $\delta=0$ in region C, ψ in C must be a sum of retarded [Eq. (1.5)] and advanced [Eq. (1.6)] fields. The only fields in region C which cannot be eliminated by a choice of boundary data consistent with $\psi=0$ in region A are fields which are advanced and are not retarded.[5] Hence our definition of nonspreading can be replaced by the statement that ψ is nonspreading if and only if ψ is a retarded field in C. But a retarded field is, from Eq. (1.5), seen to be a finite series in $1/r$ of the form of Eq. (1.8) and, conversely, every finite series of the form Eq. (1.8) that solves $\Box\psi=0$ is a retarded field of the form Eq. (1.5). Therefore, ψ is nonspreading if and only if ψ is a finite series in $1/r$ in region C.

Second, any discontinuity in ψ across the surface $u=u_2$ (Fig. 1) must have the structure of a retarded field, and these are necessarily finite series in $1/r$. Thus ψ is a finite series in $1/r$ in C if and only if it is a finite series in $1/r$ in B. *We conclude that ψ is nonspreading (in* C*) if and only if it is a finite series (in* B*). We are looking for those δ's for which this is the case.*

In the next section we derive a simple condition, Eqs. (2.6) and (2.12), on the $d_n(u)$ of Eq. (1.7) which is equivalent to nonspreading.

In Sec. 3 we consider a particular application of our condition. If we treat Einstein's empty-space equations as indicated above, δ's are obtained which can be substituted into Eq. (2.12). The resulting equation [Eq. (3.4)] involves Clebsch–Gordon coefficients (since the δ's are bilinear in spherical harmonics) and can be read as a possible identity whose verification would be equivalent to a proof of the nonspreading of gravitational waves, to the second perturbative order.

In Sec. 4, we consider Eq. (3.4) in detail. Since it has already been shown[6,7] that a finite number of cases involving quadrupole, octupole, and 16-pole gravitational radiation fields *are* nonspreading, Eq. (3.4) must be identically satisfied in certain cases, which it is, and we conjecture it to hold in general. We actually prove here that it is an identity for a twofold infinity of new special cases, but our rather direct approach has not established it in the general case, although there can be little doubt if its validity. It is not clear if the relationship is of mathematical interest in its own right, or merely an adjunct to the type of spreading wave problems we have been discussing.

2. THE INHOMOGENEOUS WAVE EQUATION

We begin with Eq. (1.4) where δ is restricted by Eq. (1.3) and Eq. (1.7). In order to study particular solutions of the inhomogeneous equation it is sufficient, and convenient, to assume

$$\psi=\sum_{n=2}^{\infty}\frac{f_n(u)}{r^n}. \tag{2.1}$$

Substituting these series [Eq. (1.7) and (2.1)], we obtain

$$\sum_{n=3}\frac{2(n-2)}{r^n}\dot{f}_{n-1}+\sum_{n=4}\frac{(n-3-L)(n-2+L)}{r^n}f_{n-2}=\sum_{n=3}\frac{d_n}{r^3}, \tag{2.2}$$

where the dot stands for differentiation with respect to u. Equation (2.2) is equivalent to

$$2\dot{f}_2=d_3, \tag{2.3a}$$

$$2(n-2)\dot{f}_{n-1}+(n-3-L)(n-2+L)f_{n-2}=d_n,\qquad 4\leq n\leq 2+L, \tag{2.3b}$$

and

$$2(n-2)\dot{f}_{n-1}+(n-3-L)(n-2+L)f_{n-2}=d_n,\qquad 3+L\leq n. \tag{2.4}$$

It is easy to see that Eqs. (2.3) determine the f_n, $2\leq n\leq L+1$, in terms of the d_n, $3\leq n\leq 2+L$ (or vice versa). Thus we have the simple result that if the driving term for the Lth multipole stops at the $L+2$ power of $1/r$, the then the Lth multipole solution, itself, stops at the $L+1$ power of $1/r$. In addition it is clear that whether the solution is a terminating series depends only on the d_n, $3+L\leq n$. Since this is the question which interests us, we can restrict our attention to Eq. (2.4).

We now assume that ψ is a terminating series in $1/r$, that is we assume that

$$f_n=0,\quad L+3\leq T\leq n, \tag{2.5}$$

where T is a positive integer. It follows from Eqs. (2.4) and (2.5) that

$$d_n=0,\quad T+2\leq n, \tag{2.6}$$

$$d_{T+1}=(T-2-L)(T-1+L)f_{T-1}, \tag{2.7}$$

$$d_n=(n-3-L)(n-2+L)f_{n-2}+2(n-2)\dot{f}_{n-1},\qquad L+4\leq n\leq T, \tag{2.8}$$

and

$$d_{3+L}=2(L+1)\dot{f}_{2+L}. \tag{2.9}$$

It can be seen that Eqs. (2.7) and (2.8) determine the f_n, $2+L\leq n\leq T-1$, which are *all* the f_n which have not been assumed to vanish, in terms of the d_n, $4+L\leq n\leq T+1$, which are *all* the d_n which have not been shown to vanish, *except* for d_{3+L}. In particular f_{2+L} is determined, and its substitution into Eq. (2.9) must not lead to a contradication. In other words, ψ can terminate if and only if Eq. (2.6) is satisfied *and* the d_n, $3+L\leq n\leq T+1$, satisfy a single condition which must now be derived.

If we differentiate Eq. (2.8) $n-L-3$ times and define

$$\chi_j=\frac{d^j}{du^j}d(u)_{L+3+j},\quad 0\leq j\leq T-L-2,$$

and

$$\eta_i=\frac{d^i}{du^i}f(u)_{L+1+i},\quad 1\leq i\leq T-L-2,$$

Eqs. (2.7) and (2.8) can be combined and written in the form

$$\chi_i = \sum_{j=1}^{T-L-2} M_{ij}\eta_j, \tag{2.10}$$

where

$$M_{ij} = \begin{array}{c} \\ 0 \\ \\ \\ 0 \end{array} \begin{array}{c} \begin{array}{ccc} & & 0 \end{array} \\ \begin{array}{ccc} i(i+2L+1) & & 2(i+L+1) \end{array} \\ \begin{array}{ccc} & & 0 \end{array} \end{array}$$

Solving Eq. (2.10) for η_1 yields, after some calculation,

$$\eta_1 = \sum_{j=1}^{T-L-2} \frac{(-1)^{j+1}2^{j-1}(L+j)!\,(2L+1)!}{j!\,(j+2L+1)!\,(L+1)!}\chi_j. \tag{2.11}$$

In terms of the χ_i and η_i Eq. (2.9) becomes $\chi_0 = 2(L+1)\eta_1$ and this, with Eq. (2.11), gives

$$\sum_{j=0}^{T-L-2} \frac{(-2)^j(L+j)!}{j!\,(j+2L+1)!}\frac{d^j}{du^j}d(u)_{L+3+j}, \tag{2.12}$$

where some nonvanishing factors present in every term have been removed. Equation (2.12), along with

$$d_n = 0, \quad T+2 \leq n, \tag{2.6}$$

are necessary and sufficient for ψ to terminate at the $T-1$ power of $1/r$.

3. AN EXAMPLE OF A NONSPREADING WAVE IN GENERAL RELATIVITY

In this section we apply Eq. (2.12) to a problem arising in general relativity. The nonspreading condition resulting therefrom is discussed on its own merit in Sec. 4. A reading of that discussion does not require all of the details of the calculations of this section.

The problem we investigate is whether a linearized retarded gravitational field composed of a set of radiating multipoles gives rise to a nonspreading gravitational field at second perturbative order. In other words, we ask whether the first-order radiation scatters at second order. This is a generalization of previous work[6,7] in which the radiating multipoles concerned were specific ones of low order.

In order to fit the problem into the framework of Sec. 2 we collect together here some well-known facts concerning general relativity in a weak field approximation scheme. The Einstein equations for the first-order part of the metric tensor can be replaced by the linearized Bianchi identities regarded as field equations for the Weyl tensor, and these field equations are the usual ones for a spin-S field,[8] $S=2$. The higher order corrections to the linearized field satisfy the spin-2 field equations with driving terms. Solutions to the spin-2 field equations can be generated from a potential[9] satisfying the scalar wave equation, and similarly solutions to the driven spin-2 equations can be generated from a potential that satisfies an appropriately driven scalar wave equation. Hence we need to deal only with Eqs. (1.1) and (1.2). This is true even for the question of spreading because the procedure whereby the components of the field are generated involve, as regards operations with respect to r, only integration and differentiation and do not change finite series in $1/r$ into infinite series (or vice versa).

We take the linearized axially symmetric gravitational field to be a retarded 2^l-pole field ($l \geq 2$) plus a retarded $2^{l'}$-pole field ($l' \geq 2$) with complex profile functions of compact support $a(u)$ and $a'(u)$, respectively. [The real parts of $a(u)$ and $a'(u)$ give the electric type moments and the imaginary parts give the magnetic type moments.] An answer to the question of nonspreading for this field of two arbitrary multipoles immediately provides an answer for a field composed of any number of different multipoles.

Expressed in terms of first-order complex quantities U, Ψ_2, X^i, etc., of the null tetrad formulation of general relativity[10] the driving term of Eq. (1.2) is

$$\begin{aligned}\delta = \frac{2}{r}\frac{\partial}{\partial r}\Bigg\{r^3\Bigg[&-U\frac{\partial\Psi_2}{\partial r} - X^i\frac{\partial}{\partial x^i}\Psi_2 + \omega\frac{\partial\Psi_3}{\partial r} \\ &+ \left(\xi^i\frac{\partial}{\partial x^i} - 2\beta + 2\tau\right)\Psi_3 + 2\nu\Psi_1 - 3\mu\Psi_2 + \sigma\Psi_4\Bigg]\Bigg\} \\ &- r\sqrt{2}\eth\left[\bar{\xi}^i\frac{\partial}{\partial x^i}\Psi_2 - 2\lambda\Psi_1\right],\end{aligned} \tag{3.1}$$

where $\xi^i\partial/\partial x^i = \xi^\theta\partial/\partial\theta + \xi^\phi\partial/\partial\phi$, and similarly for $X^i\partial/\partial x^i$, the bar denotes complex conjugation, and $\eth$ is an angular operator,[11] which in this instance has the form

$$\eth = -\left(\cot\theta + \frac{\partial}{\partial\theta} + i\frac{\partial}{\partial\phi}\right).$$

For the retarded 2^l-pole field each of the tetrad quantitites U, Ψ_2, X^i, etc., is a finite power series in $1/r$ and can be simply expressed linearly in terms of the retarded 2^l-pole scalar wave, ψ, given by

$$\psi = \sum_{\alpha=0}^{l}\frac{C_{l\alpha}}{r^{\alpha+1}}\frac{d^{l-\alpha}}{du^{l-\alpha}}a(u)Y_{l0}.$$

For example, $\Psi_2 = r^{-2}\psi$. The explicit form of the other quantities may be found in Ref. 7. For the 2^l-pole field some of these quantities have the angular dependence of spin-weighted spherical harmonics[12] ${}_sY_{l0}$, $-2 \leq s \leq 2$, rather than simply Y_{l0} dependence (${}_0Y_{l0} = Y_{l0}$); e.g., Ψ_3 has ${}_{-1}Y_{l0}$ dependence. However, because of the axial symmetry, ${}_sY_{l0}$ is the associated Legendre polynomial, $P_l^s = Y_{ls}\exp(-is\phi)$, so that we have to deal only with ordinary spherical harmonics.

Now consider the tetrad quantities to be those of our problem; namely a 2^l plus $2^{l'}$-pole field. Then Eq. (3.1) involves the products $P_l^s P_{l'}^{-s} = Y_{ls}Y_{l',-s}$, $-2 \leq s \leq 2$, of spherical harmonics. We expand[13] these products themselves in spherical harmonics Y_{L0}:

$$\begin{aligned}Y_{ls}Y_{l's'} = &\left(\frac{(2l+1)(2l'+1)}{4\pi}\right)^{1/2} \\ &\times \sum_{L=|l-l'|}^{l+l'}\sqrt{2L+1}\begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} l & l' & L \\ -s & -s' & 0 \end{pmatrix} Y_{L0}, \quad s+s' = 0,\end{aligned} \tag{3.2}$$

$\begin{pmatrix} l & l' & L \\ -s & -s' & 0 \end{pmatrix}$ are the $3j$ symbols[14]; and we see that δ is a finite sum of spherical harmonics,

$$\delta = \sum_{L=|l-l'|}^{l+l'} \delta_L Y_{L0}.$$

From Eq. (3.1) we find δ_L to be[13]

$$\delta_L = \sum_{\alpha=0}^{l+2} \sum_{\alpha'=0}^{l'+2} \frac{\tilde{C}_{l\alpha}\tilde{C}_{l'\alpha'}(\alpha+\alpha'-1)(\alpha+\alpha'-2)Q}{r^{\alpha+\alpha'}} \times \frac{d^{l+2-\alpha}}{du^{l+2-\alpha}} a(u) \frac{d^{l'+2-\alpha'}}{du^{l'+2-\alpha'}} a'(u), \tag{3.3}$$

where

$$Q \equiv \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} (K_2 K'_2)^2 (\alpha^2 + \alpha'^2 - 4\alpha\alpha' + \alpha + \alpha')$$

$$+ 2K_1 K'_1 \begin{pmatrix} l & l' & L \\ 1 & -1 & 0 \end{pmatrix} (K_2 K_{-1} K'_2 K'_{-1})^2 [l'(l'+1) \times (\alpha^2 - \alpha\alpha' - 2\alpha + \alpha') + l(l+1)(\alpha'^2 - \alpha\alpha' - 2\alpha' + \alpha)]$$

$$+ K_2 K'_2 \begin{pmatrix} l & l' & L \\ 2 & -2 & 0 \end{pmatrix} [(l'+2)(l'+1)l'(l'-1)\alpha(\alpha-3) + (l+2)(l+1)l(l-1)\alpha'(\alpha'-3)],$$

$$\tilde{C}_{l\alpha} \equiv (K_{\alpha-2})^2/2^\alpha \alpha!, \quad K_p \equiv K_p(l), \quad K'_p \equiv K_p(l').$$

We omit any overall factors in δ_L that depend only on l, l', and L.

We have actually written down in Eq. (3.3) only a part of δ_L. We have not shown some terms that may be ignored anyway, as regards the question of spreading, for part of the set of possible values of L, namely, whenever $L \geq m$, $m = \max[l+3, l'+3]$. Also we have not shown terms arising from Eq. (3.1) that involve $\bar{a}$ or $\bar{a}'$. Such terms occur in a series similar to Eq. (3.3). It can be shown that if there is no spreading then the two sets of terms, one with and one without complex conjugation, must *separately* give no spreading. Hence Eq. (3.3) is a prototype of δ_L and is an independent part of δ_L for a large class of L values, l and l' remaining arbitrary. In what follows it will be seen that interesting results may be obtained from Eq. (3.3) alone.

We now substitute Eq. (3.3) into Eq. (2.12). Coefficients of powers of r^{-1} less than $(r^{-1})^{L+3}$ in Eq. (3.3) do not contribute to Eq. (2.12) as shown in Sec. 2. The jth derivative of

$$\frac{d^{l+2-\alpha}}{du^{l+2-\alpha}} a(u) \frac{d^{l'+2-\alpha'}}{du^{l'+2-\alpha'}} a'(u)$$

occurs in Eq. (2.12), and we write it as a sum involving binomial coefficients. Then Eq. (2.12) becomes a quadruple sum. There are, however, two constraints on the sums. One constraint ($L+3+j = \alpha+\alpha'$) arises from picking out the coefficient of $r^{-(L+3+j)}$ in Eq. (3.3). The second constraint arises from using the fact that $a(u)$ and $a'(u)$ are arbitrary within the interval of support so that each coefficient of

$$\frac{d^N}{du^N} a(u) \frac{d^{M-N}}{du^{M-N}} a'(u)$$

occurring in Eq. (2.12) must vanish separately. When these two constraints are properly applied the nonspreading condition on the driving term of general relativity becomes the following unconstrainted double sum:

$$\sum_{\beta=0}^{N} \sum_{\beta'=0}^{M-N} \frac{(-1)^{\beta+\beta'}(l+l'+3-\beta-\beta')!(2l-\beta)!(2l'-\beta')!Q}{(l+l'+L+2-\beta-\beta')!\beta!\beta'!(l+2-\beta)!(l'+2-\beta')!(N-\beta)!(M-N-\beta')!} = 0, \tag{3.4}$$

where $M \equiv l+l'+1-L$ and N is any integer for which $0 \leq N \leq M$. In arriving at Eq. (3.4) we have shifted the sums in Eq. (3.3) by $\beta \equiv l+2-\alpha$, $\beta' \equiv l'+2-\alpha'$ and have used $L \geq m$. Note that Q is independent of N, and its dependence on β and β' is simply quadratic.

4. CONCLUSION

Equation (3.4) is our main result for general relativity. In the case $L = l+l'$, Eq. (3.4) is easily proven to hold by straightforward evaluation. The sums may be performed and simple expressions[14] used for $\begin{pmatrix} l & l' & l+l' \\ -s & s & 0 \end{pmatrix}$. Furthermore, we have found that for $L = l+l'$ the corresponding expression for the complex conjugate terms also holds, so that there is no spreading in the $L = l+l'$ part of the whole second-order field.

We conjecture that Eq. (3.4) holds for all possible L values[13] satisfying $m \leq L \leq l+l'$, for all integers $l \geq 2$, $l' \geq 2$, and for all integers N, $0 \leq N \leq M$. More generally, we conjecture that the whole second-order field is nonspreading. Equation (3.4) has several obvious symmetries, e.g., $N \leftrightarrow M-N$ so that one only need prove it for $N < \frac{1}{2}M$.

The $3j$ symbols occurring in Q are independent of β and β' and so may be taken outside of the sums so that Eq. (3.4) may be regarded as a linear identity on the $3j$ symbols. Equation (3.4) was derived by basing the analysis on the Y_{L0} part of the field, but we could have placed a finite series condition on any one of the ${}_sY_{l0}$ $s = 0, \pm 1, \pm 2$ parts of the spin-2 field. In this way four further conditions (identities?) similar to Eq. (3.4) would be obtained on $3j$ symbols $\begin{pmatrix} l & l' & L \\ s & s' & -(s+s') \end{pmatrix}$, $-2 \leq s+s' \leq 2$, $-3 \leq s \leq 3$.

In addition there must be more, simpler, identities related to the Einstein–Maxwell equations which are also known to have nonspreading radiation fields in the sense used above.[15] A systematic presentation of all of these identities may be justified by a more elegant derivation of them *and* their verification. Both are being investigated.

*This work has been supported by the National Research Council of Canada.

[1]W. Kundt and E.T. Newman, J. Math. Phys. **12**, 2193 (1968).

[2]We shall use spherical polar coordinates and the retarded time, $u=t-r$, throughout. The advanced time will be denoted by $v=u+2r$.

[3]It is obvious that boundary data can always be chosen so that ψ vanishes in A, and this is done, as indicated in Fig. 1.

[4]The value of the lower limit on the sum is consistent with a variety of particular problems, including all those in general relativity which motivated this work. A lower value would materially change the analysis which follows.

[5]A special subclass of multipole fields, even some radiative ones, are *both* retarded and advanced.

[6]W.E. Couch, R.J. Torrence, A.I. Janis, and E.T. Newman, J. Math. Phys. **9**, 484 (1968).

[7]W.E. Couch and R.J. Torrence, J. Math. Phys. **11**, 2096 (1970).

[8]See, for example, R. Penrose, J. Math. Phys. **10**, 38 (1969).

[9]R. Penrose, Proc. Roy. Soc. (London) A **284**, 159 (1965).

[10]E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

[11]E.T. Newman and R. Penrose, J. Math. Phys. **7**, 863 (1966).

[12]J.N. Goldberg, A.J. Macfarlane, E.T. Newman, F. Rohrlich, and E.C.G. Sudarshan, J. Math. Phys. **8**, 2155 (1967). Note that $\eth {}_sY_{l0}=[(l-s)\ (l+s+1)]^{1/2}{}_{s+1}Y_{l0}$.

[13]Because of axial symmetry L takes on only even integer values if $(l+l')$ is even, or only odd integer values if $(l+l')$ is odd.

[14]D.M. Brink and G.R. Satchler, *Angular Momentum* (Clarendon Press, Oxford, 1968), 2nd ed., Appendix I.

[15]W.E. Couch and W.H. Hallidy, J. Math. Phys. **12**, 2170 (1971).

Factorization-method treatment of the perturbed Morse oscillator*

J. N. Huffaker and P. H. Dwivedi

Department of Physics and Astronomy, Oklahoma University, Norman, Oklahoma 73069
(Received 27 September 1974)

By transforming the Morse oscillator from type B to type F factorization, we obtain operators for raising and lowering the vibrational quantum number v, and a recursion relation. This permits the calculation of matrix elements needed for perturbation of the Morse oscillator to any order for perturbations of the form $(e^{au}-1)^n$. Explicit calculations are presented for $n=3$ and $n=4$, analogous to the usual cubic and quartic anharmonicity perturbations of the harmonic oscillator.

I. INTRODUCTION

There are at present three standard theoretical approaches for treating the vibrational motion of a diatomic molecule. First is the Dunham method,[1] in which the vibrational potential energy is expressed as a power of series,

$$U(\xi)=hca_0\xi^2(1+a_1\xi+a_2\xi^2+a_3\xi^3+\cdots), \tag{1}$$

where $\xi=(r-r_e)/r_e$, and where r is the instantaneous internuclear separation and r_e its equilibrium value. The energy eigenvalues and rotation-vibration parameters for this potential have been calculated via the WKB approximation,[2] and can be matched with empirical values to determine the coefficients a_n of the series. Drawbacks of this method are the unverified reliability of the WKB approximation and the lack of analytic eigenfunctions. The second approach involves the use of a "realistic" potential with analytic solutions, such as the Morse potential,[3] given by

$$U(u)=D_e[\exp(-2au)-2\exp(-au)], \tag{2}$$

where $u=r-r_e$, involving the three parameters D_e (well depth), r_e, and a. The drawback to this approach is that there are not enough parameters to accurately reproduce experimental results. The third approach, called the RKR method,[4] is a computer calculation in two steps: first producing $U(r)$ from the observed vibrational spectrum via "classical" turning points and the WKB approximation, then obtaining eigenfunctions.

An alternative approach would be the application of perturbation theory to the Morse oscillator, permitting as good a fit to experiment as the Dunham method, while retaining analytic eigenfunctions. This approach has not been pursued very far, however; only first-order energy corrections have been published.[5] Off-diagonal matrix elements of powers of u have been calculated,[6] but since they are nonvanishing between all pairs of states, higher-order perturbation calculations are impractical.

The factorization method described by Infeld and Hull[7] (hereinafter referred to as IH), is a powerful algebraic technique for handling certain second-order linear differential equations, including such exactly solvable quantum-mechanical problems as the Morse oscillator. Using a variation of this method, we discovered a way to perturb the Morse oscillator in a manner analogous to the perturbation of a harmonic oscillator. In our method, all matrix elements can be calculated, and all but a few off-diagonal matrix elements vanish, so that perturbation can be carried out to all orders.

II. FACTORIZABILITY OF THE MORSE OSCILLATOR

The factorization method involves replacing a second-order differential operator with two equivalent products of first-order operators. Thus, following IH, we define the equation

$$d^2Y_l^m(x)/dx^2+r(x,m)\,Y_l^m(x)=-\lambda_l Y_l^m(x), \tag{3}$$

where λ_l is an eigenvalue and l and m are positive-valued parameters (which are to be varied in integer steps), to be *factorizable* if it is equivalent to the two equations

$$H^+(m+1)H^-(m+1)\,Y_l^m=[\lambda_l-L(m+1)]\,Y_l^m, \tag{4a}$$

$$H^-(m)H^+(m)\,Y_l^m=[\lambda_l-L(m)]\,Y_l^m, \tag{4b}$$

where $L(m)$ is independent of x, and where $H^\pm(m)$ are first-order differential operators of the form

$$H^\pm(m)=k(x,m)\pm d/dx. \tag{4c}$$

The operators $H^\pm(m)$ play the role of raising and lowering operators, but they act on the parameter m, *not* the eigenvalue index l:

$$H^-(m)\,Y_l^{m-1}\propto Y_l^m, \tag{5a}$$

$$H^+(m)\,Y_l^m\propto Y_l^{m-1}, \tag{5b}$$

where $Y_l^{m\pm1}$ is the solution of a *different* eigenvalue equation with the *same* eigenvalue as Eq. (3):

$$d^2Y_l^{m\pm1}/dx^2+r(x,m\pm1)\,Y_l^{m\pm1}=-\lambda_l Y_l^{m\pm1}. \tag{6}$$

By investigating the possible forms of $k(x,m)$, IH showed that there are six general types of factorizable equations, which they labeled with the letters A, B, C, D, E, and F. For each factorization type, they obtained explicit expressions for $r(x,m)$, $k(x,m)$, and $L(m)$. For example, type B factorization is specified by

$$r(x,m)=-d^2\exp(2ax)+2ad(m+c+\tfrac{1}{2})\exp(ax), \tag{7a}$$

$$k(x,m)=d\exp(ax)-m-c, \tag{7b}$$

$$L(m)=-a^2(m+c)^2. \tag{7c}$$

Writing the Schrödinger equation for a Morse oscillator in the form

$$d^2\psi/du^2 + (2\mu/\hbar^2)\{E - D_e[\exp(-2au) - 2\exp(-au)]\}\psi = 0, \tag{8}$$

IH showed that the definitions

$$s + \tfrac{1}{2} = (2\mu D_e)^{1/2}/(a\hbar), \tag{9a}$$

$$n^2 = -2\mu E/(a\hbar)^2, \tag{9b}$$

$$x = -au + \ln 2(s + \tfrac{1}{2}), \tag{9c}$$

permit one to rewrite Eq. (8) in the form

$$d^2R(x)/dx^2 + [-n^2 - (1/4)\exp(2x) + (s + \tfrac{1}{2})\exp(x)]R(x) = 0, \tag{10}$$

which is recongnizable as type B factorization with $a = 1$, $c = 0$, and $d = \frac{1}{2}$, and where m is replaced by s, and λ_l by $-n^2$. From Eqs. (7b) and (7c) we obtain

$$k(x, s) = \tfrac{1}{2}\exp(x) - s, \tag{11a}$$

$$L(s) = -s^2. \tag{11b}$$

III. IDENTIFICATION OF CLASSES AND ORTHONORMAL EIGENFUNCTIONS

Having determined that a differential equation is factorizable, the next step is to determine whether it is what IH call a class I or a class II problem. If $L(m)$ is an *increasing* function of m, one has a class I problem, for which the eigenvalue λ_l is given by

$$\lambda_l = L(l+1), \tag{12a}$$

where l can have any of the infinite set of values

$$l = l_0, \quad l_0 + 1, \quad l_0 + 2, \cdots, \quad 0 < l_0 \leq 1,$$

and where, for fixed l, m can range over the finite set of values

$$m = l_0, \quad l_0 + 1, \ldots, \quad l - 1, \; l.$$

The solution for $m = l$ satisfies the first-order differential equation

$$H^-(l+1)\, Y_l^{\,l} = 0. \tag{12b}$$

If, on the other hand, $L(m)$ is a *decreasing* function of m, one has a class II problem, for which λ_l is given by

$$\lambda_l = L(l), \tag{13a}$$

where l has the same range as before, but where m can range over the infinite set of values

$$m = l, \quad l + 1, \quad l + 2, \cdots.$$

For class II problems, $Y_l^{\,l}$ satisfies

$$H^+(l)\, Y_l^{\,l} = 0. \tag{13b}$$

Given one normalized eigensolution, such as obtained from Eq. (12b) or (13b), one can generate others, also normalized, if one uses the *normalized* raising and lowering operators $\mathcal{H}_l^{\pm}(m)$ defined by

$$\mathcal{H}_l^{\pm}(m) = [\lambda_l - L(m)]^{-1/2}[k(x, m) \pm d/dx], \tag{14}$$

where λ_l is given by either Eq. (12a) or (13a) depending on whether one has a class I or a class II problem.

For the Morse oscillator we recognize that, by Eq. (11b), $L(s)$ is a decreasing function of s, so that we have a class II problem. Thus by Eqs. (11b) and (13a) we find that

$$\lambda_l = L(l) = -l^2,$$

and we recognize that l coincides with the quantity n defined in Eq. (9b). Using n in place of l, we see that for fixed n the minimum value of s is n. The corresponding eigensolution $R_n^{\,n}(x)$ satisfies

$$(d/dx + \tfrac{1}{2}\exp(x) - n)\, R_n^{\,n}(x) = 0, \tag{15a}$$

with normalized solution

$$R_n^{\,n}(x) = [\Gamma(2n)]^{-1/2}\exp(nx - \tfrac{1}{2}e^x). \tag{15b}$$

Defining the appropriate normalized raising and lowering operators by

$$\mathcal{B}_n^{\pm}(s) = [(s+n)(s-n)]^{-1/2}(\tfrac{1}{2}e^x - s \pm d/dx), \tag{16a}$$

we can raise and lower s for fixed n (so long as $s \geq n$) according to

$$R_n^{\,s} = \mathcal{B}_n^{-}(s)\, R_n^{\,s-1}, \tag{16b}$$

$$R_n^{\,s-1} = \mathcal{B}_n^{+}(s)\, R_n^{\,s}. \tag{16c}$$

For a given Morse oscillator, the parameter s is a constant [see Eq. (9a)], while n takes the values

$$n = s, s-1, \ldots, n_0, \quad 0 < n_0 \leq 1.$$

The vibrational quantum number v is defined by $v = s - n$, and thus takes values $v = 0, 1, 2, \ldots, s - n_0$, showing that the number of bound states for a Morse oscillator is the greatest integer in $s + 1$. Writing the eigenvalue $-n^2$ as $-(s - v)^2$, we see from Eq. (9b) that the energy eigenvalue can be written

$$E_v + D_e = (s + \tfrac{1}{2})t(v + \tfrac{1}{2}) - \tfrac{1}{2}t(v + \tfrac{1}{2})^2, \tag{17a}$$

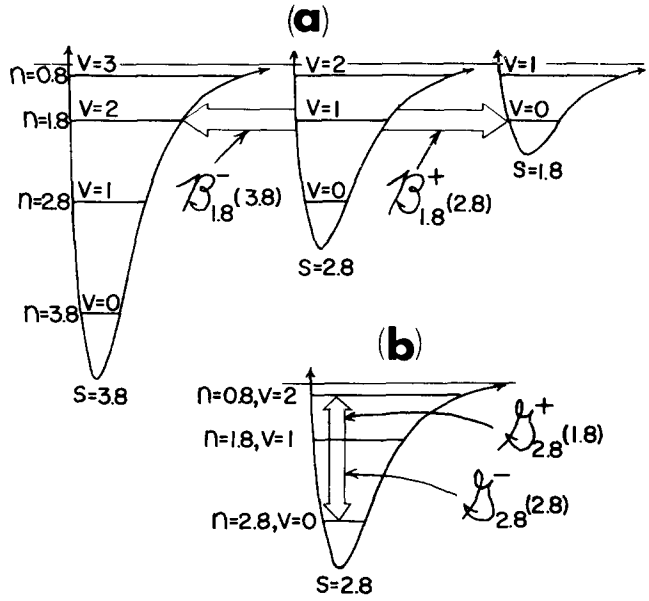

FIG. 1. Effects of various raising and lowering operators on Morse potential eigenfunction. In (a), effects of the s-changing operators $\mathcal{B}_n \pm (s)$ are shown, while (b) shows the effects of the n-changing operators $\mathcal{G}_s \pm (n)$.

where

$$t=(\hbar a)^2/\mu. \tag{17b}$$

Thus the parameter $s+\frac{1}{2}$ can be related to empirical parameters[8] by the equation

$$s+\tfrac{1}{2}=\tfrac{1}{2}\omega_e/\omega_e x_e. \tag{18}$$

The procedure for obtaining the normalized eigenfunction $\psi_v(x)$ is as follows: Noting that $\psi_v(x)=R_{s-v}{}^s(x)$, first obtain $R_{s-v}{}^{s-v}(x)$, using Eq. (15b), then apply Eq. (16b) over and over a total of v times. Here, $R_{s-v}{}^{s-v}$ is the ground state of a *different* Morse oscillator (say with a different well depth D_e), and each intermediate stage in the calculation will be an excited state of a different Morse oscillator. The process is illustrated in Fig. 1(a). Note that the orthonormality properties of the functions $R_n{}^s=\psi_{s-n}$ are

$$\int_{-\infty}^{\infty} R_n{}^s R_{n'}{}^s\,dx=\delta_{n,n'}, \tag{19a}$$

corresponding to the physical orthonormality condition

$$\int_{-\infty}^{\infty} \psi_v\psi_{v'}\,dx=\delta_{v,v'}. \tag{19b}$$

In addition to producing the eigenvalues and eigenfunctions of the Morse oscillator, the above approach can also be used to calculate certain matrix elements. In addition to some obtained by IH, we present in the Appendix a calculation of the diagonal matrix elements $\langle v|e^x|v\rangle$ and $\langle v|e^{2x}|v\rangle$. These results can be used to calculate the first-order perturbations obtained by Pekeris.[5] Unfortunately, matrix elements $\langle v'|e^x|v\rangle$ are nonvanishing for all v', so that higher-order perturbation calculations in e^x are not practicable.

IV. TRANSFORMATION FROM CLASS II TO CLASS I

Given a factorizable class II problem, it should be possible to transform to a factorizable Class I problem, and *vice versa*. In this process, the roles of the parameters l and m are reversed, so that m labels the "eigenvalues" and l is raised and lowered. Starting with Eq. (10), we consider a transformation of the type

$$x=f(y),\quad R(x)=g(y)\,W(y), \tag{20}$$

and consider the differential equation satisfied by W:

$$\frac{d^2W}{dy^2}+\left(\frac{f''}{f'}-\frac{2g'}{g}\right)\frac{dW}{dy}-(f')^2\left[(1/4)\,e^{2f}-(s+\tfrac{1}{2})\,e^f+n^2\right]W - \left(\frac{f''g'}{f'g}-\frac{g''}{g}\right)W=0, \tag{21}$$

where primes denote differentiation with respect to y. IH performed a transformation to C-type factorization, but this did not lead to an exactly factorizable result. Following a suggestion by Carlstone,[9] we considered a transformation to F-type factorization, which IH specified by

$$r(x,m)=-2q/x-m(m+1)/x^2, \tag{22a}$$

$$k(x,m)=m/x+q/m, \tag{22b}$$

$$L(m)=-(q/m)^2. \tag{22c}$$

Making the substitutions

$$f(y)=\ln[y/(s+\tfrac{1}{2})],\quad g(y)\propto[(s+\tfrac{1}{2})/y]^{1/2}, \tag{23}$$

so that

$$y=(s+\tfrac{1}{2})\,e^x,\quad W(y)\propto e^{x/2}R(x), \tag{24}$$

we obtain

$$d^2W/dy^2+W/y-(n-\tfrac{1}{2})(n+\tfrac{1}{2})\,y^{-2}W-(2s+1)^{-2}W=0, \tag{25}$$

which is equivalent to Eq. (22a) with $q=-\frac{1}{2}$, $m=n-\frac{1}{2}$, and $\lambda_l=-(2s+1)^{-2}$. Equations (22b) and (22c) thus take the form

$$k(y,m)=m/y-(2m)^{-1}, \tag{26a}$$

$$L(m)=-(2m)^{-2}. \tag{26b}$$

As $L(m)$ is an increasing function of m, this is a class I problem with eigenvalues

$$\lambda_l=L(l+1)=-(2l+2)^{-2}, \tag{27}$$

and we see that $l=s-\frac{1}{2}$. Labeling the function W with n and s, as $W_s{}^n$, we observe that $W_s{}^s$ satisfies

$$[(s-\tfrac{1}{2})/y-(2s-1)^{-1}-d/dy]\,W_s{}^s=0, \tag{28a}$$

with normalized solution

$$W_s{}^s(y)=[2\Gamma(s+\tfrac{1}{2})]^{-1/2}(s+\tfrac{1}{2})^{-(s+1)}y^{s+1/2} \times\exp[-y/(2s+1)]. \tag{28b}$$

Other normalized solutions are related by

$$W_s{}^n=\mathcal{J}_s{}^-(n)\,W_s n-1, \tag{28c}$$

$$W_s{}^{n-1}=\mathcal{J}_s{}^+(n)\,W_s{}^n, \tag{28d}$$

where the appropriate F-type raising and lowering operators are given by

$$\mathcal{J}_s{}^{\pm}(n)=\frac{2(n-\frac{1}{2})(s+\frac{1}{2})}{[(s+n)(s-n+1)]^{1/2}}\left(\frac{n-\frac{1}{2}}{y}-\frac{1}{2n-1}\pm\frac{d}{dy}\right). \tag{28e}$$

Note that these raising and lowering operators act on n while leaving s unchanged, thereby raising and lowering the vibrational quantum number for a particular Morse oscillator.

Since the "eigenvalue" of Eq. (25) depends on s, the orthonormality condition for $W_s{}^n$ is that

$$\int_0^{\infty} W_s W_{s'}{}^n\,dy=\delta_{s,s'}, \tag{29}$$

in contrast to the physical normalization of $R_n{}^s$ [Eq. (19)]. In order to relate $W_s{}^n$ with $R_n{}^s$, we introduce a constant $C_s{}^n$ into Eq. (24) and write

$$W_s{}^n(y)=C_s{}^n\,e^{x/2}R_n{}^s(x). \tag{30a}$$

Obtaining the differential relationship

$$dy=(s+\tfrac{1}{2})\,e^x\,dx \tag{30b}$$

from Eq. (24) and substituting into Eq. (29), we obtain for $s=s'$

$$\int_0^{\infty}(W_s{}^n)^2\,dy=C_s{}^{n2}(s+\tfrac{1}{2})\int_{-\infty}^{\infty}e^{2x}(R_n{}^s)^2\,dx=1, \tag{31a}$$

$$C_s{}^n=[(s+\tfrac{1}{2})\int_{-\infty}^{\infty}e^{2x}(R_n{}^s)^2\,dx]^{-1/2}. \tag{31b}$$

Using the value of the integral from Eq. (A11), we obtain

$$C_s^n=[4n(s+\tfrac{1}{2})^2]^{-1/2},$$

$$W_s^n(y)=[4n(s+\tfrac{1}{2})^2]^{-1/2}e^{x/2}R_n^s(x). \tag{32}$$

This result is easily checked by comparing Eqs. (15b) and (28b).

Substituting this result into Eq. (28e), we obtain another set of raising and lowering operators for n (or v), but which now act on the physically normalized solutions R_n^s:

$$R_{n-1}^s=\mathcal{G}_s^+(n)R_n^s, \tag{33a}$$

$$R_n^s=\mathcal{G}_s^-(n)R_{n-1}^s, \tag{33b}$$

where

$$\mathcal{G}_s^{\pm}(n)=\left(\frac{4(n-\tfrac{1}{2}\mp\tfrac{1}{2})(n-\tfrac{1}{2})^2}{n-\tfrac{1}{2}\pm\tfrac{1}{2})(s+n)(s-n+1)}\right)^{1/2}$$

$$\times\left[(n-\tfrac{1}{2}\pm\tfrac{1}{2})\,e^{-x}-\frac{s+\frac{1}{2}}{2n-1}\pm e^{-x}\frac{d}{dx}\right]. \tag{33c}$$

These raising and lowering operators produce a finite ladder of eigenfunctions, as shown in Fig. 1(b), consisting of the bound states of a particular Morse oscillator.

V. ANALOGY WITH HARMONIC OSCILLATOR AND PERTURBATION CALCULATION

The harmonic oscillator was one of the first systems treated by the use of raising and lowering operators,[10] albeit of a simpler sort than those of the factorization method. Where the oscillator has mass m and potential energy $U(u)=\frac{1}{2}ku^2$, one defines a dimensionless coordinate

$$Q=\alpha u, \tag{34a}$$

where

$$\alpha^2=m\omega/\hbar,\quad \omega=(k/m)^{1/2}. \tag{34b}$$

The groundstate eigenfunction $\varphi_0(Q)$ satisfies

$$(d/dQ+Q)\,\varphi_0(Q)=0, \tag{34c}$$

with normalized solution

$$Q_0(Q)=\pi^{-1/4}\exp(-\tfrac{1}{2}Q^2). \tag{34d}$$

The other normalized eigenfunctions are generated by

$$\varphi_v(Q)=\mathcal{A}^+(v)\,\varphi_{v-1}(Q), \tag{35a}$$

$$\varphi_{v-1}(Q)=\mathcal{A}^-(v)\,\varphi_v(Q), \tag{35b}$$

where

$$\mathcal{A}^{\pm}(v)=(2v)^{-1/2}(Q\mp d/dQ). \tag{35c}$$

A recursion relation satisfied by the harmonic oscillator eigenfunctions, which is important for perturbation calculations, is obtained by the following procedure: In Eq. (35a) replace v by $v+1$ and multiply by $(2v+2)^{1/2}$ to obtain

$$(2v+2)^{1/2}\varphi_{v+1}=(Q-d/dQ]\,\varphi_v. \tag{36a}$$

Multiply Eq. (35b) by $(2v)^{1/2}$ to obtain

$$(2v)^{1/2}\varphi_{v-1}=(Q+d/dQ)\,\varphi_v. \tag{36b}$$

Finally, add Eqs. (36a) and (36b) and solve for $Q\varphi_v$, to obtain the desired recursion relation,

$$Q\varphi_v=[\tfrac{1}{2}(v+1)]^{1/2}\varphi_{v+1}+(\tfrac{1}{2}v)^{1/2}\varphi_{v-1}. \tag{36c}$$

Repeated use of this recursion relation, together with the orthonormality condition,

$$\int_{-\infty}^{\infty}\varphi_v\varphi_{v'}\,dQ=\delta_{v,v'},$$

permits the algebraic calculation of matrix elements $\langle v'|Q^n|v\rangle$ for any desired power n of the coordinate.

In light of this procedure, note the similarity between Eqs. (33) and (35). In an analogous fashion to the derivation of Eq. (36c), we can derive a recursion relation satisfied by Morse eigenfunctions: Rewriting (33a) and (33b) by replacing n by $n+1$ in the former and taking the quantities in square brackets to the other side, then adding and solving for $(e^{au}-1)\,\psi_v$, one can obtain

$$(e^{au}-1)\,\psi_v=B_{v+1}\psi_{v+1}+A_v\psi_v+B_v\psi_{v-1}, \tag{37a}$$

where

$$B_v=\frac{1}{2}\frac{(s+\frac{1}{2})}{(s+\frac{1}{2}-v)}\left(\frac{v(2s+1-v)}{(s-v)(s+1-v)}\right)^{1/2}, \tag{37b}$$

$$A_v=\frac{2(s+\frac{1}{2})(v+\frac{1}{2})-v(v+1)}{(s+\frac{1}{2}-v)(s-\frac{1}{2}-v)}. \tag{37c}$$

Repeated applications of Eq. (37), together with the orthonormality condition of Eq. (19), permit the calculation of matrix elements of the type $\langle v'|(e^{au}-1)^n|v\rangle$, hence perturbations in powers of $(e^{au}-1)$. Another formula needed for perturbation calculations involves the energy differences between levels of the Morse oscillator, which is obtained from Eq. (17a):

$$E_v-E_{v-n}=nt[(s+\tfrac{1}{2})-v+\tfrac{1}{2}(n-1)],\quad n=\pm1,\pm2,\cdots. \tag{38}$$

It can easily be shown that Eq. (36c) is a limiting case of Eq. (37), just as a harmonic oscillator is a limiting case of a Morse oscillator. Expanding the Morse potential [Eq. (2)] in a power series in au, we obtain

$$U(u)=D_e[-1+(au)^2-(au)^3+(7/12)(au)^4+\cdots]. \tag{39}$$

Thus the force constant of the equivalent harmonic oscillator is

$$k=2D_e\,a^2,$$

and the harmonic oscillator parameter α^2 is related to the Morse oscillator parameter a^2 by

$$\alpha^2=a^2(s+\tfrac{1}{2}). \tag{40}$$

Using this relationship, along with the approximation $(e^{au}-1)\approx au$ and the limit $s\gg v$, we see that Eq. (37) reduces to Eq. (35).

In order to illustrate the perturbation method, we consider a perturbation

$$V(u)=\lambda(e^{au}-1)^3+\mu(e^{au}-1)^4,$$

which should correspond in the above limit to the usual cubic and quartic anharmonic perturbation of a harmonic oscillator. Multiplying Eq. (37a) by $(e^{au}-1)$ and expanding the right-hand side, we obtain

$$(e^{au}-1)^2\psi_0 = B_2B_1\psi_2 + B_1(A_1+A_0)\psi_1 + (B_1^2+B_0^2+A_0^2)\psi_0 + B_0(A_0+A_{-1})\psi_{-1} + B_0B_{-1}\psi_{-2},$$

where A_n, B_n, and ψ_n stand for A_{v+n}, B_{v+n}, and ψ_{v+n}, respectively. Repeating this procedure and then using the orthogonality of the wavefunctions, we obtain the following expression for the first-order energy correction due to the "cubic anharmonicity" term:

$$E_v^{(1)} = \lambda[B_1^2(A_1+A_0) + A_0(B_1^2+B_0^2+A_0^2) + B_0^2(A_0+A_{-1})]. \tag{41}$$

Substitution of the exact expressions for the quantities A_n and B_n from Eq. (37) leads to an intractible result. Instead, one can expand in powers of $\nu = (v+\frac{1}{2})/(s+\frac{1}{2})$, recalling that the unperturbed energy [Eq. (17a)] can be written

$$E_v^{(0)} = D_e(-1+2\nu-\nu^2), \tag{42}$$

where we used Eqs. (9a) and (17b) to obtain

$$(s+\tfrac{1}{2})^2 t = 2D_e.$$

Making the approximation $s^2 \gg 1$, we obtained the following expansions for A_n and B_n^2:

$$A_n \approx 2\,\frac{v+n+\frac{1}{2}}{s+\frac{1}{2}} + 3\left(\frac{v+n+\frac{1}{2}}{s+\frac{1}{2}}\right)^2 + \cdots, \tag{43a}$$

$$B_n^2 \approx \frac{1}{2}\,\frac{v+n}{s+\frac{1}{2}} + \frac{7}{4}\left(\frac{v+n}{s+\frac{1}{2}}\right)^2 + \cdots. \tag{43b}$$

To this order, Eq. (41) can be approximated by

$$E_v^{(1)} \approx \lambda(6\nu^2+38\nu^3), \tag{44a}$$

which in spectroscopic notation[8] involves contributions to $\omega_e x_e$ and $\omega_e y_e$. By a similar process, the second-order energy correction was found to be

$$E_v^{(2)} \approx -(\lambda^2/8D_e)(15\nu^2+662\nu^3). \tag{44b}$$

Finally, the "quartic anharmonicity" produces a first-order correction

$$E_v'^{(1)} \approx \tfrac{1}{2}\mu(3\nu^2+69\nu^3). \tag{44c}$$

Defining dimensionless perturbation parameters

$$\eta = \tfrac{1}{2}\lambda/D_e, \quad \gamma = \tfrac{1}{2}\mu/D_e,$$

we obtain the following expression for the perturbed energy level to second order in η and first order in γ:

$$E_v = D_e\{-1+2\nu-[1-12\eta-3\gamma+(15/2)\eta^2]\nu^2 + [76\eta+69\gamma-331\eta^2]\nu^3+\cdots\}. \tag{45}$$

As a partial check of the above perturbation result, we considered a perturbation which changes the parameter a to $a' = a(1+\Delta)$ and D_e to $D_e' = D_e(1+\Delta)^{-2}$, which is equivalent to

$$(s'+\tfrac{1}{2}) = (s+\tfrac{1}{2})(1+\Delta)^{-2}, \tag{46a}$$

$$t' = t(1+\Delta)^2. \tag{46b}$$

Since in this case the perturbed oscillator is still a Morse oscillator, the energy shifts are exactly known, and given by

$$\Delta E_v = -D_e(2\Delta+\Delta^2)\nu^2. \tag{46c}$$

Recalling Eq. (39), this perturbation is equivalent to the power series perturbation,

$$V(u) = -D_e\Delta(au)^3 + (7/12)D_e(2\Delta+\Delta^2)(au)^4 + \cdots. \tag{47a}$$

The quantity $(e^{au}-1)^3$ has the power series expansion

$$(e^{au}-1)^3 = (au)^3 + (3/2)(au)^4 + \cdots, \tag{47b}$$

from which we deduce that the perturbation of Eq. (47a) is equivalent to our cubic plus quartic perturbation with the following values for the perturbation parameters:

$$\eta = -\tfrac{1}{2}\Delta, \quad \gamma = (4/3)\Delta + (7/24)\Delta^2. \tag{47c}$$

Substituting these values into Eq. (45), we obtain

$$\Delta E_v = D_e(-2\Delta-\Delta^2)\nu^2 + [54\Delta - (641/8)\Delta^2]\nu^3 + \cdots, \tag{48}$$

which agrees with Eq. (46c) to order ν^2. (To obtain agreement to order ν^3, one would have to include higher-order perturbations and higher-order power series terms.)

VI. CONCLUSIONS

We have demonstrated a practicable method for applying perturbations of the form $(e^{au}-1)^n$ to a Morse oscillator and obtaining perturbations of any desired order. Since a linear combination of such perturbations is equivalent to a power series for small au, the method may conveniently be applied to potentials describing actual diatomic molecules, yielding analytic expressions for both eigenfunctions and eigenvalues. The resulting expressions are power series in $(v+\frac{1}{2})/(s+\frac{1}{2})$, which makes for easy comparison with empirical formulas, as well as indicating the convergence properties of the approximations.

APPENDIX: EVALUATION OF INTEGRALS

In order to relate the type-B and type-F solutions in Eq. (31), we need the value of the integral

$$\int_{-\infty}^{\infty} |R_n^s|^2 e^{2x}\,dx.$$

In a manner analogous to our derivations of Eqs. (36c) and (37), we can derive the following recurrence relation from Eq. (16):

$$e^x R_n^s = [(s+n+1)(s-n+1)]^{1/2} R_n^{s+1} + (2s+1)R_n^s + [(s+n)(s-n)]^{1/2} R_n^{s-1}. \tag{A1}$$

Multiplying this expression by e^x and expanding each term of the form $e^x R_n^{s'}$ on the right-hand side, we obtain

$$\begin{aligned} e^{2x}R_n^s = {} & [(s+n+1)(s+n+2)(s-n+1)(s-n+2)]^{1/2} R_n^{s+2} \\ & + 4(s+1)[(s+n+1)(s-n+1)]^{1/2} R_n^{s+1} \\ & + [(s+n+1)(s-n+1) + (2s+1)^2 + (s+n)(s-n)] R_n^s \\ & + 4s[(s+n)(s-n)]^{1/2} R_n^{s-1} \\ & + [(s+n)(s-n)(s+n-1)(s-n-1)]^{1/2} R_n^{s-2}. \end{aligned} \tag{A2}$$

Multiplying Eq. (A2) by R_n^s and integrating, we obtain integrals of the form $\int R_n^s R_n^{s+k}\,dx$, with $k = 0, \pm 1, \pm 2$. For $k=0$ the integral is unity, due to the normalization of R_n^s. The other integrals do not vanish, as the orthogonality property of R_n^s is for different n, not different s.

We evaluate the integrals for $k \neq 0$ by using a modification of a technique used by IH, involving an extensive

use of raising and lowering operators. For $k=-1$ we replace R_n^s with $\beta_n^-(s)R_n^{s-1}$, and write

$$\int R_n^{s-1}R_n^s\,dx=[(s+n)(s-n)]^{-1/2}\times\int R_n^{s-1}(\tfrac{1}{2}e^x-s-d/dx)R_n^{s-1}\,dx. \quad \text{(A3)}$$

Using the mutually adjoint properties of the raising and lowering operators, we integrate by parts, then add and subtract a term:

$$\begin{aligned}\int R_n^{s-1}R_n^s\,dx&=[(s+n)(s-n)]^{-1/2}\int[(\tfrac{1}{2}e^x-s+d/dx)R_n^{s-1}\,dx\\&=[(s+n)(s-n)]^{-1/2}\int\{[\tfrac{1}{2}e^x-(s-1)\\&\quad+d/dx]R_n^{s-1}\}R_n^{s-1}\,dx-[(s+n)(s-n)]^{-1/2}\\&\quad\times\int(R_n^{s-1})^2\,dx.\end{aligned} \quad \text{(A4)}$$

The last integral has the value unity while by Eq. (16a) the operator in the other term is proportional to $\beta_n^+(s-1)$. Thus we obtain

$$\int R_n^{s-1}R_n^s\,dx=\left(\frac{(s+n-1)(s-n-1)}{(s+n)(s-n)}\right)^{1/2}\times\int R_n^{s-2}R_n^{s-1}\,dx-[(s+n)(s-n)]^{-1/2}. \quad \text{(A5)}$$

If we apply this procedure over and over a total of $(s-n)$ times, we finally obtain

$$\begin{aligned}\int R_n^{s-1}R_n^s\,dx&=\left(\frac{2n+1}{(s+n)(s-n)}\right)^{1/2}\\&\quad\times\int[(\tfrac{1}{2}e^x-n+d/dx)R_n^n]R_n^n\,dx\\&\quad-[(s+n)(s-n)]^{-1/2}(s-n).\end{aligned} \quad \text{(A6)}$$

The first term on the right-hand side vanishes because R_n^n satisfies Eq. (15a), and we obtain

$$\int R_n^{s-1}R_n^s\,dx=-[(s-n)/(s+n)]^{1/2}. \quad \text{(A7)}$$

In similar fashion, we evaluate $\int R_n^{s-2}R_n^s\,dx$ by replacing R_n^s with $\beta_n^+(s)$, then integrating by parts, to obtain

$$\begin{aligned}\int R_n^{s-2}R_n^s\,dx&=[(s+n)(s-n)]^{-1/2}\\&\quad\times\int\{[\tfrac{1}{2}e^x-(s-2)+d/dx]R_n^{s-2}R_n^{s-1}\,dx\\&\quad-2[(s+n)(s-n)]^{-1/2}\int R_n^{s-2}R_n^{s-1}\,dx\\&=\left(\frac{(s+n-2)(s-n-2)}{(s+n)(s-n)}\right)^{1/2}\int R_n^{s-3}R_n^{s-1}\,dx\\&\quad+\left(\frac{4(s-n-1)}{(s+n-1)(s+n)(s-n)}\right)^{1/2},\end{aligned} \quad \text{(A8)}$$

where we used Eq. (A7) to evaluate an integral. Applying this procedure over and over $(s-n-1)$ times, we finally obtain

$$\begin{aligned}\int R_n^{s-2}R_n^s\,dx&=(\text{const})\int\beta_n^+(n)R_n^nR_n^{n+1}\,dx\\&\quad+2[(s+n)(s-n)(s+n-1)(s-n-1)]^{-1/2}\\&\quad\times\sum_{k=1}^{s-n-1}(s-n-k)\\&=\left(\frac{(s-n)(s-n-1)}{(s+n)(s+n-1)}\right)^{1/2}.\end{aligned} \quad \text{(A9)}$$

Multiplying Eqs. (A1) and (A2) by R_n^s and integrating, and then using Eqs. (A7) and (A9) to evaluate integrals of the form $\int R_n^sR_n^{s'}\,dx$, we obtain

$$\int_{-\infty}^{\infty}R_n^s\,e^xR_n^s\,dx=2n, \quad \text{(A10)}$$

$$\int_{-\infty}^{\infty}R_n^s\,e^{2x}R_n^s\,dx=(2s+1)2n. \quad \text{(A11)}$$

*This work based in part on a M.S. Thesis by P.H. Dwivedi at Oklahoma University, Norman, Oklahoma, 1973.

[1] J. L. Dunham, Phys. Rev. **41**, 721 (1932).
[2] G. Wentzel, Z. Phys. **38**, 518 (1926); H.A. Kramers, Z. Phys. **39**, 828 (1926); L. Brillouin, Compt. Rend. **183**, 24 (1926).
[3] P.M. Morse, Phys. Rev. **34**, 57 (1929).
[4] R. Rydberg, Z. Phys. **73**, 376 (1931); O. Klein, Z. Phys. **76**, 226 (1932); J.T. Vanderslice *et al.*, J. Mol. Spectrosc. **3**, 17 (1959).
[5] C. L. Pekeris, Phys. Rev. **45**, 98 (1934).
[6] H.S. Heaps and G. Herzberg, Z. Phys. **133**, 48 (1952); R. Hermann and R.J. Rubin, Astrophys. J. **121**, 533 (1955).
[7] L. Infeld and T.E. Hull, Rev. Mod. Phys. **23**, 21 (1951), referred to in this work as IH.
[8] G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, New York, 1950), 2nd ed.
[9] D.S. Carlstone (private communication).
[10] P.A.M. Dirac, *Principles of Quantum Mechanics* (Clarendon, Oxford, 1958), 4th ed., pp. 136 ff.

The variational approach to the two-body density matrix

C. Garrod

University of California, Davis, California

M. V. Mihailović

J. Stefan Institute, University of Ljubljana, Ljubljana, Yugoslavia

Department of Theoretical Physics, University of Oxford, Oxford, England

M. Rosina

Faculty for Natural Sciences and Technology and J. Stefan Institute, University of Ljubljana, Ljubljana, Yugoslavia

(Received 20 June 1974)

A variational method for the two-body density matrix is developed for practical calculations of the properties of many-fermion systems with two-body interactions. In this method the energy $E = \Sigma H_{ijkl}\rho_{ijkl}$ is minimized using the two-body density matrix elements $\rho_{ijkl} = \langle\psi|(a_j^\dagger a_i^\dagger a_k a_l)|\psi\rangle$ as variational parameters. The approximation consists in satisfying only a subset of necessary conditions—the nonnegativity of the following matrices: the two-body density matrix, the "two-hole matrix" $Q_{ijkl} = \langle\Psi|a_j a_i a_k^\dagger a_l^\dagger|\Psi\rangle$ and the particle-hole matrix $G_{ijkl} = \langle\Psi|(a_i^\dagger a_j - \rho_{ij})^+ (a_k^\dagger a_l - \rho_k)|\Psi\rangle$. The idea of the method was introduced earlier; here some further physical interpretation is given and a numerical procedure for calculations within a small single-particle model space is described. The method is illustrated on the ground state of Be atom using $1s$, $2s$, $2p$ orbitals.

I. INTRODUCTION

We shall concern ourselves with the problem of calculating the physical properties of a many-fermion system in the ground state or certain excited states. We shall consider systems where the Hamiltonian has one-body and two-body interactions:

$$\hat{H} = \sum T_{ij} a_i^\dagger a_j + \tfrac{1}{2}\sum V_{ijkl} a_j^\dagger a_i^\dagger a_k a_l. \tag{1.1}$$

The operators $a_i^\dagger$ and a_i are creation and annihilation operators in a chosen single-particle representation. In the matrix elements T_{ij} the kinetic energy and the one-body interaction are contained. We shall express the energy associated with any N-particle state $|\psi\rangle$ as a linear function of the elements of the two-body density matrix

$$\rho_{ijkl} = \langle\psi|\, a_j^\dagger a_i^\dagger a_k a_l \,|\psi\rangle \tag{1.2}$$

in the form

$$E = \sum_{\substack{i<j \\ k<l}} H_{ijkl}\rho_{ijkl}. \tag{1.3}$$

The coefficients H_{ijkl} are given by

$$H_{ijkl} = (N-1)^{-1}(T_{ik}\delta_{jl} - T_{il}\delta_{jk} + \delta_{ik}T_{jl} - \delta_{il}T_{jk}) + V_{ijkl} - V_{ijlk}. \tag{1.4}$$

In this paper we present the elements of a method of computing the two-body density matrix ρ_{ijkl} directly without using the wavefunction (Sec. II). We shall refer to the method as the density matrix approach. In the density matrix approach we minimize the energy with respect to the two-body density matrix elements. The calculated two-body density matrix can then be used to compute several properties of the system. The idea of the method was introduced in Ref. 1, where several formal properties are discussed. Here we develop the method for practical calculations.

The motivation for this method comes from the fact that the two-body density matrix contains a much smaller number of independent parameters than the wavefunction (unless N is quite small). In order to illustrate this let us quote the number of parameters in both methods for the case of N fermions having at their disposal L single-particle states. There are $\frac{1}{4}L(L-1)[\frac{1}{2}L(L-1)+1]$ two-body density matrix elements while there are $\binom{L}{N}$ parameters needed to define the wavefunctions. Furthermore the symmetry properties of the system (rotational, spin, isospin, space inversion invariance, etc., if applicable) reduce the number of independent density matrix elements more efficiently than the number of parameters in the wavefunction.

However, variational calculations of density matrices have the major disadvantage that the two-body density matrix, in order to correspond to an N-fermion state, must satisfy certain complicated subsidiary conditions which are called in the literature N-representability conditions. This mathematical problem has been studied extensively by mathematicians, physicists, and quantum chemists[1–4] (and further references therein). The full set of necessary and sufficient conditions is not yet known explicitly. We present in Sec. III a set of necessary conditions which are manageable and with whose effectiveness we have some good experience.[5] By satisfying only a set of known conditions we can calculate an approximate solution to the variational problem. Because the set of restrictions is incomplete too much freedom is given to the variational parameters; therefore the approximate energy lies below the exact energy value obtainable with the chosen single-particle basis.

We discuss in Sec. IV the computational problems in the variational calculation of density matrices and we describe an algorithm based on linear programming. As an illustration we present in Sec. V the results of some calculations on the Be atom to show the feasibility of the method.

The density matrix approach can be used not only to calculate the two-body density matrix of the ground state, but also of those lowest excited states which have a different set of quantum numbers compared with the ground state. In this case one has to add the subsidiary conditions that the corresponding symmetry operators have the prescribed expectation values.

We would like to mention that there have been several attempts to calculate the properties of the N-particle system using the elements of the two-body density matrix as variational parameters. In the early attempts fewer conditions were used which were reasonable for simpler systems. The first lower bound formula was derived by Bopp[6] and it was successfully applied to 3-electron ions. Weidemann[7] and Hall and Post[7] made variational calculations of systems of particles interacting by different kinds of potentials, but without a central field. In particular they calculated a lower bound to triton energy. While these attempts dealt mostly with 3-particle systems, some more recent approaches introduce necessary conditions important for many-body systems (e.g. Refs. 8–10).

The status of all direct calculations of the two-body density matrix is still in a pioneering stage.

II. FORMULATION OF THE METHOD

While a wavefunction ψ uniquely determines the two-body density matrix the inverse is not true in general. There may exist no wavefunction, one or several wavefunctions related to a given matrix ρ_{ijkl} by the Eq. (1.2). Those matrices ρ_{ijkl} which have a solution for ψ are acceptable for an exact description of physical states.

The central problem in the variational calculations of density matrix is to find and satisfy the conditions which insure that the trial two-body density matrix corresponds to an N-fermion wavefunction.

It was shown[2] that the set of acceptable density matrices is a convex set and therefore all necessary conditions may be expressed as linear equalities and inequalities.[1]

A. Inequality constraints

We shall write the linear inequalities in the form

$$\sum_{\substack{i<j\\k<l}} h^{(\nu)}_{ijkl}\rho_{ijkl} \geq \epsilon_\nu, \quad (\nu = 1, \ldots, \infty). \tag{2.1}$$

The right-hand sides can be evaluated in principle for any choice of the coefficients $h^{(\nu)}_{ijkl}$ by introducing the two-body operator

$$\hat{h}^{(\nu)} = \sum_{\substack{i<j\\k<l}} h^{(\nu)}_{ijkl}\, a_j^\dagger a_i^\dagger a_k a_l \tag{2.2}$$

and by taking for ϵ_ν the lowest eigenvalue of $\hat{h}^{(\nu)}$ in the N-body space.[1] For any choice of coefficients $h^{(\nu)}_{ijkl}$, Eq. (2.1) is a necessary condition because for any N-body wavefunction ψ the expectation value $\langle\psi|\hat{h}^{(\nu)}|\psi\rangle$ is larger than or equal to the lowest eigenvalue of $\hat{h}^{(\nu)}$ and the same is true for $\sum h^{(\nu)}_{ijkl}\rho_{ijkl} \equiv \langle\psi|\hat{h}^{(\nu)}|\psi\rangle$ if ρ_{ijkl} is derived from ψ. The theorem has been proved[1] that the set of conditions (2.1) is also sufficient if $\hat{h}^{(\nu)}$ are all possible two-body operators.

The above theorem in the form presented does not seem useful, because in order to solve the desired N-body problem, one has to know the solution of an infinity of equally difficult N-body problems defined by $\hat{h}^{(\nu)}$, $(\nu = 1, \ldots, \infty)$. However, the theorem is a useful guide, if one is looking for a good approximate solution in which case one might employ only a subset of necessary conditions. The basic approximation is then defined by the choice of the subset $\hat{h}^{(\mu)}$.

Let us call $\tilde{E}$ the energy of the approximate ground state obtained with the conditions arising from the chosen set of operators $h^{(\mu)}$. As the number of conditions defined by $h^{(\mu)}$ may still be infinite one has to construct a procedure for selecting a finite sequence of $h^{(\mu_i)}$ so that the successive approximations $\tilde{E}_i$ converge to $\tilde{E}$. A possible procedure will be described in Sec. IV.

B. Equality constraints

In one type of equalities we impose the desired expectation values of the symmetry operators such as the number operator $\hat{N}$ and the angular momentum operator $\hat{\mathbf{J}}$

$$\langle\psi|\mathbf{N}^2|\psi\rangle = N^2, \tag{2.3}$$

$$\left.\begin{aligned}\langle\psi|\hat{\mathbf{J}}_2|\psi\rangle &= J(J+1)\\ \langle\psi|\hat{\mathbf{J}}_3|\psi\rangle &= M\end{aligned}\right\}, \tag{2.4}$$

$$\langle\psi|\hat{Q}(\hat{J}_3 - M)|\psi\rangle = 0. \tag{2.5}$$

Here $\hat{Q}$ is any one-body operator. These equalities are linear equalities for the two-body density matrix.

By imposing these equalities we are looking for the solution only within a chosen subspace. Equation (2.3) normalizes the two-body density matrix corresponding to N particles. With Eqs. (2.4) and (2.5) we can distinguish the calculation of the lowest excited state with chosen quantum numbers J and M from the calculation of the ground state.

If necessary and sufficient conditions (2.1) and (2.3) are satisfied the variational calculation without restrictions (2.4) and (2.5) would automatically give the ground state with the correct expectation value for the expressions (2.4) and (2.5). In the calculation of the ground state these restrictions reduce the number of independent variational parameters. If, however, only a subset of conditions (2.1) is taken into account, the expectation values (2.4) and (2.5) would sometimes come out wrong; imposing the *a priori* known correct values then improves the approximate result.

The second type of equalities refers to those N-body states $|\psi\rangle$ whose energy is stationary with respect to one-body transformations $|\psi\rangle \to \exp(\alpha\hat{Q})|\psi\rangle$, so that in the expansion

$$\langle\exp(\alpha\hat{Q})\psi|\hat{H}|\exp(\alpha\hat{Q})\psi\rangle = \langle\psi|\hat{H}|\psi\rangle + \alpha\langle\psi|[\hat{H},\hat{Q}]|\psi\rangle + (\alpha^2/2)\langle\psi|[\hat{Q},[\hat{H},\hat{Q}]]|\psi\rangle + \cdots$$

the linear term vanishes:

$$\langle\psi|[\hat{H},\hat{Q}]|\psi\rangle=0. \tag{2.6}$$

For eigenstates of the Hamiltonian, such a relation is valid for any operator $\hat{Q}$, but we can use the relation only with one-body operators $\hat{Q}$ because only then is the relation expressible in terms of the two-body density matrix. If the two-body density matrix is a solution of a variational calculation, the energy is a fortiori minimized with respect to one-body transformations and the relation (2.6) is satisfied automatically. But it is a useful restriction because it reduces the number of free parameters for trial density matrices.

III. BASIC APPROXIMATION—RESTRICTION TO SOME MANAGEABLE CONDITIONS

We are able to satisfy only some necessary conditions for the trial two-body density matrix. Therefore there will in general exist no wavefunction ψ corresponding to the trial two-body density matrix through the relation (1.2). The resulting two-body density matrix has a physical meaning in the sense that it offers an approximation to the expectation values of one and two-body operators.

We present here a subset of necessary conditions which is numerically manageable, with whose relevance we have had some good experience[5] and for which we can give a physical interpretation. The conditions have the form (2.1) and are defined by the following operators:

$$\hat{h}^{(\alpha)}=A_\alpha^\dagger A_\alpha,\ A_\alpha=\sum_{i<j}x_{ij}^\alpha a_i a_j, \tag{3.1}$$

$$\hat{h}^{(\beta)}=A_\beta A_\beta^\dagger, \tag{3.2}$$

$$\hat{h}^{(\gamma)}=B_\gamma^\dagger B_\gamma,\ B_\gamma=\sum_{i,j}z_{ij}^\gamma(a_i^\dagger a_j-c_{ij}^\gamma). \tag{3.3}$$

Here the coefficients x_{ij}, z_{ij}, and c_{ij} assume all possible values. The lowest eigenvalues of the operators $\hat{h}^{(\alpha)}$ and $h^{(\beta)}$ in the N-body space are $\epsilon_\alpha=0$ and $\epsilon_\beta=0$. The eigenvalues of the operators $h^{(\gamma)}$ cannot be obtained easily, but they are obviously larger than or equal to zero. In this paper we replace ϵ_γ on the r.h.s. of Eq. (2.1) by zero, which leads to a slightly weaker necessary condition.

It has been shown[1] that the conditions generated by the operators $h^{(\gamma)}$ with ϵ_γ put equal to zero are all contained in the subset in which one takes $c_{ij}=\rho_{ij}$, where

$$\rho_{ij}=\sum_k\rho_{ikjk}/(N-1). \tag{3.4}$$

It would be sufficient to consider only operators $\hat{h}^{(\gamma)}$ with $c_{ij}=\rho_{ij}$, but the corresponding inequalities would then be nonlinear. As we use an iterational procedure, we keep the conditions linear by choosing c_{ij} equal to the value of ρ_{ij} from the previous iteration. When ρ_{ij} converges towards the solution this is equivalent to choosing $c_{ij}=\rho_{ij}$.

Let us give some further interpretation of these conditions. The condition generated by Eq. (3.1) is equivalent to the nonnegativity of the two-body density matrix. This can be seen by writing the coefficients $h_{ijkl}^{(\alpha)}$ in the form $h_{ijkl}^{(\alpha)}=x_{ij}^\alpha x_{kl}^\alpha$, so that the corresponding inequality can be written as

$$\sum_{i<j,k<l}x_{ij}^\alpha\rho_{ijkl}x_{kl}^\alpha\geq 0. \tag{3.5}$$

This implies that all eigenvalues are nonnegative.

The condition generated by Eq. (3.2) is equivalent to the nonnegativity of the "two-hole density matrix"

$$Q_{ijkl}=\rho_{ijkl}-\rho_{ki}\delta_{jl}+\rho_{li}\delta_{jk}+\delta_{ik}(\delta_{jl}-\rho_{lj})-\delta_{il}(\delta_{jk}-\rho_{kj}). \tag{3.6}$$

By rewriting the operator (3.2) so that the creation and annihilation operators appear in normal order one gets the inequality (2.1) in the form

$$\sum x_{ij}Q_{ijkl}x_{kl}\geq 0. \tag{3.7}$$

Let us note that when a wavefunction ψ exists the two-hole density matrix takes the form:

$$Q_{ijkl}=\langle\psi|a_j a_i a_k^\dagger a_l^\dagger|\psi\rangle. \tag{3.8}$$

Similarly, the condition generated by Eq. (3.3) where $c_{ij}=\rho_{ij}$ is equivalent to the nonnegativity of the "particle—hole matrix"

$$G_{ijkl}=\rho_{jkil}+\delta_{ik}\rho_{jl}-\rho_{ij}\rho_{kl} \tag{3.9}$$

in the following way

$$\sum z_{ij}G_{ijkl}z_{kl}\geq 0. \tag{3.10}$$

It is instructive to write also the particle—hole matrix in terms of the wavefunction.

$$G_{ijkl}=\langle\psi|(a_i^\dagger a_j-\rho_{ij})^*(a_k^\dagger a_l-\rho_{kl})|\psi\rangle. \tag{3.11}$$

It is worthwhile to point out that for N-representable ρ_{ijkl} the first subset of conditions (3.1) guarantees the nonnegativity of the norms of the states $A|\psi\rangle$ having $N-2$ particles, which is evident from the form $\langle\psi|(\sum x_{ij}a_i a_j)^*(\sum x_{kl}a_k a_l)|\psi\rangle\geq 0$. Similarly, the second subset of conditions guarantees the nonnegative norms of the "$(N+2)$-particle" states $A^\dagger|\psi\rangle$ and the third guarantees the nonnegative norms of "particle—hole" states $B|\psi\rangle$. Let us conclude by listing three types of manageable inequality constraints which we know so far.

(i) The constraints generated by the operators $\hat{h}^{(\alpha)}$, $\hat{h}^{(\beta)}$, and $\hat{h}^{(\gamma)}$, Eqs. (3.1), (3.2), and (3.3) which we use in the present paper.

(ii) The constraints generated by the Casimir operators for certain Lie algebras or such operators which mix only few representations of the group. Important inequality constraints are probably generated by those groups, which have already been used to derive approximate wave functions for the problem under consideration.

(iii) The constraints generated by general two-body operators which have nonzero matrix elements in a smaller single particle basis and hence may be diagonalized numerically. These constraints ensure all necessary conditions at least in the subspace in which the two-body density matrix has dominant components. The con-

TABLE I. The Hamiltonian and the two-body density matrix elements of the Be atom. [a]

$n_1 l_1$	$n_2 l_2$	$n_3 l_3$	$n_4 l_4$	L S	$H^{LS}_{ijkl}/\eta_{ij}\eta_{kl}$ [b]	$\rho^{LS}_{ijkl}/\eta_{ij}\eta_{kl}$	
						Density matrix approach	Complete diagonalization
1 0	1 0	1 0	1 0	0 0	−3.0217238	0.999918	0.999916
2 0	1 0	1 0	1 0	0 0	−0.1767351	−0.002355	−0.002382
2 0	1 0	2 0	1 0	0 0	−2.6707742	0.929191	0.929222
2 0	2 0	1 0	1 0	0 0	0.0253498	0.000495	0.000498
2 0	2 0	2 0	1 0	0 0	0.0843677	−0.000016	−0.000017
2 0	2 0	2 0	2 0	0 0	−0.7160670	0.929116	0.929145
2 1	2 1	1 0	1 0	0 0	−0.0250858	0.002017	0.002025
2 1	2 1	2 0	1 0	0 0	−0.0394407	0.008525	0.008622
2 1	2 1	2 0	2 0	0 0	−0.1325608	0.256489	0.256437
2 1	2 1	2 1	2 1	0 0	−0.5878038	0.070887	0.070859
2 0	1 0	2 0	1 0	0 1	−2.7214738	0.929113	0.929142
2 1	2 1	2 1	2 1	1 1	−0.6990588	0.000000	0.000000
2 1	1 0	2 1	1 0	1 0	−2.6516514	0.023615	0.023605
2 1	2 0	2 1	1 0	1 0	0.0440854	−0.000559	−0.000565
2 1	2 0	2 1	2 0	1 0	−0.7682196	0.000014	0.000015
2 1	1 0	2 1	1 0	1 1	−2.6226850	0.023615	0.023605
2 1	2 0	2 1	1 0	1 1	0.0762886	−0.000559	0.000565
2 1	2 0	2 1	2 0	1 1	−0.6151516	0.000014	0.000015
2 1	2 1	2 1	2 1	2 0	−0.6545568	0.000000	0.000000

[a] For notation see Appendix B.
[b] $\eta_{ij} = (1+\delta_{ij})^{1/2}$.

straints (ii) and (iii) are to be studied in future.

IV. NUMERICAL PROCEDURE

In the variational calculation of the two-body density matrix we use an iterative numerical procedure which contains linear programming. We were motivated to use this procedure because the energy (1.3) to be minimized is a linear function of the variational parameters ρ_{ijkl} and the subsidiary conditions can be written as linear equalities and inequalities.

In order to obtain the zeroth approximation we impose all equalities of the type (2.3), (2.4), (2.5), and (2.6) and we confine each matrix element ρ_{ijkl} with inequalities $0 \leq \rho_{ijij} \leq 1$, $-1 \leq \rho_{ijkl} \leq 1$ which are contained in the inequalities (3.5) and (3.7). With these conditions, the minimum of the energy is calculated with linear programming.

The successive approximations are obtained by the following iterative cycle: we construct the most violated condition, add it to the previous ones and minimize the energy with linear programming. In order not to work with an increasing number of conditions, we then discard one of the old conditions. A program for linear programming which at each iteration adds one new condition and discards one old condition is presented in Appendix A.

The most violated condition (3.5) is obtained by diagonalizing the two-body density matrix from the previous iteration. The eigenvector $x^{\min}$ corresponding to the most negative eigenvalue $\lambda_{\min}$ then generates the condition $\lambda_{\min} = \sum x^{\min}_{ij} \rho_{ijkl} x^{\min}_{kl} \geq 0$ which is violated by the amount $\lambda_{\min}$. The coefficients of the inequalities in the form (2.1) are $h_{ijkl} = x^{\min}_{ij} x^{\min}_{kl}$. Optionally one can add several conditions in each iteration by constructing them from the eigenvectors of several lowest negative eigenvalues. New conditions (3.7) and (3.10) for the two-hole density matrix Q and the particle-hole matrix G are constructed in a similar way. One constructs the Q matrix or G matrix from the parameters ρ_{ijkl}, diagonalizes it and constructs the coefficients for the inequality from the eigenvector corresponding to the most negative eigenvalue. The construction of the G matrix and of the corresponding coefficients h_{ijkl} usually requires the recoupling of angular momentum. The corresponding formulas are given in Appendix B. In our program we add the ρ-matrix, Q-matrix and G-matrix conditions sequentially in consecutive iterations.

V. ILLUSTRATION OF THE METHOD

The proposed method faces two major problems: (i) As the approximation we satisfy only some necessary conditions on the two body density matrix. The question is whether the conditions proposed in this paper are adequate for a system of physical interest. (ii) The iterative procedure described in Sec. IV selects a finite sequence from an infinite number of conditions. It should be examined whether and how fast this procedure converges.

Our present experience is that both answers depend on the properties of the physical system. The results of our variational calculations on the nuclei ^{16}O and ^{20}Ne using a model with four valence particles are quite satisfactory compared with several other methods. In calculations with more valence particles (^{24}Mg and ^{28}Si) further conditions seem to be needed.

For illustration of the method we present here a calculation for the Be atom. As a model we restrict the single-particle space to three orbitals ($1s$, $2s$, $2p$) similar to the oribitals $1s$, $2s$, and p_I in Ref. 11. The corresponding matrix elements of the Hamiltonian are given in Table I. The small single-particle basis is not

TABLE II. Ground state energy of the Be atom, calculated within the 1s, 2s, 2p shells.

Density matrix approach	−14.60999 atomic units
Complete diagonalization	−14.609987
Hartree–Fock	−14.57299
Experimental	−14.66745

sufficient for a precise description of Be, but it does give the ground state energy half-way between the Hartree–Fock value and the experimental value. Thus the illustration has some physical relevance. In addition, it contributes to the compilation of examples which have as a purpose to test the new method. Results are given in Tables I and II. The agreement with the exact result of the model is good which shows that the chosen conditions are adequate for this model.

In the calculation of the Be atom the convergence of the algorithm is satisfactory (270 iterations for the relative accuracy of 10^{-6}). We have used this algorithm for systems of up to 70 variational parameters. For a larger number of parameters we are preparing a faster procedure.

VI. CONCLUSION

In this paper we have shown the feasibility of the density matrix approach. The method provides the energy and the two-body density matrices of the ground state and some excited states.

Regarding the calculation of the energy, this method gives a lower bound to the eigenenergy of the Hamiltonian restricted to a chosen single-particle basis. In this sense it is complementary to the variational methods with wavefunctions (such as configuration mixing, projected Hartree–Fock, generator coordinate method) which yield an upper bound to the energy. In cases where the results of a wavefunction calculation are available and where the gap between the lower and upper bound is small the two methods provide a rather complete answer which is useful especially for those models of physical systems where a complete diagonalization is no longer feasible.

Since the energy determined by this method will increase as the number of restrictions is increased but decrease as the orbital basis is increased it may turn out to be either larger or smaller than the true ground state energy.

The calculated two-body density matrix provides the expectation value of any one and two-body operator. This suffices to calculate most static properties of physical interest. In addition the two-body density matrix of the ground state offers the required input data for the calculation of those excited states which can be described within the particle–hole space.[12] Recently excellent ionization energy calculations have been made[13] using a method which requires only the two-particle density matrix of the neutral atom as input.[14]

Our present experience with the approximation of satisfying only some necessary conditions is encouraging in most cases. In some cases, for which preliminary calculations have been performed, some important class of conditions still seems to be lacking. We have, however, not used all presently known explicit conditions in these calculations. Only further study will show which conditions are relevant for individual physical systems. Some examples of classes of conditions which have not been employed in the calculations of the authors are:

(i) The constraints of the form

$$\sum B_{ij} G_{ijkl} B_{kl} \geq \epsilon_B,$$

where B_{ij} is any Hermitian matrix and ϵ_B is a positive constant which can be explicitly calculated.[9] In this paper we have used the weaker condition $\epsilon_B = 0$.

(ii) The constraints generated by the Casimir operators for certain Lie algebras or such operators which mix only a few representations of the group.

(iii) The constraints generated by general two-body operators which have nonzero matrix elements in a smaller single particle basis and hence may be diagonalized numerically.

ACKNOWLDGMENTS

The authors C. G. and M. R. would like to thank Professor A. J. Coleman and R. M. Erdahl for the stimulating interest and for the fine hospitality they received at Queen's University, Kingston, Ontario where this work was initiated. One of the authors (M. R.) would like to acknowledge the fine hospitality at the University of California at Davis where part of this work was done. Thanks are also due to N. Mankoč-Borštnik for some critical remarks. M. V. M. would like to acknowledge some critical comments of R. E. Peierls.

APPENDIX A

An algorithm for linear programming with inequalities generated in consecutive iterations. We minimize the function

$$E = \sum_{i=1}^{n} H_i V_i,$$

where H_i are given coefficients and V_i are variational parameters. The variational parameters must satisfy the following equalities and inequalities:

$$\sum_i a_i^\alpha V_i = b^\alpha, \quad \alpha = 1, \ldots, e$$

$$\sum_i a_i^\beta V_i \geq b^\beta, \quad \beta = e+1, \ldots, \infty.$$

The coefficients of equalities a_i^α and b^α are given in advance, while the coefficients of inequalities a_i^β and b^β are generated in consecutive iterations.

(i) In the zeroth iteration, the function E is minimized with the constraints $l_i \leq V_i \leq u_i$. The lower and upper bound l_i and u_i are given in advance. They are not taken care of in consecutive iterations unless the program which generates inequalities presents them as an in-

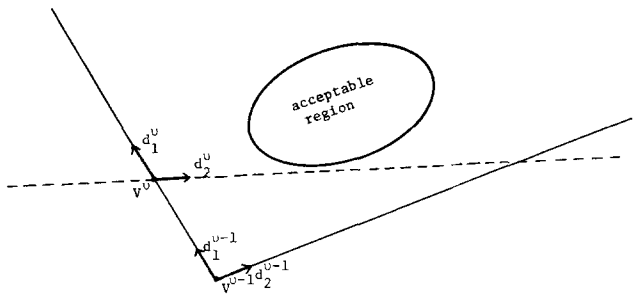

FIG. 1.

equality when then get violated. In the zeroth iteration, we get

$$\begin{cases} V_i^0 = & l_i \\ & u_i \end{cases} \text{ if } \begin{matrix} H_i \geq 0 \\ H_i < 0 \end{matrix}$$

$$\begin{cases} d_{mi}^0 = & \delta_{mi} \\ & -\delta_{mi} \end{cases} \text{ if } \begin{matrix} H_i \geq 0 \\ H_i < 0 \end{matrix}, \quad m = 1, \ldots n.$$

The quantity d has the geometrical interpretation as the set of m edges pointing upwards from the vertex V (Fig. 1).

(ii) The equalities are imposed one in each iteration by intersecting the edges with the corresponding hyperplane and choosing the lowest intersection

$$v_{mi}^\nu = V_i^{\nu-1} + d_{mi}^{\nu-1}(b^\nu - \sum_j a_j V_j^{\nu-1}) / \sum_j a_j^\nu d_{mj}^{\nu-1}.$$

$V_i^\nu = v_{mi}^\nu$ for that index $m = \tilde{m}_\nu$ for which $\sum_i v_{mi}^\nu H_i = \min$ under the condition that

$$(b^\nu - \sum_j a_j^\nu V_j^{\nu-1}) / \sum_j a_j^\nu d_{mj}^{\nu-1} > 0.$$

$$\tilde{d}_{mi}^\nu = \pm (v_{mi}^\nu - V_i^\nu) \text{ if } (b^\nu - \sum_j a_j^\nu V_j^{\nu-1}) / \sum_j a_j^\nu d_{mj}^{\nu-1} \begin{matrix} > 0 \\ < 0 \end{matrix}$$

$$d_{mi}^\nu = \tilde{d}_{mi}^\nu \left[\sum_j (\tilde{d}_{mj}^\nu)^2 \right]^{-1/2}.$$

In each iteration, the index m runs over $m = 1, \ldots, n$, $m \neq \tilde{m}_1, \tilde{m}_2 \ldots \tilde{m}_{\nu-1}$ so in each iteration one additional value of m is omitted.

(iii) After having introduced all equalities, in each iteration one inequality is imposed by the same algorithm as in step (ii) except that the index $m = \tilde{m}_\nu$ is no longer omitted. The index runs $m = 1, \ldots, n; m \neq \tilde{m}_1 \ldots \tilde{m}_e$. In this way, the inequalities for $\beta = \nu - n, \ldots \nu$ are satisfied while some of the previous ones may get violated again.

(iv) The program is terminated when one of the following conditions is fulfilled:

(a) $E^\nu \leq E^{\nu-10} + \epsilon$ (we take $\epsilon = 10^{-6}$),

(b) when no inequality violated by more than ϵ is found,

(c) $\nu > \nu_{\max}$, where $\nu_{\max}$ is given in advance.

In the calculation, precaution is taken against divisions with too small denominators. If for any $\bar{m}$, $|\sum_j a_j^\nu d_{\bar{m}j}^{\nu-1}| < \epsilon$, it is avoided to choose $\tilde{m} = \bar{m}$ and we put put $\tilde{d}_{\bar{m}i}^\nu = d_{\bar{m}i}^{\nu-1}$. If an equality is almost linearly dependent on the previous ones (if $|\sum_j a_j^\nu d_{mj}^{\nu-1}| < \epsilon$ for all m and $|b^\nu - \sum_j a_j^\nu V_j^{\nu-1}| < \epsilon$) it is ignored. If an equality is incompatible with the previous ones (if $|\sum_j a_j^\nu d_{mj}^{\nu-1}| < \epsilon$ for all m and $|b - \sum_j a_j^\nu V_j^{\nu-1}| > \epsilon$) the calculation is terminated.

APPENDIX B

Recoupling of angular momenta for the Q and G matrix and the coefficients h. (We present the formulas only for orbital angular momentum coupling. Similar coupling must be done for spin, leading to the matrices ρ^{LS}, Q^{LS}, and G^{LS}.) Single particle wavefunctions are defined by the quantum numbers $i = (n_i, l_i)$ and m_i. Due to the time reversal symmetry, all quantities are taken to be real. The following definitions and phase conventions are used:

$$\rho_{ijkl}^L = \frac{1}{2L+1} \sum_M \langle \psi | \left(\sum_{m_i m_j} C_{l_i m_i l_j m_j}^{LM} a_{i m_i} a_{j m_j} \right)^+ \times \left(\sum_{m_k m_l} C_{l_k m_k l_l m_l}^{LM} a_{k m_k} a_{l m_l} \right) | \psi \rangle,$$

$$Q_{ijkl}^L = \frac{1}{2L+1} \sum_M \langle \psi | \left(\sum_{m_i m_j} C_{l_i m_i l_j m_j}^{LM} a_{i m_i} a_{j m_j} \right) \times \left(\sum_{m_k m_l} C_{l_k m_k l_l m_l}^{LM} a_{k m_k} a_{l m_l} \right)^+ | \psi \rangle,$$

$$G_{ijkl}^L = \frac{1}{2L+1} \sum_M \langle \psi | \left\{ \sum_{m_i m_j} (-1)^{l_j + m_j} C_{l_i m_i l_j m_j}^{LM} \times (a_{i m_i}^+ a_{j -m_j} - \delta_{L0} \rho_{ij}) \right\}^+ \times \left\{ \sum_{m_k m_l} (-1)^{l_l + m_l} C_{l_k m_k l_l m_l}^{LM} (a_{k m_k}^+ a_{l -m_l} - \delta_{L0} \rho_{kl}) \right\} | \psi \rangle,$$

$$\rho_{ij} = \delta_{l_i l_j} \frac{1}{2L+1} \sum_M \langle \psi | a_{iM}^+ a_{jM} | \psi \rangle,$$

$$\sum_{\substack{i \leq j \\ k \leq l}, L} h_{ijkl}^L \rho_{ijkl}^L \geq \epsilon.$$

The relations are as follows:

$$\rho_{ij} = \delta_{l_i l_j} \frac{1}{N-1} \sum_{kL} \frac{2L+1}{2l_i+1} \rho_{ikjk}^L,$$

$$Q_{ijkl}^L = \rho_{klij}^L - \delta_{ik}\rho_{lj} - \delta_{jl}\rho_{ki} + \delta_{ik}\delta_{jl} - (-1)^{L-l_k-l_l}(-\delta_{il}\rho_{kj} - \delta_{jk}\rho_{li} + \delta_{il}\delta_{jk}),$$

$$G_{ijkl}^L = -\sum_J (-1)^{l_i - l_j + l_k - l_l} (2J+1) W(l_j l_i l_k l_l, LJ) \rho_{kjil}^J + \delta_{ik}\rho_{jl} - [(2l_i+1)(2l_k+1)]^{1/2} \delta_{L0} \rho_{ij} \rho_{kl}.$$

The coefficients for inequalities are constructed from the following eigenvectors:

$\sum_{kl} \rho_{ijkl}^J x_{kl}^J = \lambda x_{ij}^J$ for the inequality corresponding to (3.1) to (3.1),

$\sum_{kl} Q_{ijkl}^J y_{kl}^J = \lambda' y_{ij}^J$ for the inequality corresponding to (3.2),

$\sum_{kl} G_{ijkl}^J z_{kl}^J = \lambda'' z_{ij}^J$ for the inequality corresponding to (3.3);

$$h^L_{ijkl}=\{\tilde{h}_{ijkl}-(-1)^{L-l_i-l_j}\tilde{h}_{jikl}-(-1)^{L-l_k-l_l}\tilde{h}_{ijlk}$$
$$+(-1)^{l_i+l_j-l_k-l_l}\tilde{h}_{jilk}\}/(1+\delta_{ij})(1+\delta_{kl});$$

(i) $\tilde{h}^L_{ijkl}=\delta_{LJ}x^J_{ij}x^J_{kl}, \quad \epsilon=0,$

(ii) $\tilde{h}^L_{ijkl}=\delta_{LJ}y^J_{ij}y^J_{kl}-\sum_m y^J_{mj}y^J_{ml}\delta_{l_jl_l}\delta_{ik}(2L+1)/$
$$(2l_j+1)(N-1), \quad \epsilon=-2,$$

(iii) $\tilde{h}^L_{ijkl}=-(-1)^{l_i-l_j+l_k-l_l}(2L+1)\,W(l_jl_kl_il_l,JL)\,z^J_{kj}z^J_{il}$
$$+\sum_m z^J_{mj}z^J_{ml}\,\delta_{l_jl_l}\delta_{ik}\,(2L+1)/(2l_j+1)(N-1)$$
$$-2[(2l_i+1)(2l_k+1)]^{1/2}\delta_{J0}\left[\sum_{mn}z_{mn}\rho_{mn}\right]z_{jl}\,\delta_{l_jl_l}\delta_{ik}$$
$$\times(2L+1)/(2l_j+1)(N-1), \quad \epsilon=-[(2l_i+1)(2l_k+1)]^{1/2}$$
$$\times\delta_{J0}\left[\sum_{mn}z_{mn}\rho_{mn}\right]^2.$$

[1]C. Garrod and J.K. Percus, J. Math. Phys. **5**, 1756 (1964).
[2]A.J. Coleman, Rev. Mod. Phys. **35**, 668 (1963).
[3]H. Kummer, J. Math. Phys. **8**, 2063 (1967).
[4]A.J. Coleman and R.M. Erdahl, Eds., *Reduced Density Matrices with Applications to Physical and Chemical Systems*, Queen's Papers on Pure and Applied Mathematics No. 11 (Queen's University, Kingston, Ontario, 1968).
[5]M. Rosina, in *The Nuclear Many-Body Problem* (Proceedings of the Symposium, Rome, 19—23 September 1972) edited by F. Calogero and C. Ciofi degli Atti (Editrice Compository, Rome, 1973). M. Rosina, in *Sur de Recents Developpements en Physique Nucléaire Théorique* (Session d'Etudes de La Toussuire, 5—10 February 1973), edited by E. El Baz (Université Claude Bernard, Villeurbanne, France, 1973); M.V. Mihailović, in *Correlations in Nuclei* (Proceedings of the Symposium, Balatonfüred, Hungary, 3—8, September 1973), edited by J. Nemeth (OMKDK-Technoinform, Budapest, 1974).
[6]F. Bopp, Z. Physik **156**, 348 (1959).
[7]E.G. Weidemann, Nucl. Phys. **65**, 559 (1965); R.L. Hall and H.R. Post, Proc. Phys. Soc. A **69**, 936 (1956); **79**, 819 (1962); **90**, 381 (1967); R.L. Hall, Proc. Phys. Soc. **91**, 16 (1967).
[8]M.V. Mihailović and M. Rosina, Nucl. Phys. A **130**, 386 (1969).
[9]E.R. Davidson, J. Math. Phys. **10**, 725 (1969).
[10]L. Kijewski, Phys. Rev. **6**, 31 (1972).
[11]R.E. Watson, Phys. Rev. **119**, 170 (1960).
[12]M. Bouten, P. van Leuven, M.V. Mihailović, and M. Rosina, Nucl. Phys. A **202**, 127 (1973).
[13]O. Day and D.W. Smith, *Proceedings of the* 1974 *Density Matrix Conference at Queen's University*, edited by A.J. Colemand and R.M. Erdahl (Queen's University, Kingston, Ontario, Canada, to be published).
[14]O. Day, D.W. Smith, and C. Garrod, Int. J. Quant. Chem. (1974 Symposium Issue) (to be published).

Adiabatic expansions of solutions of coupled second-order linear differential equations. I*

S. A. Fulling†

Physics Department, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201
(Received 30 July 1974)

A generalized higher-order WKB approximation is found for the set of equations $h_j''(t) + u^2 \sum_{k=1}^{N} M_{jk}(t)h_k(t) = 0$ $(u \to \infty)$, when the coefficients M_{jk} form a positive definite Hermitian matrix $\mathbf{M}$ satisfying a smoothness condition as a function of t. In the construction, essential use is made of a transformation introduced by Kato to connect smoothly the eigenvectors of $\mathbf{M}(t)$ at different values of t. Eigenvalue degeneracies which exist for all t are covered by the method. The expansion breaks down at points t where the multiplicities of the eigenvalues of $\mathbf{M}(t)$ change; this phenomenon, analogous to the "turning point" problem of the ordinary WKB method, will be studied in a second paper. The asymptotic nature of the expansion is proved; error bounds can be extracted from the proof but are not studied here.

1. INTRODUCTION

We shall consider a system of coupled differential equations,

$$\frac{d^2h_j}{dt^2} + u^2 \sum_{k=1}^{N} M_{jk}(t)h_k = 0 \quad (j = 1, \ldots, N), \tag{1}$$

and seek approximate solutions which are valid in the limit of large u. (M_{jk} and h_j may take complex values; t is real; u is a positive real number.) Equation (1) can be written

$$\mathbf{h}''(t) + u^2\mathbf{M}(t)\mathbf{h}(t) = 0, \tag{2}$$

where $\mathbf{h}(t)$ is an N-component vector ($\mathbf{h} \in \mathbb{C}^N$) and $\mathbf{M}(t)$ is an $N \times N$ matrix. Setting $\tau = ut$ converts the equation to

$$\frac{d^2\mathbf{h}}{d\tau^2} + \mathbf{M}\left(\frac{\tau}{u}\right)\mathbf{h}(\tau) = 0. \tag{3}$$

The problem of the limit of large u in Eq. (2) is thus equivalent to the problem of the limit of slowly varying coefficients, or adiabatic limit, in an equation of the same form. The distinguishing feature of either limit is that the "wavelengths" characteristic of the solution are small compared to lengths characteristic of the variation of the coefficients. We use the word "adiabatic" to designate this particular sort of problem in asymptotic analysis.

When $N = 1$, the familiar WKB approximation is valid up to terms which decrease as u^{-1}, provided the function $M(t)$ is twice differentiable and bounded away from zero. Higher-order approximations, forming an asymptotic sequence with the WKB as first term, have been studied rigorously by Blumenthal[1] and Olver.[2] The results are summarized in Appendix A for the case that $M(t)$ is strictly positive. [In that appendix $M(t)$ is allowed to depend on u and is denoted by $p(u, t)$.] Our aim is to derive similar expansions for systems of equations ($N > 1$).

A standard method of studying second-order differential equations is to pass to an equivalent system of (twice as many) first-order equations. Indeed, many of the results of this paper could be extracted from the extensive literature on the adiabatic problem for first-order systems. (Especially relevant are the books of Feshchenko *et al.*[3]—discussed further in Appendix B—and of Wasow.[4]) That approach is probably the most efficient for proving theorems on the existence and uniqueness of asymptotic expansions. From the point of view of the physicist (or other user of applied mathematics), however, there are advantages, aesthetic and practical, in working with the second-order equations directly. The solutions and approximate solutions are more easily visualized—i.e., their qualitative features more profoundly appreciated—both because they are more intimately related to the original motivating problem, and because the space of the dependent variables has smaller dimension. Our formulas may appear complicated at first glance, but after close study they are seen to have a simple and elegant structure.

Only a special class of matrices $\mathbf{M}$ will be considered here (generalizations being discussed briefly in Sec. 7):

Positivity condition: $\mathbf{M}(t)$ is a positive definite Hermitian matrix for each t. [Thus $\mathbf{M}(t)$ has an orthonormal complete set of eigenvectors, and the eigenvalues $p_k(t)$ are strictly positive.]

As in the one-dimensional case (Appendix A), the validity of the mth order adiabatic approximation depends on differentiability of $\mathbf{M}(t)$ to a certain order. In fact, one is compelled to make a more cumbersome technical assumption, to the effect that the eigenvectors of $\mathbf{M}(t)$ at different values of t are related to each other in a sufficiently differentiable way:

Smoothness condition (Lth order): There is a family of projection operators, $\{\mathbf{P}_k(t)\}$ $(k = 1, 2, \ldots, K \leq N)$, such that: (1) $\sum_{k=1}^{K} \mathbf{P}_k(t) = \mathbf{1}$ (the identity matrix); (2) each $\mathbf{P}_k(t)$ is the orthogonal projection[5] onto a space of eigenvectors of $\mathbf{M}(t)$ with eigenvalue $p_k(t)$; (3) all the $\mathbf{P}_k(t)$ and $p_k(t)$ are differentiable L times, and the Lth derivatives are at least bounded on the interval considered.

A simpler but stronger smoothness assumption[6] is that $\mathbf{M}(t)$ is an analytic function of t [i.e., each $M_{jk}(t)$ is analytic for t in some neighborhood of the real axis]. In such a case the eigenvalues of $\mathbf{M}(t)$ are also analytic functions; since $\mathbf{M}$ is Hermitian, these functions have no branch points at real t values.[7] As a consequence of analyticity, if two eigenvalues are distinct at one t, they remain distinct except possibly at isolated points of "crossing" (defined precisely in Sec. 6). Let $p_k(t)$ $(k = 1, \ldots, K)$ be the distinct eigenvalues in this sense. Then the corresponding $\mathbf{P}_k(t)$, which are unambiguously defined except at the crossing points, are analytic, and they can be defined at the crossing points by analytic continuation.

The complications which can arise when $\mathbf{M}(t)$ is not analytic are discussed by Kato.[8] The eigenvalues may

split and merge in a complicated way instead of simply crossing or touching. Also, the eigenprojections $\mathbf{P}_k(t)$ may be less smooth than the matrix elements of $\mathbf{M}$, even discontinuous. It is the latter pathology which motivates our complicated statement of the smoothness condition. However, Lth order smoothness of $\mathbf{M}(t)$ implies that of $\mathbf{P}_k(t)$ except in the neighborhood of a point of crossing or splitting.[9]

The adiabatic expansions constructed in this paper apply only when $p_k(t) \neq p_{k'}(t)$ for all t ($k \neq k'$). [Note that any p_k may be a degenerate (multiple) eigenvalue, provided that the degeneracy is "permanent."] When two eigenvalues cross, a different method is needed, very much as at the turning points [zeros of $M(t)$] in the one-dimensional problem. This situation is described in Sec. 6, and a full treatment of the simplest special case will appear separately.[10]

2. KATO'S ADIABATIC TRANSFORMATION

If $\mathrm{M}(t)$ had eigenvectors which were independent of t, then an adiabatic expansion of a particular solution of Eq. (2) could be constructed by multiplying such an eigenvector by the one-dimensional adiabatic expansion (A3) with $p = p_k(t)$, the corresponding eigenvalue. In the general case, we shall find, as one would expect, that the t-dependent instantaneous eigenvectors of $\mathbf{M}(t)$ play an important role in the adiabatic expansion. But how are those eigenvectors to be specified uniquely? The phase of an eigenvector is always arbitrary, and when the eigenvalue is degenerate, there is even greater freedom in choosing an orthonormal set of eigenvectors. In the special case first mentioned, it would clearly be perverse to choose an eigenvector with (for instance) a t-dependent phase, when a constant vector is available. In general, however, there seems at first glance to be no natural way to choose the eigenvectors.

Nevertheless, there is a very useful way to specify a canonical set of orthonormal eigenvectors at each t in terms of an arbitrary set given at an initial value of t. This procedure was introduced by Kato in the study of the adiabatic problem in quantum mechanics[11] and treated in detail in his book on perturbation theory.[12] The eigenvectors for a general t are related to those for the initial value, $t = c$, by an operator $\mathbf{U}(t)$, the Kato adiabatic transformation:

$$\mathrm{a}(t) = \mathbf{U}(t)\mathrm{a}(c). \tag{4}$$

The guiding principle behind the definition of $\mathbf{U}(t)$ is that as t varies, the eigenvectors should change only in a minimal manner; specifically, that the derivative of an eigenvector should contain no component parallel to the vector itself [see Eq. (9)]. In Sec. 3 this condition will arise naturally in our heuristic derivation of the adiabatic expansions. The appearance of Kato's transformation in the approximate solutions is the most distinctive feature of our approach to the adiabatic analysis of coupled equations.

Before giving a formal definition of the Kato transformation, we review some properties of projection operators. A *projection* is an operator P satisfying $\mathbf{P}^2 = \mathbf{P}$. It is intimately associated with a certain subspace, its range $\mathbf{P}\mathbb{C}^N$. If a is a vector in $\mathbf{P}\mathbb{C}^N$, then $\mathbf{P}\mathrm{a} = \mathrm{a}$. P is called *orthogonal* if it annihilates the vectors orthogonal to $\mathbf{P}\mathbb{C}^N$:

$$\mathbf{P}\mathrm{a} = 0 \quad \text{if} \quad \mathrm{a} \in (\mathbf{P}\mathbb{C}^N)^{\perp}. \tag{5}$$

A projection is orthogonal if and only if it is Hermitian.

If $\{\mathbf{P}_k\}$ are the eigenprojections of $\mathbf{M}$ (see the smoothness condition, Sec. 1), and if $\mathbf{D}\mathbf{M}\mathbf{D}^{-1}$ is a diagonal matrix, then each $\mathbf{D}\mathbf{P}_k\mathbf{D}^{-1}$ is a diagonal matrix with 1's and 0's on the diagonal. Some readers may find it helpful to re-express various statements of this paper in terms of such a diagonal representation of $\mathbf{M}$ and the $\mathbf{P}$'s. In fact, we shall see that $\mathbf{U}(t)^{-1}$ can be regarded as a t-dependent diagonalizing transformation in a representation where $\mathbf{M}(c)$ is diagonal.

If $\{\mathrm{e}_k^{(j)}\}$ ($j = 1, 2, \ldots, N_k \equiv \dim \mathbf{P}_k\mathbb{C}^N$) is an orthonormal basis for the eigenvectors of eigenvalue p_k, then in the notation common in quantum mechanics one has

$$\mathbf{P}_k = \sum_{j=1}^{N_k} |\mathrm{e}_k^{(j)}\rangle\langle \mathrm{e}_k^{(j)}|. \tag{6}$$

For examples of eigenprojections in explicit matrix notation see the beginning of Sec. 4. $\mathbf{P}_k$ is an intrinsic, uniquely defined object, independent of the particular choice of the complete orthonormal set $\{\mathrm{e}_k^{(j)}\}$; this is one of the advantages of working in terms of eigenprojections. Nevertheless, even when one avoids choosing a particular basis, Kato's transformation $\mathbf{U}(t)$ still is defined, as an abstract operator, and is important.

For clarity we shall define $\mathbf{U}(t)$ first as a transformation of eigenvectors, in accord with the motivation given at the beginning of this section, and later characterize it more abstractly. Let $\mathbf{M}(t)$, $p_k(t)$, and $\mathbf{P}_k(t)$ be as described in the positivity and smoothness conditions of Sec. 1. For a particular k let a vector a_0 (independent of t) satisfy $\mathbf{M}(c)\mathrm{a}_0 = p_k(c)\mathrm{a}_0$ [equivalently, $\mathbf{P}_k(c)\mathrm{a}_0 = \mathrm{a}_0$]. Then $\mathrm{a}(t)$, defined by

$$\mathrm{a}'(t) = \mathbf{P}_k'(t)\mathrm{a}(t) \quad \text{and} \quad \mathrm{a}(c) = \mathrm{a}_0 \tag{7}$$

(where the primes denote differentiation), satisfies

$$\mathbf{M}(t)\mathrm{a}(t) = p_k(t)\mathrm{a}(t) \quad [\text{i.e.}, \ \mathbf{P}_k(t)\mathrm{a}(t) = \mathrm{a}(t)] \tag{8}$$

and

$$\mathbf{P}_k(t)\mathrm{a}'(t) = 0. \tag{9}$$

Proof: $\mathbf{P}^2 = \mathbf{P}$ implies $\mathbf{P}\mathbf{P}' + \mathbf{P}'\mathbf{P} = \mathbf{P}'$, which implies $\mathbf{P}\mathbf{P}'\mathbf{P} = 0$ and $\mathbf{P}\mathbf{P}'\mathrm{a} = \mathbf{P}'\mathrm{a} - \mathbf{P}'\mathbf{P}\mathrm{a}$. Let $\mathrm{w} = \mathbf{P}\mathrm{a}$. Then one has $\mathrm{w}(c) = \mathrm{a}_0$ and $\mathrm{w}' = \mathbf{P}'\mathrm{a} + \mathbf{P}\mathrm{a}' = \mathbf{P}'\mathrm{a} + \mathbf{P}\mathbf{P}'\mathrm{a} = 2\mathbf{P}'\mathrm{a} - \mathbf{P}'\mathbf{P}\mathrm{a} = 2\mathrm{a}' - \mathbf{P}'\mathrm{w}$; these two equations form a first-order initial-value problem for w which is satisfied by a itself. Therefore, by the standard uniqueness theorem, $\mathrm{a} = \mathrm{w} = \mathbf{P}\mathrm{a}$. Moreover, it follows that $\mathbf{P}\mathrm{a}' = \mathbf{P}\mathbf{P}'\mathrm{a} = \mathbf{P}\mathbf{P}'\mathbf{P}\mathrm{a} = 0$.

This construction can be applied to all the eigenvectors of $\mathbf{M}$ and extended by linearity to the whole vector space $\mathbb{C}^N$, thereby defining a linear operator $\mathbf{U}(t)$ [Eq. (4)]. This operator, the Kato transformation, has the properties

$$\mathbf{U}(t)\mathbf{P}_k(c)\mathbf{U}(t)^{-1} = \mathbf{P}_k(t) \quad \text{for all } k, \tag{10}$$

$$\mathbf{P}_k(t)\mathbf{U}'(t)\mathbf{P}_k(c) = 0 \quad \text{for all } k, \tag{11}$$

$$\mathbf{U}(c) = 1, \tag{12}$$

$$\mathbf{U}'(t)=\sum_{k=1}^{K}\mathbf{P}_k'(t)\mathbf{P}_k(t)\mathbf{U}(t)\equiv\mathbf{Q}(t)\mathbf{U}(t). \tag{13}$$

[Equations (12) and (13) can serve as a definition of U. Equations (10) and (11) express the fundamental properties (8) and (9) of an a satisfying Eq. (4).] Furthermore, U is unitary (when M is Hermitian, as assumed here). If D diagonalizes M(c) [i.e., $\mathbf{DM}(c)\mathbf{D}^{-1}$ is diagonal], then $\mathbf{DU}(t)^{-1}$ diagonalizes M(t).

In the absence of degeneracy, the Kato transformation can be written down explicitly. If the eigenvalue p_k is not degenerate, then a normalized eigenvector a(t) is already determined up to phase. The proper phase is found as follows. Let e(t) be an arbitrary differentiable normalized eigenvector of M(t) with $\mathbf{e}(c)=\mathbf{a}_0$, and let

$$\mathbf{a}(t)=\exp(i\theta(t))\mathbf{e}(t). \tag{14}$$

By Eq. (9) the scalar product $(\mathbf{e}(t),\mathbf{a}'(t))=(\mathbf{P}_k(t)\mathbf{e}(t),\ \mathbf{a}'(t))$ must vanish. ($\mathbf{P}_k$ is Hermitian since M is). Differentiating Eq. (14), one therefore obtains $\theta'(t)=i(\mathbf{e}(t),\ \mathbf{e}'(t))$, or

$$\theta(t)=i\int_c^t dt'(\mathbf{e}(t'),\mathbf{e}'(t')). \tag{15}$$

Thus the action of U(t) on a nondegenerate eigenvector has been determined. For a (permanently) multiple eigenvalue one must solve a system of coupled first-order equations.

Note that the possibility of crossing of eigenvalues of M(t) is irrelevant to the construction of the Kato transformation, as long as the smoothness condition is satisfied by the eigenprojections to order $L\geq 1$. In fact, the Kato transformation is determined by the system of eigenprojections and has nothing to do with the eigen*values* at all.

3. CALCULATION OF COEFFICIENTS

It is a natural conjecture that for each eigenvalue $p_k(t)$ there exist solutions of Eq. (2) which possess adiabatic expansions analogous to Eq. (A3):

$$\mathbf{h}^{\pm}(t)=p_k^{-1/4}(t)\exp[\pm iu\int_c^t p_k^{1/2}(t')\,dt']\times\sum_{s=0}^{m}(\pm iu)^{-s}\mathbf{a}_s^{\pm}(t)+O(u^{-(m+1)}), \tag{16}$$

where the $\mathbf{a}_s^{\pm}$ are now vectors and $\mathbf{M}\mathbf{a}_0^{\pm}=p_k\mathbf{a}_0^{\pm}$. (We shall omit the indices k and $\pm$ and the argument t whenever there is no chance of confusion. A prime will denote differentiation with respect to t.) Let us determine the coefficients $\mathbf{a}_s$ formally, postponing the question of validity of the expansion to Sec. 5.

Substituting the conjectured expansion (16) into Eq. (2) [see Eq. (52) below] yields, order by order, the equations

$$(\mathbf{M}-p)\mathbf{a}_0=0, \tag{17}$$

$$(\mathbf{M}-p)\mathbf{a}_1=2p^{1/2}\mathbf{a}_0', \tag{18}$$

$$(\mathbf{M}-p)\mathbf{a}_{s+2}=2p^{1/2}\mathbf{a}_{s+1}'+p^{1/2}\frac{d}{dt}(p^{-1/2}\mathbf{a}_s')-pf\mathbf{a}_s, \tag{19}$$

where

$$f=f_k(t)=\frac{1}{4}p^{-3/4}\frac{d}{dt}(p^{-5/4}p')=\frac{p''}{4p^2}-\frac{5(p')^2}{16p^3}. \tag{20}$$

Equation (17) says that $\mathbf{a}_0$ is indeed an eigenvector in $H=H_k(t)\equiv\mathbf{P}_k(t)\mathbb{C}^N$. Denote by $H^{\perp}$ the orthogonal complement of this subspace; every vector can be decomposed as

$$\mathbf{a}=\mathbf{P}(t)\mathbf{a}+\mathbf{a}^{\perp}(t),\quad \mathbf{P}\mathbf{a}\in H,\ \mathbf{a}^{\perp}\in H^{\perp}.$$

We have

$$\mathbf{a}_0^{\perp}=0. \tag{21}$$

Equation (18) can be divided into two equations by operating on both sides with P and with $\mathbf{1}-\mathbf{P}$:

$$\mathbf{P}(\mathbf{a}_0')=0, \tag{22}$$

$$\mathbf{a}_1^{\perp}=(\mathbf{M}-p)^{-1}\,2p^{1/2}(\mathbf{a}_0')^{\perp}. \tag{23}$$

The second of these equations makes sense at any t at which p is distinct from all the other eigenvalues, since $(\mathbf{M}-p)^{-1}$ is then a well-defined operator in $H^{\perp}$. (That is, "crossing" is excluded from the present discussion.) In the same way, Eq. (19) for each s yields a recursive formula for $\mathbf{P}(\mathbf{a}_{s+1}')$ and one for $\mathbf{a}_{s+2}^{\perp}$. When $N=1$, Eqs. (A4) are recovered.

The perpendicular part of each coefficient, $\mathbf{a}_s^{\perp}$, is thus completely determined when the coefficients for all smaller s are known. To complete the recursive determination of the coefficient, therefore, it remains to determine the parallel part, $\mathbf{P}\mathbf{a}_s$, using the known expression for $\mathbf{P}(\mathbf{a}_s')$. Since

$$\mathbf{P}(\mathbf{a}_s')=\mathbf{P}[(\mathbf{P}\mathbf{a}_s)']+\mathbf{P}[(\mathbf{a}_s^{\perp})'] \tag{24}$$

and the latter term is known, the problem is to solve for a vector (namely, $\mathbf{b}\equiv\mathbf{P}\mathbf{a}_s$) which at all times lies in the t-dependent space H, when that portion of its derivative which lies in H is prescribed. When this "parallel derivative" is zero, as is the case for $s=0$, the solution is given by the Kato adiabatic transform of an initial value:

$$\mathbf{b}(t)=\mathbf{U}(t)\mathbf{b}(c).$$

Indeed, U is designed precisely to guarantee properties (17) and (22) [cf. Eqs. (8) and (9)]. To solve the more general problem where $\mathbf{P}(\mathbf{b}')$ is a prescribed function of t, we write

$$\mathbf{b}(t)=\mathbf{U}(t)\hat{\mathbf{a}}(t)\quad(\mathbf{b}\equiv\mathbf{P}\mathbf{a}_s), \tag{25}$$

where $\hat{\mathbf{a}}(t)$ is in $H(c)$ and $\hat{\mathbf{a}}(c)=\mathbf{b}(c)$. Then $\mathbf{P}(\mathbf{b}')=\mathbf{P}\mathbf{U}'\mathbf{P}(c)\hat{\mathbf{a}}+\mathbf{P}\mathbf{U}\hat{\mathbf{a}}'=\mathbf{U}\mathbf{P}(c)\hat{\mathbf{a}}'=\mathbf{U}(\hat{\mathbf{a}}')$, where Eqs. (11) and (10) have been used. Hence one has

$$\hat{\mathbf{a}}(t)=\int_c^t dt'\mathbf{U}(t')^{-1}\mathbf{P}(t')\mathbf{b}'(t')+\hat{\mathbf{a}}(c). \tag{26}$$

In particular, from Eq. (24) with $s=1$ and the parallel part of Eq. (19) with $s=0$ one obtains [using Eqs. (17) and (22)]

$$\mathbf{P}[(\mathbf{P}\mathbf{a}_1)']=-\mathbf{P}[(\mathbf{a}_1^{\perp})']+\tfrac{1}{2}[p^{1/2}f\mathbf{a}_0-p^{-1/2}\mathbf{P}(\mathbf{a}_0')], \tag{27}$$

where $\mathbf{a}_1^{\perp}$ is given by Eq. (23). One then finds $\mathbf{P}\mathbf{a}_1$ by substituting into Eqs. (25) and (26).

When (as in the example in Sec. 4) a calculation is done in terms of a particular t-dependent basis of eigenvectors satisfying Eq. (4), the effect of the U operators in Eqs. (25) and (26) will be simply to move the basis vectors outside of the integral [see, e.g., Eq. (42)].

The only nonmechanical part of this construction is finding $\mathbf{U}(t)$. For a given p_k only the part of $\mathbf{U}(t)$ that maps $H_k(c)$ onto $H_k(t)$ is needed. The differential equations defining it [Eqs. (13) or (7)] reduce, once the purely algebraic task of finding a complete set of eigenvectors for $\mathbf{M}(t)$ has been completed, to a set of coupled equations, $\dim H_k$ in number, which can often be solved by inspection. In particular, when p_k is not degenerate only a quadrature is required [Eqs. (14) and (15)].

The general solution of Eq. (2) is

$$\mathbf{h}(t)=\sum_{k=1}^{K}[{}^k\mathbf{h}^+(t)+{}^k\mathbf{h}^-(t)], \tag{28}$$

where the ${}^k\mathbf{h}^\pm$ have the form (16) ($\mathbf{a}_s^\pm$ now carrying an additional index, k, which we shall write as a superscript on the left). The still undetermined initial values $P_k(c)[{}^k\mathbf{a}_s^+(c)]$ can be fixed by matching given initial values of $\mathbf{h}(c)$ and $u^{-1}\mathbf{h}'(c)$ [treated as of order $O(u^0)$] up through order u^{-m}, just as in Appendix A.

4. AN EXAMPLE

Let

$$C=\cos t,\quad S=\sin t, \tag{29}$$

and consider

$$\mathbf{M}(t)=\begin{bmatrix} t & 0 & 0 \\ 0 & tC^2+S^2 & (t-1)CS \\ 0 & (t-1)CS & tS^2+C^2 \end{bmatrix}, \tag{30}$$

which is analytic and satisfies the positivity condition when $0<t<\infty$. In the usual way one finds that $\mathbf{M}$ has the eigenvalues

$$p_1=t \text{ (double)} \quad \text{and} \quad p_2=1. \tag{31}$$

An orthonormal basis of eigenvectors is

$$\mathbf{e}_1^{(1)}=\begin{bmatrix}1\\0\\0\end{bmatrix},\quad \mathbf{e}_1^{(2)}=\begin{bmatrix}0\\C\\S\end{bmatrix},\quad \mathbf{e}_2=\begin{bmatrix}0\\-S\\C\end{bmatrix}. \tag{32}$$

Hence one has

$$\mathbf{P}_1=\begin{bmatrix}1&0&0\\0&C^2&CS\\0&CS&S^2\end{bmatrix},\quad \mathbf{P}_2=\begin{bmatrix}0&0&0\\0&S^2&-CS\\0&-CS&C^2\end{bmatrix}, \tag{33}$$

and also

$$\mathbf{e}_1^{(1)\prime}=0,\quad \mathbf{e}_1^{(2)\prime}=\mathbf{e}_2,\quad \mathbf{e}_2'=-\mathbf{e}_1^{(2)}. \tag{34}$$

It follows that the vectors (32) all satisfy Eq. (7) without further adjustment. If we choose as the initial point

$$c=\pi, \tag{35}$$

then the operator which maps $\mathbf{e}_1^{(1)}(\pi)$ onto $\mathbf{e}_1^{(1)}(t)$, etc., is

$$\mathbf{U}=\begin{bmatrix}1&0&0\\0&-C&S\\0&-S&-C\end{bmatrix} \tag{36}$$

[which indeed satisfies Eqs. (12) and (13)].

Let us find the first two terms of the adiabatic expansion of a solution of the ${}^1\mathbf{h}^+$ type for $t>1$. Equation (16) becomes

$${}^1\mathbf{h}^+=t^{-1/4}\exp[\tfrac{2}{3}iu(t^{3/2}-\pi^{3/2})][{}^1\mathbf{a}_0^+ +(iu)^{-1}\,{}^1\mathbf{a}_1^+] + O(u^{-2}). \tag{37}$$

From Eq. (21) we know that

$${}^1\mathbf{a}_0^+(t)=\xi_1^+\mathbf{e}_1^{(1)}(t)+\xi_2^+\mathbf{e}_1^{(2)}(t); \tag{38}$$

ξ_1^+ and ξ_2^+ are independent of t, because the t development of $\mathbf{a}_0(t)$ is given entirely by the Kato transformation $\mathbf{U}(t)$ [see Eqs. (22), (25), and (26)]. We then have (omitting the index +)

$$\mathbf{a}_0'=\mathbf{a}_0'^{\perp}=\xi_2\mathbf{e}_2. \tag{39}$$

Thus, by Eq. (23),

$$\mathbf{a}_1^{\perp}=2t^{1/2}(1-t)^{-1}\xi_2\mathbf{e}_2. \tag{40}$$

Equation (27) now yields

$$\mathbf{P}_1[(\mathbf{P}_1\mathbf{a}_1)']=2t^{1/2}(1-t)^{-1}\xi_2\mathbf{e}_1^{(2)} +\tfrac{1}{2}t^{-1/2}\xi_2\mathbf{e}_1^{(2)}-\tfrac{5}{32}t^{-5/2}\mathbf{a}_0. \tag{41}$$

So, by Eqs. (25) and (26), we have

$$\mathbf{P}_1\mathbf{a}_1=\mathbf{U}(t)\hat{\mathbf{a}}_1(c)+F(t)\xi_2\mathbf{e}_1^{(2)}+(5/48)(t^{-3/2}-\pi^{-3/2})\mathbf{a}_0, \tag{42}$$

where

$$F(t)=\tfrac{1}{2}\int_\pi^t dt'(t')^{-1/2}(1-t')^{-1}(1+3t'). \tag{43}$$

In analogy to Eq. (38), $\mathbf{U}(t)\hat{\mathbf{a}}_1(c)$ can be written

$$\mathbf{U}(t)\,{}^1\hat{\mathbf{a}}_1^+(c)=\eta_1^+\mathbf{e}_1^{(1)}+\eta_2^+\mathbf{e}_1^{(2)}. \tag{44}$$

Finally, we assemble the desired approximation (suppressing the t dependence of all the vectors):

$${}^1\mathbf{h}^+=t^{-1/4}\exp[\tfrac{2}{3}iu(t^{3/2}-\pi^{3/2})]\{{}^1\mathbf{a}_0^+ +(iu)^{-1}[\eta_1^+\mathbf{e}_1^{(1)}+\eta_2^+\mathbf{e}_1^{(2)}+F(t)\xi_2^+\mathbf{e}_1^{(2)} +(5/48)(t^{-3/2}-\pi^{-3/2})\,{}^1\mathbf{a}_0^+ +2t^{1/2}(1-t)^{-1}\xi_2^+\mathbf{e}_2]\} + O(u^{-2}), \tag{45}$$

where ${}^1\mathbf{a}_0^+$ is given in Eq. (38).

Similarly, one finds

$${}^2\mathbf{h}^+=\exp[iu(t-\pi)]\{\xi_0^+\mathbf{e}_2+(iu)^{-1}[\eta_0^+\mathbf{e}_2+G(t)\xi_0^+\mathbf{e}_2 -2(t-1)^{-1}\xi_0^+\mathbf{e}_1^{(2)}]\}+O(u^{-2}), \tag{46}$$

where

$$G(t)=\tfrac{1}{2}\int_\pi^t dt'(t'-1)^{-1}(3+t') \tag{47}$$

and ξ_0^+ and η_0^+ are arbitrary constants. The expressions for ${}^1\mathbf{h}^-$ and ${}^2\mathbf{h}^-$ are the same except for the sign of iu, with different coefficients, ξ_j^- and η_j^-.

The solution of the form (28) which satisfies

$$\mathbf{h}(\pi)=\pi^{-1/4}\mathbf{e}_1^{(2)}(\pi)+O(u^{-2}),\qquad \mathbf{h}'(\pi)=iu\pi^{1/4}\mathbf{e}_1^{(2)}(\pi)+O(u^{-1}) \tag{48}$$

is found to be

$$\mathbf{h}(t)=t^{-1/4}\exp[\tfrac{2}{3}iu(t^{3/2}-\pi^{3/2})]\{\mathbf{e}_1^{(2)}+(iu)^{-1} \times[\tfrac{1}{8}\pi^{-3/2}\mathbf{e}_1^{(2)}+F(t)\mathbf{e}_1^{(2)} +(5/48)(t^{-3/2}-\pi^{-3/2})\mathbf{e}_1^{(2)}+2t^{1/2}(1-t)^{-1}\mathbf{e}_2]\}$$

$$+t^{-1/4}\exp[-\tfrac{2}{3}iu(t^{3/2}-\pi^{3/2})](-iu)^{-1}\tfrac{1}{8}\pi^{-3/2}\mathbf{e}_1^{(2)}$$
$$+\exp[iu(t-\pi)](iu)^{-1}[\tfrac{1}{2}\pi^{-1/4}(\pi+1)+\pi^{1/4}](\pi-1)^{-1}\mathbf{e}_2$$
$$+\exp[-iu(t-\pi)](-iu)^{-1}[\tfrac{1}{2}\pi^{-1/4}(\pi+1)-\pi^{1/4}](\pi-1)^{-1}\mathbf{e}_2$$
$$+O(u^{-2}). \tag{49}$$

Note that terms proportional to $\mathbf{e}_2$ enter in the order u^{-1}, despite the "pure $\mathbf{e}_1^{(2)}$" initial conditions (48).

Equation (49) is valid only on closed intervals which lie to the right of the point $t=1$, where the eigenvalues cross. On closed subintervals between $t=0$ and $t=1$ the solutions have expansions of the same form as Eqs. (45) and (46), of course; to determine the coefficients (analogous to $\xi_j^{\pm}, \eta_j^{\pm}$) corresponding to the solution satisfying Eq. (48) requires investigation of the behavior of that solution near $t=1$ (see Sec. 6 and Ref. 10).

5. PROOF THAT THE SERIES IS ASYMPTOTIC

We shall now establish to what order L the smoothness condition (Sec. 1) must be satisfied in order that the error term in Eq. (16) really be of order $u^{-(m+1)}$.

Theorem: Let $p(t)=p_k(t)$, one of the eigenvalues of a matrix function $\mathbf{M}(t)$ which satisfies the positivity condition, let $j=\pm i$, and let

$$\mathbf{h}_m(t)=p^{-1/4}\exp[ju\int_c^t p^{1/2}(t')\,dt']\sum_{s=0}^{m}(ju)^{-s}\mathbf{a}_s(t), \tag{50}$$

where the coefficients satisfy Eqs. (17)—(20). Here t varies in a closed interval containing c and *containing no point of crossing of the eigenvalues*. Let $\mathbf{h}(t)$ be the solution of Eq. (2) such that $\mathbf{h}(c)=\mathbf{h}_m(c)$, $\mathbf{h}'(c)=\mathbf{h}_m'(c)$. Then if $\mathbf{M}$ satisfies the Lth-order smoothness condition with $L=m+3$, the error $\mathbf{Z}_m$ in the approximation,

$$\mathbf{Z}_m=\mathbf{h}-\mathbf{h}_m, \tag{51}$$

is $O(u^{-(m+1)})$ (i.e., $u^{m+1}\|\mathbf{Z}_m\|$ is bounded as $u\to\infty$, where $\|\ \|$ denotes the Hilbert-space norm or 2-norm). The same statement holds for $u^{-1}(\mathbf{h}'-\mathbf{h}_m')$ [cf. Eq. (A7)].

We begin the proof by finding a differential equation satisfied by $\mathbf{Z}_m$. One calculates that

$$\mathbf{h}_m''+u^2\mathbf{M}\mathbf{h}_m$$
$$=\exp(ju\int_c^t p^{1/2}(t')\,dt')\Big(p^{3/4}\sum_{s=-2}^{m-2}(ju)^{-s}\mathbf{a}_{s+2}$$
$$+2p^{1/4}\sum_{s=-1}^{m-1}(ju)^{-s}\mathbf{a}_{s+1}'-fp^{3/4}\sum_{s=0}^{m}(ju)^{-s}\mathbf{a}_s$$
$$-\tfrac{1}{2}p^{-5/4}p'\sum_{s=0}^{m}(ju)^{-s}\mathbf{a}_s'$$
$$+p^{-1/4}\sum_{s=0}^{m}(ju)^{-s}\mathbf{a}_s''-p^{-1/4}\sum_{s=-2}^{m-1}(ju)^{-s}\mathbf{M}\mathbf{a}_{s+2}\Big). \tag{52}$$

The $\mathbf{a}_s$ are constructed so that the lower-order terms cancel; using Eqs. (17)—(20) up to $s=m-1$, one reduces Eq. (52) to

$$\mathbf{h}_m''+u^2\mathbf{M}\mathbf{h}_m$$
$$=\exp(ju\int_c^t p^{1/2}(t')\,dt')$$
$$\times\{(ju)^{-(m-1)}p^{-1/4}(\mathbf{M}-p)\mathbf{a}_{m+1}$$
$$+(ju)^{-m}p^{-1/4}(\mathbf{a}_m''-\tfrac{1}{2}p^{-1}p'\mathbf{a}_m'-fp\mathbf{a}_m)\}$$
$$\equiv\exp(ju\int_c^t p^{1/2}(t')\,dt')$$
$$\times[(ju)^{-(m-1)}\mathbf{g}_m^{(1)}(t)+(ju)^{-m}\mathbf{g}_m^{(0)}(t)]$$
$$\equiv-\mathbf{g}_m(u,t). \tag{53}$$

Hence one has

$$\mathbf{Z}_m''+u^2\mathbf{M}\mathbf{Z}_m=\mathbf{g}_m,\quad \mathbf{Z}(c)=\mathbf{Z}'(c)=0. \tag{54}$$

Since the construction of $\mathbf{a}_s'$ [according to Eqs. (17)—(20), (25)—(26), and (13)] requires derivatives of the p's and $\mathbf{P}$'s of order $s+1$, g_m involves derivatives of order $m+2$. The term in Eq. (53) proportional to $u^{-(m-1)}$ (absent in the one-dimensional case treated in Refs. 1 and 2) will eventually force us to increase by 1 the order of differentiability assumed.

The solution of Eq. (54) may be represented in the form

$$\mathbf{Z}_m(t)=\frac{1}{u}\int_c^t dt'\mathbf{G}(t,t')\mathbf{g}_m(t'), \tag{55}$$

where $\mathbf{G}$ is a matrix defined by

$$\frac{\partial^2}{\partial t^2}\mathbf{G}(t,t')+u^2\mathbf{M}(t)\mathbf{G}(t,t')=0, \tag{56}$$

$$\mathbf{G}(t,t)=0,\quad \frac{\partial}{\partial t}\mathbf{G}(t,t')\Big|_{t=t'}=u\mathbf{1}. \tag{57}$$

We have

$$\mathbf{Z}_m'(t)=\frac{1}{u}\int_c^t dt'\frac{\partial}{\partial t}\mathbf{G}(t,t')\mathbf{g}_m(t'). \tag{58}$$

If the operator norms $\|\mathbf{G}(t,t')\|$ and $u^{-1}\|\partial\mathbf{G}/\partial t\|$ have upper bounds independent of u, one finds immediately that $\mathbf{Z}_m=O(u^{-m})$ and $u^{-1}\mathbf{Z}_m'=O(u^{-m})$. To prove that these error terms are $O(u^{-(m+1)})$, we must let $L=m+3$ and use the above argument for $\mathbf{Z}_{m+1}$; then combining the $u^{-(m+1)}$ term in $\mathbf{h}_{m+1}$ with $\mathbf{Z}_{m+1}$ yields the desired result.

To show that $\mathbf{G}$ and $\partial\mathbf{G}/\partial t$ behave as desired, we note that $\mathbf{G}$ satisfies a matrix version of Eq. (2) and hence possesses a formal expansion of the type we are studying. Let $\{\mathbf{d}_i(t)\}$ $(i=1,\ldots,N)$ be a basis of eigenvectors of $\mathbf{M}(t)$ with the Kato t dependence [Eq. (4)]. Denote the corresponding eigenvalues by $p_i(t)$. (In the present context p's with distinct indices may coincide.) Incorporating the initial conditions (57), we find that $\mathbf{G}$ has the form

$$\mathbf{G}(t,t')=\sum_{i=1}^{N}\sin(u\int_{t'}^t p_i(t'')^{1/2}\,dt'')$$
$$\times[p_i(t)^{-1/4}\mathbf{d}_i(t)\otimes\mathbf{d}_i^*(t')p_i(t')^{-1/4}$$
$$+u^{-1}\mathbf{A}_i(t,t')]$$
$$+\sum_{i=1}^{N}\cos(u\int_{t'}^t p_i(t'')^{1/2}\,dt'')u^{-1}\mathbf{B}_i(t,t')+\mathbf{Z}_1, \tag{59}$$

where $\mathbf{Z}_1$ is expected to be of order u^{-2}, although it would be circular to assert that at this point. $\mathbf{A}_i$ and $\mathbf{B}_i$ do not concern us except that they are independent of u. Now $\mathbf{Z}_1$ must satisfy Eq. (55) (where $\mathbf{Z}_1$ and $\mathbf{g}_1$ are now matrices). One therefore has from Eq. (59) a bound of the form

$$\|\mathbf{G}(t,t')\|\le C(t,t')+u^{-1}D(t,t')$$
$$+u^{-1}\int_{t'}^t dt''\|\mathbf{G}(t,t'')\|\,\|\mathbf{g}_1(t'')\|.$$

Recall [see Eq. (53)] that $\mathbf{g}_1=O(u^0)$ if the smoothness

condition holds to order $L=3$. Introducing

$$G_{\max}=\sup\|\mathbf{G}(t,t')\| \tag{60}$$

(sup over all values of t and t' in the "closed interval" of the theorem), one obtains

$$G_{\max}\le C+u^{-1}D+u^{-1}G_{\max}E,$$

where C, D, and E are independent of u, and thus for sufficiently large u

$$G_{\max}\le\frac{C+u^{-1}D}{1-u^{-1}E}=O(u^0). \tag{61}$$

A similar argument applies to the derivative. This completes the proof.

Remark: This proof corresponds to the method used in Ref. 1, rather than that of Ref. 2, which does not generalize so easily.

6. THE PROBLEM OF CROSSING OF EIGENVALUES

By "crossing" we mean any change in the multiplicity structure of the eigenvalues of $\mathbf{M}(t)$. The simplest case is the first-order crossing of two eigenvalues at a point t_0:

$$p_1(t)-p_2(t)=C(t-t_0)+O[(t-t_0)^2], \tag{62}$$

where C is a nonzero constant. For complete generality one must also be prepared for tangency,

$$p_1(t)-p_2(t)\sim(t-t_0)^2,$$

and for higher-order intersections. When $\mathbf{M}(t)$ is not analytic, $p_1(t)$ and $p_2(t)$ may even coincide on a whole interval—e.g.,

$$p_1=t^3+1,\quad p_2=|t|^3+1\quad(t>-1).$$

Of course, in the most general case more than two eigenvalues may be involved.

The expansions derived in this paper do not apply near a crossing point t_0. Right at such a point Eq. (23), for instance, is meaningless. Near the point, Eq. (23), because of its small "denominator", contributes (in general) a large term to the error $\mathbf{Z}_1(t)$ [see Eqs. (55) and (53)]. For a fixed $t\neq t_0$ the series is still asymptotic as $u\to\infty$, but it is not asymptotic [in the case (62)] in a limit such as $u\to\infty$, $t-t_0\propto u^{-\epsilon}$, $\epsilon\ge\frac{1}{2}$. The lowest-order term in the series, $p_k^{-1/4}\exp(\pm iu\int p_k^{1/2})\,{}^k\mathbf{a}_0$ ($k=1$ or 2), is still meaningful at t_0, however, and one can show, using Eq. (55) with $m=0$ for $|t-t_0|\le\lambda u^{-\epsilon}$, $\epsilon\approx\frac{1}{2}$, and using the previous estimate outside that region, that the error still vanishes uniformly as $u\to\infty$. In general it will not vanish as fast as u^{-1}. That is, not only is it impossible to construct the higher-order terms in the series, but also the first term cannot be expected to be as good an approximation as it normally is. An analogous situation is encountered in the lowest-order adiabatic approximation to the Schrödinger equation in quantum mechanics (an equation of first order in t), where it is found[13] that one cannot obtain a uniform error bound of the order $O(u^{-1})$ near a point of eigenvalue crossing, but only one of the type $o(u^0)$. [The notation $\mathbf{Z}=o(u^{-m})$ means that $u^m\mathbf{Z}\to 0$ as $u\to\infty$.]

When two eigenvalues cross as in Eq. (62), the trouble in the adiabatic series associated with one eigenvalue arises from the appearance in the higher-order approximations of anomalously large terms proportional to the eigenvectors of the other eigenvalue. Evidently there is strong "mixing" of the two modes near the crossing point. A solution which to the left of t_0 has the leading term $p_1^{-1/4}\exp(iu\int p_1^{1/2})\,{}^1\mathbf{a}_0$ should be expected to behave to the right of t_0 like

$$R(u)p_1^{-1/4}\exp(iu\int p_1^{1/2})\,{}^1\mathbf{a}_0+S(u)p_2^{-1/4}\exp(iu\int p_2^{1/2})\,{}^2\mathbf{a}_0,$$

where $S(u)$ approaches zero as u grows, but more slowly than u^{-1}. One must, therefore, study the behavior of the solution near t_0 in order to know its correct continuation from one region of validity of the adiabatic expansion into another. The problem is similar to that of finding the WKB connection formulas, which continue a given exponential solution of Eq. (A2), valid in a region where $p<0$, through a zero of $p(t)$ into the correct linear combination of oscillatory solutions in the region where $p>0$.

A sequel (Ref. 10) to this paper will present a procedure for dealing with the special case (62) of the crossing problem.

7. GENERALIZATIONS

Some of the restrictions placed on the coefficient matrix $\mathbf{M}(t)$ in this work are surely unnecessary. Even if it were in the author's power to cover all possible cases, however, the effect would be to complicate the formulas and proofs inordinately. It seems wiser to let each reader construct the generalization needed for his specific problem. A few remarks are offered here concerning various directions in which the present work might be generalized or extended.

Explicit error bounds and additional u-dependence: From Eqs. (55) and (58) we have

$$\|\mathbf{Z}_m(t)\|\le u^{-1}|t-c|\,G_{\max}\sup\|\mathbf{g}_m(t')\|, \tag{63a}$$

$$\|\mathbf{Z}_m'(t)\|\le u^{-1}|t-c|\sup\left\|\frac{\partial}{\partial t'}\mathbf{G}(t',t'')\right\|\sup\|\mathbf{g}_m(t')\|, \tag{63b}$$

where $G_{\max}$, defined in Eq. (60), satisfies Eq. (61), and the derivative is similarly bounded. From a detailed study of Eq. (59) for $\mathbf{G}$, one could obtain upper bounds on the constants C, D, and E in Eq. (61) and the analogous constants in the bound on $\partial\mathbf{G}/\partial t$. Thus one would have rigorous upper bounds on the error terms $\mathbf{Z}_m$ and their derivatives—unfortunately much more complicated, in all probability, than those in Appendix A.

As in Olver's study of the one-dimensional problem (see Appendix A of the present paper), error bounds could be used to judge the accuracy of the adiabatic approximations $\mathbf{h}_m$ when $\mathbf{M}$ itself is allowed to depend on u. For example, if all the derivatives of the p_k and $\mathbf{P}_k$ which appear in $\mathbf{Z}_m$ are bounded as $u\to\infty$ and if the p_k themselves and their differences are bounded below, then the series will still be asymptotic. If some of the derivatives approach zero for large u, then the approximation $\mathbf{h}_m$ may be valid to higher than mth order.

An alternative approach to u-dependent coefficients, adopted in Ref. 3, is to expand them in power series in u^{-1}. The formulas for the terms $\mathbf{a}_s$ in the asymptotic se-

ries become rather complicated for $s>0$, but the method is straightforward in principle.

Infinite intervals: The error bounds provided by Eqs. (63) increase linearly with the length of the integration interval. They are unnecessarily pessimistic if $\mathbf{M}(t)\to$ constant (with its derivatives) as $t\to\pm\infty$, since each term in g_m involves a derivative of, ultimately, a p_k or a $\mathbf{P}_k$. In the one-dimensional case one obtains simple bounds of the total variation type, Eq. (A5). In the present more complicated context it will still turn out for some $\mathbf{M}(t)$ that the integrals (55) and (58) converge when extended over the whole real line, yielding bounds which are uniform in t. In such a case, moreover, c could be chosen to be $\pm\infty$.

Relaxation of the positivity condition: We consider three successive degrees of complication.

If the eigenvalues $p_k(t)$ can be negative or complex (but not yet zero), the proof in Sec. 5 will require modifications, because the trigonometric functions in Eq. (59) are no longer bounded by 1 as $u\to\infty$. A promising remedy (cf. Ref. 2, Theorems 1, 3, and 5) is to get control over these factors by choosing c to be an end point of the interval of t considered. (*Which* end point depends on the sign of $jp_k^{1/2}$, and hence will be different for the two solutions ${}^k\mathbf{h}^+$ and ${}^k\mathbf{h}^-$.)

If $\mathbf{M}(t)$ is not normal, but is diagonalizable, then the eigenprojections, defined from the resolvent by a contour integral,[14] will not be orthogonal.[15] Again, some points in the construction and the proof will require modification.

Finally, let us consider to lowest order the simplest example of nondiagonalizability, the case of a block

$$\begin{bmatrix} p(t) & 1 \\ 0 & p(t) \end{bmatrix} \quad [p(t)>0] \tag{64}$$

in the Jordan canonical form of $\mathbf{M}(t)$. Let $\mathbf{a}_1(t)$ and $\mathbf{a}_2(t)$ be vectors such that

$$\mathbf{M}\mathbf{a}_1 = p\mathbf{a}_1, \quad \mathbf{M}\mathbf{a}_2 = p\mathbf{a}_2 + \mathbf{a}_1. \tag{65}$$

As with any eigenvector, there are solutions whose lowest-order approximations are

$${}^1\mathbf{h}_0^\pm = p^{-1/4}\exp(\pm iu\int_c^t p^{1/2}(t')\,dt')\mathbf{a}_1. \tag{66}$$

To obtain linearly independent approximate solutions which permit fitting initial values proportional to $\mathbf{a}_2$, one must include terms of order u^{-1}:

$${}^2\mathbf{h}_0^\pm = \tfrac{1}{2}p^{-3/4}(t-c)\exp(\pm iu\int_c^t p^{1/2}(t')\,dt')\mathbf{a}_1$$

$$\pm(iu)^{-1}p^{-1/4}\exp(\pm iu\int_c^t p^{1/2}(t')\,dt')\mathbf{a}_2. \tag{67}$$

The form of Eq. (67) is suggested by the known exact solution of a system of two equations with a *constant* coefficient matrix $\mathbf{M}$ of the form (64). The notation "term of order u^{-m}" becomes ambiguous in this situation. One easily shows that [contrast Eq. (53)]

$${}^2\mathbf{h}_0^{\pm\prime\prime} + u^2\mathbf{M}\,{}^2\mathbf{h}_0^\pm = O(u^1(t-c)) + O(u^0). \tag{68}$$

For an approximation *near* c which need not satify the equation uniformly well, therefore, one may consider $\pm iu\,{}^2\mathbf{h}_0^\pm$, rather than ${}^2\mathbf{h}_0^\pm$, to be zeroth-order quantities; then the fitting of initial conditions proceeds as in the cases studied earlier. Otherwise, in fitting initial conditions order by order one must treat the components along $\mathbf{a}_2(c)$ of $u\mathbf{h}(c)$ and $\mathbf{h}'(c)$, rather than of $\mathbf{h}(c)$ and $u^{-1}\mathbf{h}'(c)$, as zeroth-order quantities. Finally, the phases of $\mathbf{a}_1(t)$ and $\mathbf{a}_2(t)$ should be determined by studying the approximations of next highest order, in keeping with the philosophy of Sec. 3. We shall not carry the analysis any further here, wishing only to demonstrate that the general method can be applied to such problems. First-order systems with nondiagonal Jordan forms are studied in Ref. 3.

Vanishing eigenvalues: When an eigenvalue passes through zero, an entirely different approach to approximate solutions of the equation is needed. The connection formulas used with the first-order WKB method in this situation are well known, and several higher-order generalizations are available.[16] It should be possible to extend such methods to systems of equations, but the problem is beyond the scope of this paper.

Other generalizations which are not discussed here are to equations of more general form (e.g., with inhomogeneous and first-derivative terms—cf. Ref. 3) and possibly to equations in infinite-dimensional vector spaces.

ACKNOWLEDGMENTS

I thank W.C. Hammel, Jr., D.A. Lutz, F.J. Narcowich, and L. Parker for comments on the manuscript, and Professor Narcowich and F.W.J. Olver for pointing out references.

APPENDIX A: EXPANSION FOR A SINGLE EQUATION

Combining Theorems 4 and 6 of Ref. 2, one obtains the following: Let $p(u,t)$ be a strictly positive function which is (piecewise continuously) differentiable $m+2$ times with respect to t. Let

$$f(u,t) = -p^{-3/4}\frac{d^2}{dt^2}(p^{-1/4}) = \frac{p''}{4p^2} - \frac{5(p')^2}{16p^3}. \tag{A1}$$

Then the equation

$$\frac{d^2h}{dt^2} + u^2p(u,t)h = 0 \tag{A2}$$

has solutions $h_\pm(u,t)$ of the form

$$h_\pm = p^{-1/4}\exp(\pm iu\int_c^t p^{1/2}(u,t')\,dt')$$
$$\times\left\{\sum_{s=0}^{m}(\pm iu)^{-s}a_s^\pm(u,t) + (\pm iu)^{-(m+1)}\right.$$
$$\left.\times[a_{m+1}^\pm(u,t) - a_{m+1}^\pm(u,c)] + \epsilon_m^\pm(u,t)\right\}. \tag{A3}$$

Here c is an arbitrary number in the interval of t considered; the coefficients satisfy the equations

$$\frac{da_0^\pm}{dt} = 0 \tag{A4a}$$

and

$$\frac{da_{s+1}^\pm}{dt} = \frac{1}{2}p^{1/2}fa_s^\pm - \frac{1}{2}\frac{d}{dt}\left[p^{-1/2}\frac{da_s^\pm}{dt}\right]; \tag{A4b}$$

and the magnitude of the error is

$$|\epsilon_m^\pm| \le u^{-(m+1)}V(a_{m+1}^\pm)\{2\exp[2V(a_1^\pm)/u] - 1\}, \tag{A5}$$

where the total variation $V(\phi)$ of a function ϕ between c and t can be defined adequately for our purposes as

$$V(\phi)=\left|\int_c^t|\phi'(t')|\,dt'\right|. \tag{A6}$$

Moreover, the derivatives have the expansion

$$\begin{aligned}h_\pm'=&-\frac{p'}{4p}h\pm iup^{+1/4}\exp(\pm iu\textstyle\int_c^t p^{1/2}\,dt')\\&\times\Big[\sum_{s=0}^{m}(\pm iu)^{-s}\left(a_s^\pm+p^{-1/2}\frac{da_{s-1}^\pm}{dt}\right)\\&+(\pm iu)^{-(m+1)}\left(a_{m+1}^\pm+p^{-1/2}\frac{da_m^\pm}{dt}\right.\\&\left.-a_{m+1}^\pm(c)\right)+\eta_m^\pm(u,t)\Big],\end{aligned} \tag{A7}$$

where $\eta_m^\pm$ satisfies the same bound as $\epsilon_m^\pm$ [Eq. (A5)]. The differentiability condition on p assures that the coefficients $a^\pm$ and the error bounds $\epsilon^\pm$ and $\eta^\pm$ are finite.

The general solution of Eq. (A2) is of the form $h_+ + h_-$, where the initial values $a^\pm(u,c)$ of the solutions of Eqs. (A4) can be determined by matching the initial data $h(c)$ and $u^{-1}h'(c)$ order by order. For instance, if one requires

$$\begin{aligned}&h(c)=(2u)^{-1/2}p^{-1/4}(c),\\&h'(c)=i(u/2)^{1/2}p^{+1/4}(c)+u^{1/2}O(u^{-(m+1)})\end{aligned} \tag{A8}$$

(a choice which has applications in quantum field theory[17]), then

$$a_0^+(c)=(2u)^{-1/2},\quad a_0^-(c)=0, \tag{A9a}$$

$$a_1^+(c)=a_1^-(c)=(2u)^{-1/2}p'(c)p^{-3/2}(c)/8, \tag{A9b}$$

$$a_s^\pm(c)=-\tfrac{1}{2}(2u)^{-1/2}p^{-1/2}(c)[a_{s-1}^{\pm\prime}(c)-(-1)^s a_{s-1}^{\mp\prime}(c)]\quad(s>1). \tag{A9c}$$

APPENDIX B: RELATION TO THE APPROACH OF FESHCHENKO *ET AL.*

Adiabatic analysis of systems of equations is the subject of Ref. 3. The approach of that treatise differs from ours in several ways, of which the most important are the following: (1) Except for a preliminary chapter in which only nondegenerate eigenvalues are considered, second-order systems are treated only by reduction to a first-order system of twice the dimension. (2) The exponentiated integrand $p_k^{1/2}$ in Eq. (16) is generalized to a power series in u^{-1}. (3) The Kato transformation is not used; the eigenvectors at different t are not related uniquely. The mth-order approximations obtained consequently differ, in general, from those of this paper, but they must agree up to terms of the next higher order—laborious manipulations sometimes being required to verify the agreement. The case of crossing eigenvalues is not considered in Ref. 3, but some results along that line for first-order systems are given by Wasow (Ref. 4).

The present treatment leads rather inexorably to the Kato conditions on the eigenvectors $\mathbf{a}_0(t)$ [see Eqs. (17) and (22)]. How is it possible, then, that the eigenvector can be left arbitrary in the approach of Feshchenko *et al.*? The answer is hidden in the terms of next higher order in the exponentiated integrand. Let $\mathbf{e}(t)$ be an arbitrary normalized eigenvector of $\mathbf{M}(t)$ with eigenvalue $p(t)$. Let us carry out through the first two orders the expansion prescribed in Ref. 3 for a system of second-order equations without degeneracy.[18] After translation into the notation of this paper one has

$$\begin{aligned}\mathbf{h}^\pm(t)\sim&[\mathbf{e}_0\mp 2iu^{-1}(\mathbf{M}-p)^{-1}p^{1/2}(\mathbf{e}_0')^\perp\exp\{\pm iu\textstyle\int^t dt'\\&\times[p^{1/2}\pm\tfrac{1}{4}iu^{-1}p^{-1}p'\pm iu^{-1}(\mathbf{e},\mathbf{e}')]\}.\end{aligned} \tag{B1}$$

Because of the extra factor of u, the second and third terms in the exponential really should be considered part of the zeroth-order approximation, rather than first-order corrections. Indeed, the term involving p'/p, which can be integrated, is needed to reproduce the factor $p^{-1/4}$ in our expansion (16). (In particular, such a factor appears in the standard zeroth-order WKB approximation for a system consisting of a single equation. It is fundamental.) The term involving $(\mathbf{e},\mathbf{e}')$ yields a phase factor[19] which, when it multiplies the leading term in the first factor in Eq. (B1), converts the possibly wayward eigenvector $\mathbf{e}_0$ to the Kato eigenvector $\mathbf{a}_0$, as we have demonstrated in the discussion leading to Eq. (15). Since the Kato transformation in the event of eigenvalue degeneracy requires more than a phase change, it is not surprising that the method of Ref. 3 for second-order equations is not easily extendible to the degenerate case.

*Research supported by University of Wisconsin-Milwaukee Graduate School.

†Present address: Mathematics Department, King's College, University of London, Strand, London, WC2R 2LS, U.K.

[1]O. Blumenthal, Arch. Math. Physik (Leipzig) **19**, 136 (1912).
[2]F.W.J. Olver, Proc. Camb. Phil. Soc. **57**, 790 (1961).
[3]S.F. Feshchenko, N.I. Shkil', and L.D. Nikolenko, *Asymptotic Methods in the Theory of Linear Differential Equations* (American Elsevier, New York, 1967).
[4]W. Wasow, *Asymptotic Expansions for Ordinary Differential Equations* (Interscience, New York, 1965), Chaps. VII–VIII.
[5]For the sake of compactness and elegance we shall often work with the projections onto the eigenspaces of **M** instead of with a complete set of eigenvectors of **M**. This apparatus is often used in quantum mechanics, where the vector space is infinite-dimensional. Since some potential users of our results may feel uncomfortable with this language, we shall adopt a rather pedagogical stance (especially in Sec. 2) and work out a very concrete example (Sec. 4).
[6]Ref. 12, pp. 63–74.
[7]Ref. 12, pp. 120–21.
[8]Ref. 12, pp. 106–15, 122–24.
[9]Ref. 3, pp. 66–73, 85–90.
[10]S.A. Fulling, paper in preparation.
[11]T. Kato, J. Phys. Soc. Japan **5**, 435 (1950).
[12]T. Kato, *Perturbation Theory for Linear Operators* (Springer, New York, 1966), pp. 98–102, 104–06, 121–22.
[13]M. Born and V. Fock, Z. Physik **51**, 165 (1928); T. Kato, Ref. 11.
[14]Ref. 12, pp. 34–44, 58–60.
[15]For any diagonalizable **M** there will be a family of mutually commuting eigenprojections whose sum is the identity matrix.

(In fact, $\mathbf{P}_{k'}\mathbf{P}_k = 0$ if $k \neq k'$.) If the projections are all orthogonal, then **M** is normal (i.e., commutes with its adjoint). If, in addition, the eigenvalues are all real, then **M** is Hermitian.

[16]See references in *Handbook of Mathematical Functions* (National Bureau of Standards Applied Mathematics Series, No. 55), edited by M. Abramowitz and I.A. Stegun (U.S. Government Printing Office, Washington, D.C., 1964), p. 455. Another method is indicated by J.D. Cole, *Perturbation Methods in Applied Mathematics* (Blaisdell, Waltham, Mass., 1968), pp. 105—11.

[17]Ya. B. Zel'dovich and A.A. Starobinsky, Zh. Eksp. Teor. Fiz. **61**, 2161 (1971) [Sov. Phys. JETP **34**, 1159 (1972)]; S.A. Fulling, Ph.D. dissertation, Princeton University (1972), pp. 150—53, 336—42, 351—63.

[18]Ref. 3, pp. 34—35 with back reference to pp. 25—31. In Eq. (7.11) (p. 29) the term $\mu_1(\tau)\Omega_0'(\tau)$ carries the wrong sign.

[19]Since $(\mathbf{e},\mathbf{e}) = 1$, $(\mathbf{e},\mathbf{e}')$ is an imaginary number.

Vector and tensor fields on conformal space*

D. H. Mayer

Institut für Theoretische Physik, RWTH Aachen, Aachen, West Germany
(Received 25 March 1974; revised manuscript received 8 August 1974)

We consider in this paper vector and tensor fields on the compactified Minkowski space M_c^4 and investigate their transformation properties under the group $SO(2,4)$ of conformal transformations which are well defined on the manifold M_c^4 contrary to their singular behavior on the pseudo-Euclidean noncompact Minkowski space M_4. In writing down field equations on the manifold M_c^4, we get immediately the well-known conformal invariance of Maxwell's equations. Also the problem of gauge transformations of the vector potential is treated both from the global point of view on the manifold M_c^4 and from the local point of view on the Minkowski space M_4. There we show which gauge instead of the so-called Lorentz gauge one has to choose to get a conformal covariant formulation of Maxwell's equations on the pseudo-Euclidean noncompact Minkowski space M_4.

INTRODUCTION

Besides its application in general relativity[1,2] the conformal group plays also an important role in elementary particle physics and quantum field theory. The starting point for the application there was the discovery[3] that a field theory for very high energies could in some sense asymptotically be determined by a massless theory or that the interactions of particles become independent of their masses if the momenta are high enough. It was known already long ago[4] that the group of conformal transformations is an invariance group of such a theory, in the sense that the field equations for these theories are invariant under these transformations if the fields are transformed in a certain manner.

This problem was treated in two papers by Flato *et al.*[5] and Rosen,[6] who found the general solution for the transformation matrix acting on the fields. These authors work in the usual four-dimensional pseudo-Euclidean Minkowski space M_4. From the definition of the conformal tranformations it is clear that certain of them are singular on this space. This fact seems to be the main reason for all the difficulties arising whenever one tries to apply the global conformal transformations to physical problems.

A way out of this problem was in principle already found by Dirac[7] and mathematically formulated in a rigorous way by Penrose in general relativity.[8] One has only to compactify the usual Minkowski space by adding points at infinity. There are different mathematical formulations of this compactification in the literature, Penrose for instance calls it light cones at infinity, but they are all topologically equivalent. For our purpose the compactification of M_4 as a closed subspace of the five-dimensional projective space[9] $\mathbb{P}^5$ appears as the most convenient one.

On this compactified Minkowski space M_c^4 the conformal group can act as a well-defined group of C^∞ transformations. It is therefore of some advantage to work not on the usual space M_4 but instead on the compact manifold M_c^4 when one is going to apply the conformal group to physical problems. As a first step in this direction we wrote down in a recent paper[10] the massless Klein-Gordon equation for scalar fields and got immediately the conformal invariance of this equation on the manifold M_c^4. Furthermore, we got also the familiar transformation properties of a scalar field under the different conformal transformations on M_4 by writing the quite natural transformation laws on the manifold M_c^4 in local coordinates.

The advantage compared to the common treatment of these problems in the literature is the fact that our formulation is mathematically rigorous and indeed quite natural on the manifold M_c^4. In this paper we continue this work in the same spirit and discuss vector and tensor fields on the manifold M_c^4. Here again we can write down field equations which are easily seen to be conformally invariant. In this way we can give a rigorous and detailed discussion of the long known invariance properties of Maxwell's equations[4] under the group of conformal transformations. The difference from Dirac's treatment[7] is that we are working in four space—time dimensions whereas he is working on a five-dimensional hypercone embedded in a six-dimensional space.

In discussing Maxwell's equations for the vector potential and the related gauge transformations on the manifold M_c^4, we can then deduce the correct Maxwell equations for the vector potential in M_4 in a gauge which is, contrary to the usually used Lorentz gauge, conformally invariant. We show that this supplementary condition on the vector potential can be chosen to be a linear equation in the vector potential which gives as a special case exactly the Lorentz condition. This is in contrast to a comment of Flato *et al.* in Ref. 5 where they introduce a nonlinear equation.

In writing the transformation properties of the fields on the compactified Minkowski space M_c^4 under the conformal group in local coordinates, that means that, in the coordinates of the space M_4, we get the formal transformation properties of vector and tensor fields on the space M_4, formal because the expressions involved are generally not defined for global special conformal transformations. Compared with the result of Flato *et al.*,[5] we can give the full transformation matrix and not only an expansion of it up to order two in the group parameters. Our results coincide with the heuristically written down transformation properties of these fields in different papers.[11–13]

In detail, the problems are handled in the following way: After a brief review of the compactification of the

Minkowski space M_4 we discuss in the first section the structure of vector fields on M_c^4.

In Sec. II cotangent vectors and the tensor product of cotangent vector spaces on the manifold M_c^4 are treated, especially the symmetric tensors and the antisymmetric tensors of rank 2.

In Sec. III the different tensor fields are discussed. The results of these first three sections allow us to treat the problem of extending Maxwell's equations for the vector potential to the manifold M_c^4 in Sec. IV. It is shown how these conformal covariant equations on M_c^4 look in global coordinates and how they look if they are written in local coordinates of the space M_4.

In Sec. V the notion of gauge transformations on M_c^4 is introduced, and it is shown how their local version generalizes the Lorentz gauge in Minkowski space M_4.

In Sec. VI we extend the Maxwell tensor field $f^{ij}(x)$ from Minkowski space M_4 to an antisymmetric tensor field $F^{\mu\nu}(\eta)$ on the manifold M_c^4 and discuss the manifestly conformal covariance of the equations these fields fulfill.

In the last section, VII, finally, we investigate the transformation properties of scalar, vector, and tensor fields on the manifold M_c^4 and discuss again their local versions in Minkowski space M_4.

I. VECTOR FIELDS ON M_c^4

Let us first briefly recall the definition of the compactified Minkowski space M_c^4.[2,8-10,14] Consider the space $\mathring{\mathbb{R}}_2^6$ defined as

$$\mathring{\mathbb{R}}_2^6 := \{q = (\eta^0, \cdots, \eta^5) \in \mathbb{R}^6 \setminus \{0\}\} \tag{1}$$

together with the metric $g^{\mu\nu}$, $g^{00} = g^{55} = -g^{11} = \cdots = -g^{44} = 1$ and all the $g^{\mu\nu} = 0$ for $\mu \neq \nu$, $\mu, \nu \in (0, 1, \cdots, 5)$, and the subset $Q_0^5 \subset \mathring{\mathbb{R}}_2^6$,

$$Q_0^5 := \{q \in \mathring{\mathbb{R}}_2^6 : \eta^\mu g_{\mu\nu} \eta^\nu = \eta^\mu \eta_\mu = 0\}. \tag{2}$$

We introduce the following equivalence relation ~ in Q_0^5:

$q_1 \sim q_2$ iff $\eta_1^\mu = \rho \eta_2^\mu$ for all μ and some $\rho \in \mathbb{R}_0 := \mathbb{R} \setminus \{0\}$.

Then the compactified Minkowski space M_c^4 is defined as

$$M_c^4 := Q_0^5 / \sim. \tag{3}$$

Let be π the canonical map $\pi: Q_0^5 \to M_c^4$.

In two papers[10,14] together with Go and Kastrup the notion of conformal causality and the Klein–Gordon operator for scalar fields on this space M_c^4 were investigated. Let us now consider vector fields on M_c^4. We denote by $X(Q_0^5)$ the set of all C^∞ vector fields X on the manifold Q_0^5, i.e.,

$$X(Q_0^5) := \{X = a^\mu(\circ)\partial_\mu : \eta^\mu a_\mu(q) = 0 \quad \forall q = (\eta^0, \cdots, \eta^5) \in Q_0^5, a^\mu(q) \in C^\infty(Q_0^5)\}. \tag{4}$$

Of special interest for the following discussion is the following subset $X_1(Q_0^5) \subset X(Q_0^5)$:

$$X_1(Q_0^5) := \{X = a^\mu(\circ)\partial_\mu : X \in X(Q_0^5),\ a^\mu(\rho q) = \rho a^\mu(q) \forall \mu, \forall \rho \in \mathbb{R}_0\}, \tag{5}$$

i.e., the set of all vector fields whose components are C^∞ functions homogeneous of degree 1 in q. In the set $X_1(Q_0^5)$ an equivalence relation $\approx$ is introduced as follows:

Let $X_1 = a^\mu(\circ)\partial_\mu$ and $X_2 = b^\mu(\circ)\partial_\mu \in X_1(Q_0^5)$, then

$$X_1 \approx X_2 \text{ iff } b^\mu(\eta) = a^\mu(\eta) + \sigma(\eta)\eta^\mu$$

for some C^∞ mapping $\sigma: Q_0^5 \to \mathbb{R}$,

homogeneous of degree 0 in η. (6)

Lemma: The quotient space $\bar{X}(M_c^4) := X_1(Q_0^5)/\approx$, whose elements we denote by $[X]$, is isomorphic to the space $X(M_c^4)$ of all C^∞ vector fields on M_c^4, so that we can identify the two spaces.

Proof: It can be shown[14] that the tangent bundle of the manifold M_c^4 can be identified with the following set:

$$\bar{T}(M_c^4) := \{[(q, a^\mu \partial_\mu)],\ q \in Q_0^5, a^\mu \partial_\mu \in T_q(Q_0^5),$$

where $(q, a^\mu\partial_\mu)$, $(q', a^{\mu\prime}\partial_\mu)$ belong to the same class

$[(q, a^\mu\partial_\mu)]$ iff $\eta^{\mu\prime} = \rho\eta^\mu$ and $a^{\mu\prime} = \rho a^\mu + \sigma\eta^\mu$

for some $\rho \in \mathbb{R}_0$ and some $\sigma \in \mathbb{R}\}$.

Consider an element $[X] = [a^\mu(\circ)\partial_\mu] \in X_1(Q_0^5)/\approx$ and an element $[q] \in M_c^4$:

$$[X]([q]) := [(q, a^\mu(q)\partial_\mu)] \in \bar{T}(M_c^4). \tag{7}$$

It can be easily seen that this definition does not depend on the representative q of $[q]$ nor on the representative $a^\mu(\circ)\partial_\mu$ of $[X]$: Take any other two representatives q' and $a^{\mu\prime}(\circ)\partial_\mu$ of $[q]$ and $[X]$ respectively, then $(q', a^{\mu\prime}(q')\partial_\mu)$ determines the same class as $(q, a^\mu(q)\partial_\mu)$ in $\bar{T}(M_c^4)$ because $\eta^{\mu\prime} = \rho\eta^\mu$ and $a^{\mu\prime}(\rho q) = \rho a^{\mu\prime}(q) = \rho(a^\mu(q) + \sigma(q)\eta^\mu) = \rho a^\mu(q) + \bar{\sigma}\eta^\mu$ with $\rho \in \mathbb{R}_0$ and some $\bar{\sigma} \in \mathbb{R}$. The fact that $a^\mu(\circ) \in C^\infty(Q_0^5)$ ensures that the above mapping (7) is even a C^∞ section.

On the other hand let $[X]$ be a C^∞ vector field on M_c^4, i.e., in local coordinates $x = (x^0, x^1, x^2, x^3)$ $[X]$ has the form $[X] = A^j(x)\partial/\partial x^j$, where the functions $A^j(x) \in C^\infty(\mathbb{R}^4)$. The local vector field $A^j(\circ)\partial_j$ can be expressed as a vector field $a^\mu(\circ)\partial_\mu$, where $a^\mu(\rho\eta) = \rho a^\mu(\eta)$ and $a^\mu(\circ) \in C^\infty(Q_0^5)$ for all $\mu = 0, 1, \cdots, 5$. The components of the vector field $a^\mu(\circ)\partial_\mu \in X_1(Q_0^5)$ are given in terms of the components $A^j(x)$ in the following way[14]:

$$\begin{aligned} &a^j(\eta) = \kappa A^j(\eta/\kappa), \quad a^\kappa(\eta) = 0, \\ &a^\lambda(\eta) = 2\eta^j A_j(\eta/\kappa), \quad \eta = (\eta^0, \eta^1, \eta^2, \eta^3). \end{aligned} \tag{8}$$

This vector field $a^\mu(\circ)\partial_\mu$ determines exactly one class $[a^\mu(\circ)\partial_\mu]$ in $X_1(Q_0^5)/\approx$. This completes the proof of the lemma.

II. COTANGENT VECTORS AND TENSOR PRODUCTS

To treat the Maxwell tensor f^{ij} in a conformal way, we next have to investigate the 1- and 2-forms on the manifold M_c^4. For this reason let us first discuss the cotangent vectors ω_q of Q_0^5 in a point q.

In the coordinates η a cotangent vector ω_q at a point $q \in \mathring{\mathbb{R}}_2^6$ has the general form

$$\omega_q = b^\mu d\eta_\mu, \quad b^\mu \in \mathbb{R} \text{ for all } \mu = 0, 1, \cdots, 5. \tag{9}$$

Consider next the cotangent vector $\bar{\omega}_q = \eta^\mu d\eta_\mu$. Applying it to a general tangent vector $X_q = a^\mu \partial_\mu \in T_q(Q_0^5) \subset T_q(\mathring{\mathbb{R}}_2^6)$,

we get

$$\bar{\omega}_q(a^\mu\partial_\mu)=a^\mu\eta_\mu=0 \quad \text{because } a^\mu\partial_\mu\in T_q(Q_0^5).$$

Therefore, the cotangent vector $\eta^\mu d\eta_\mu=0$ on $T_q(Q_0^5)$. If we therefore introduce in the set $T_q^*(\mathring{\mathbb{R}}_2^6)$ of all cotangent vectors in $\mathring{\mathbb{R}}_2^6$ the equivalence relation $\sim^*$

$$b^\mu d\eta_\mu \sim^* b^{\mu\prime} d\eta'_\mu \quad \text{iff} \quad b^{\mu\prime}=b^\mu+\rho\eta^\mu, \quad \rho\in\mathbb{R}, \forall\mu, \tag{10}$$

the space $T_q^*(Q_0^5)$ can be identified with $T_q^*(\mathring{\mathbb{R}}_2^6)/\sim^*$, the elements of which we denote by $[b^\mu d\eta_\mu]$.

To construct the space $T_q^*(M_c^4)$ we apply a representative $b^\mu d\eta_\mu$ of $[b^\mu d\eta_\mu]$ to any representative $a^\mu\partial_\mu$ of an element $[a^\mu\partial_\mu]$ of the tangent space $T_q(M_c^4)$; this gives

$$b^\mu d\eta^\mu(a^\nu\partial_\nu)=b^\mu a_\mu. \tag{11}$$

As a special case consider the zero tangent vector $a^\mu\partial_\mu=\eta^\mu\partial_\mu$:

$$b^\mu d\eta_\mu(\eta^\nu\partial_\nu)=\eta^\mu b_\mu=0 \quad \text{for all } b^\mu d\eta_\mu. \tag{12}$$

Therefore $b^\mu\eta_\mu=0$ is a supplementary condition for cotangent vectors acting on tangent vectors in M_c^4.

Consider the set $T^*(Q_0^5)$

$$T^*(Q_0^5)=\{(q,[b^\mu d\eta_\mu]):q\in Q_0^5,[b^\mu d\eta_\mu]\in T_q^*(Q_0^5)\}. \tag{13}$$

This set is called the cotangent bundle of the manifold Q_0^5. To get from it the cotangent bundle of the manifold M_c^4, we introduce again an equivalence relation $\approx^*$ in $T^*(Q_0^5)$:

$$(q,[b^\mu d\eta_\mu])\approx^*(q',[b^{\mu\prime}d\eta_\mu]) \quad \text{iff} \quad \eta^{\mu\prime}=\rho\eta^\mu, \quad b^{\mu\prime}=\rho^{-1}b^\mu+\sigma\eta^\mu$$

$$\text{for some } \rho\in\mathbb{R}_0 \text{ and some } \sigma\in\mathbb{R}. \tag{14}$$

It can be seen very easily that the above definition of $\approx^*$ does not depend on the choice of the representatives $b^\mu d\eta_\mu$ and $b^{\mu\prime}d\eta_\mu$. As always we shall denote the elements of the set $\bar{T}^*(M_c^4)$ defined as $T^*(Q_0^5)/\approx^*$ by the symbol $[(q,[b^\mu d\eta_\mu])]$ or by $[(q,b^\mu d\eta_\mu)]$. In the next step we want to show that the set $\bar{T}^*(M_c^4)$ can indeed be identified with the cotangent bundle $T^*(M_c^4)$. For this we consider the subset $\bar{T}^*_{[q]}(M_c^4)\subset\bar{T}^*(M_c^4)$ which is defined in the following way:

$$\bar{T}^*_{[q]}(M_c^4):=\{[(q,[b^\mu d\eta_\mu])]\in\bar{T}^*(M_c^4):[q] \text{ fixed}\} \tag{15}$$

and the subset

$$\bar{T}_{[q]}(M_c^4):=\{[(q,a^\mu\partial_\mu)]\in\bar{T}(M_c^4):[q] \text{ fixed}\}. \tag{16}$$

Choose any $[(q,[b^\mu d\eta_\mu])]\in\bar{T}^*_{[q]}(M_c^4)$ and any $[(q,a^\mu\partial_\mu)]\in\bar{T}_{[q]}(M_c^4)$ and two representatives $(q,b^\mu d\eta_\mu)$ and $(q,a^\mu\partial_\mu)$ of these classes. Then

$$[(q,[b^\mu d\eta_\mu])]\{[(q,a^\mu\partial_\mu)]\}:=b^\mu d\eta_\mu\{(a^\mu\partial_\mu)\}=a^\mu b_\mu.$$

If $q'=\rho q$ and $b^{\mu\prime}d\eta_\mu$ and $a^{\mu\prime}\partial_\mu$ are other representatives, we get

$$(q',b^{\mu\prime}d\eta_\mu)\{(q',a^{\mu\prime}\partial_\mu)\}=b^{\mu\prime}a_\mu'=(\rho^{-1}b^\mu+\sigma_1\eta^\mu)$$
$$\times(\rho a_\mu+\sigma_2\eta_\mu)=b^\mu a_\mu,$$

because $a^\mu\eta_\mu=b^\mu\eta_\mu=\eta^\mu\eta_\mu=0$. Therefore, $\bar{T}^*_{[q]}(M_c^4)$ is contained in the dual of $\bar{T}_{[q]}(M_c^4)$.

We can express any element $[(q,[b^\mu d\eta_\mu])]\in\bar{T}^*_{[q]}(M_c^4)$ also in local coordinates x of the chart U_κ (for the definition of the different charts U_α, see Ref. 10):

$$b^\mu d\eta_\mu=b^\mu\frac{\partial\eta_\mu}{\partial x_\kappa}dx_k=V^k dx_k \tag{16'}$$

where $V^k=\kappa b^k-\kappa b^\kappa x^k$ and $x^k=\eta^k\kappa^{-1}$, $k=0,1,\cdots,3$.

On the other hand, let there be given a cotangent vector $V^j dx_j$ in local coordinates x^j; then we want to express it in the coordinates η. This can be done via the mapping $\pi^*_{[q]}$:

$$\pi^*_{[q]}: T^*_{[q]}(M_c^4)\to T_q^*(Q_0^5), \tag{17}$$

$$\pi^*_{[q]})\omega_{[q]}(X_q)$$
$$=\omega_{[q]}(\pi_*X_q), \text{ where } \omega_{[q]}\in T^*_{[q]}(M_c^4) \text{ and } X_q\in T_q(Q_0^5). \tag{18}$$

Taking $\omega_{[q]}=dx^j$, we get

$$\pi^*_{[q]}(dx^j)(a^\mu\partial_\mu)=dx^j(a^k\kappa^{-1}-\eta^k a^\kappa\kappa^{-2})\partial_k=a^j\kappa^{-1}-\eta^j a^\kappa\kappa^{-2}$$
$$=(b^k d\eta_k-2^{-1}b^\kappa d\lambda-2^{-1}b^\lambda d\kappa)(a^\mu\partial_\mu)$$
$$=a^k b_k-2^{-1}b^\kappa a^\lambda-2^{-1}b^\lambda a^\kappa.$$

From this we get

$$b^\kappa=0, \quad b_k=\kappa^{-1}\delta_{jk}, \quad b^\lambda=2\kappa^{-2}\eta^j.$$

For the general cotangent vector $V^j dx_j$ finally the result is

$$V^j dx_j\leftrightarrow b^\mu d\eta_\mu$$
$$\text{with } b^\kappa=0, \ b^k=\kappa^{-1}V^k, \ b^\lambda=2\eta^j V_j\kappa^{-2}. \tag{19}$$

This cotangent vector $b^\mu d\eta_\mu$ determines uniquely a class $[(q,[b^\mu d\eta_\mu])]$ in the set $\bar{T}^*_{[q]}(M_c^4)$ and therefore there is a one-to-one map of $\bar{T}^*_{[q]}(M_c^4)$ onto the set $T^*_{[q]}(M_c^4)$.

Next let us construct the tensor product $T^*_{[q]}(M_c^4)\otimes T^*_{[q]}(M_c^4)$. We proceed in the same way as we did in constructing the space $T^*_{[q]}(M_c^4)$. The general element of the tensor product $T_q^*(\mathring{\mathbb{R}}_2^6)\otimes T_q^*(\mathring{\mathbb{R}}_2^6)$ has the form:

$$F^{\mu\nu}d\eta_\mu\otimes d\eta_\nu. \tag{20}$$

As a special case consider the expression

$$F^{\mu\nu}=b^\mu\eta^\nu, \tag{21}$$

where (b^μ) is any point in $\mathbb{R}^6$. Applying this tensor of rank 2 to an element of $T_q(Q_0^5)\otimes T_q(Q_0^5)$, we get

$$b^\mu\eta^\nu d\eta_\mu\otimes d\eta_\nu(a^\mu\partial_\mu\otimes a^\nu\partial_\nu)=b^\mu a_\mu\eta^\nu a'_\nu=0,$$

because $a^\nu\partial_\nu$ is an element of $T_q(Q_0^5)$. The same happens for the tensor $F^{\mu\nu}d\eta_\mu\otimes d\eta_\nu$ where

$$F^{\mu\nu}=\eta^\mu b^\nu. \tag{22}$$

Therefore, the tensor $(b^\mu\eta^\nu+b^{\nu\prime}\eta^\mu)d\eta_\mu\otimes d\eta_\nu$ acts on the tensor product $T_q(Q_0^5)\otimes T_q(Q_0^5)$ as the zero tensor $\mathring{F}^{\mu\nu}\equiv 0$. It is therefore straightforward to introduce in $T_q^*(\mathring{\mathbb{R}}_2^6)\otimes T_q^*(\mathring{\mathbb{R}}_2^6)$ an equivalence relation $\sim_2^*$

$$F^{\mu\nu}d\eta_\mu\otimes d\eta_\nu\sim_2^* G^{\mu\nu}d\eta_\mu\otimes d\eta_\nu \quad \text{iff} \quad F^{\mu\nu}=G^{\mu\nu}+b^\mu\eta^\nu+b'^\nu\eta^\mu$$
$$\text{for all } \nu,\mu=0,\cdots,5 \text{ with } b,b'\in\mathbb{R}^6. \tag{23}$$

To get finally the tensor product $T^*_{[q]}(M_c^4)\otimes T^*_{[q]}(M_c^4)$, we apply any tensor $F^{\mu\nu}d\eta_\mu\otimes d\eta_\nu\in T_q^*(Q_0^5)\otimes T_q^*(Q_0^5)$ to the special elements $\eta^\mu\partial_\mu\otimes a^\mu\partial_\mu$ and $a^\mu\partial_\mu\otimes\eta^\nu\partial_\nu\in T_{[q]}(M_c^4)\otimes T_{[q]}(M_c^4)$:

$$F^{\mu\nu}d\eta_\mu\otimes d\eta_\nu(a^\mu\partial_\mu\otimes\eta^\mu\partial_\mu)=F^{\mu\nu}a_\mu\eta_\nu, \tag{24}$$

$$F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu(\eta^\mu\partial_\mu \otimes a^\mu\partial_\mu) = F^{\mu\nu}\eta_\mu a_\nu. \tag{25}$$

Since the elements $\eta^\nu\partial_\nu \otimes a^\mu\partial_\mu$ and $a^\mu\partial_\mu \otimes \eta^\nu\partial_\nu$ are the zero element in $T_{[q]}(M_c^4) \otimes T_{[q]}(M_c^4)$, the general tensor $F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu$ applied to it must give zero: $F^{\mu\nu}a_\mu\eta_\nu = 0 = F^{\mu\nu}\eta_\mu a_\nu$ for all $a^\mu\eta_\mu = 0$. From this it follows that the relations

$$F^{\mu\nu}\eta_\mu \propto \eta^\nu \tag{26}$$

and

$$F^{\mu\nu}\eta_\nu \propto \eta^\mu \quad \text{must hold.} \tag{27}$$

The cotangent vector $\eta^\nu d\eta_\nu \in T^*_{[q]}(M_c^4)$ is the zero cotangent vector, and therefore we can demand

$$F^{\mu\nu}\eta_\mu = 0 = F^{\mu\nu}\eta_\nu \quad \text{on } Q_0^5. \tag{28}$$

In the tensor bundle

$$T_2^*(Q_0^5) := \bigcup_{q\in Q_0^5} T_q^*(Q_0^5) \otimes T_q^*(Q_0^5),$$

whose elements we denote by the pair $(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)$, we can consider the following equivalence relation $\approx_2^*$:

$$\begin{aligned}&(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu) \approx_2^* (q', F^{\mu\nu\prime}d\eta_\mu \otimes d\eta_\nu)\\ &\quad \text{iff} \quad \eta^{\mu\prime} = \rho\eta^\mu, \quad F^{\mu\nu\prime} = \rho^{-2}F^{\mu\nu} + b^\mu\eta^\nu + c^\nu\eta^\mu\\ &\quad \text{with} \quad b^\mu\eta_\mu = c^\nu\eta_\nu = 0 \quad \text{and} \quad \rho \in \mathbb{R}_0.\end{aligned} \tag{29}$$

We put $\bar{T}_2^*(M_c^4) := T_2^*(Q_0^5)/\approx_2^*$ and denote the elements of this space by $[(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)]$. The space $\bar{T}_2^*(M_c^4)$ can again be identified with the bundle $T_2^*(M_c^4)$: Take any two representatives $(q, a^\mu\partial_\mu \otimes a^{\nu\prime}\partial_\nu)$ and $(q', c^\mu\partial_\mu \otimes c^{\nu\prime}\partial_\nu)$ from the class $[(q, (a^\mu\partial_\mu \otimes a^{\nu\prime}\partial_\nu))]$ and any two representatives of the class $[(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)]$, say $(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)$ and $(q', F^{\mu\nu\prime}d\eta_\mu \otimes d\eta_\nu)$:

$$(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)\{(q, a^\mu\partial_\mu \otimes a^{\nu\prime}\partial_\nu)\} = F^{\mu\nu}a_\mu a'_\nu, \tag{30}$$

$$(q', F^{\mu\nu\prime}d\eta_\mu \otimes d\eta_\nu)\{(q', c^\mu\partial_\mu \otimes c^{\nu\prime}\partial_\nu)\} = F^{\mu\nu\prime}c_\mu c'_\nu. \tag{31}$$

If $q' = \rho q$, then $F^{\mu\nu\prime} = \rho^{-2}F^{\mu\nu} + b^\mu\eta^\nu + b^{\nu\prime}\eta^\mu$ and $c^\mu = \rho a^\mu + \delta\eta^\mu$, $c^{\mu\prime} = \rho a^{\mu\prime} + \delta'\eta^\mu$, and therefore

$$\begin{aligned}F^{\mu\nu\prime}c_\mu c'_\nu &= (\rho^{-2}F^{\mu\nu} + b^\mu\eta^\nu + b^{\nu\prime}\eta^\mu)\\ &\quad \times (\rho a_\mu + \delta\eta_\mu)(\rho a'_\nu + \delta'\eta_\nu) = F^{\mu\nu}a_\mu a'_\nu,\end{aligned}$$

because $\eta_\mu F^{\mu\nu} = \eta_\nu F^{\mu\nu} = \eta_\mu a^\mu = \eta_\nu b^\nu = \eta_\nu b^{\nu\prime} = \eta_\mu a^{\mu\prime} = \eta_\mu\eta^\mu = 0$.

Next we want to give a description of the tensors of rank 2 at a point $[q] \in M_c^4$ in local coordinates. It is known[15] that any such tensor can be written as $f^{ij}dx_i \otimes dx_j$, where the dx_i constitute a basis of the cotangent space $T^*_{[q]}(M_c^4)$. The connection of the components f^{ij} and the components $F^{\mu\nu}$ can be found by using the formula

$$\begin{aligned}&d\eta^\mu = \frac{\partial\eta^\mu}{\partial x^i}dx^i \quad \text{with } \eta^i = \kappa x^i, \ \lambda = \kappa x^j x_j,\\ &\quad \kappa \text{ independent of } x^i.\end{aligned} \tag{32}$$

Then we get

$$F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu \overset{\text{loc}}{=} f^{ij}dx_i \otimes dx_j$$

with

$$f^{ij} = \kappa^2F^{ij} - \kappa^2F^{i\kappa}x^j - \kappa^2F^{\kappa j}x^i + \kappa^2F^{\kappa\kappa}x^ix^j. \tag{33}$$

From this we can also see that all representatives of an element $[(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)]$ correspond everywhere locally to the same tensor and are therefore the same tensor on M_c^4.

On the other hand, given a tensor from $T^*_{2[q]}(M_c^4)$ in local coordinates $f^{ij}dx_i \otimes dx_j$, we can easily find a representative of this tensor in the η coordinates, namely the tensor $F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu$ with

$$\begin{aligned}&F^{ij} = f^{ij}\kappa^{-2}, \quad F^{\lambda j} = \kappa^{-3}2\eta_i f^{ij},\\ &F^{i\lambda} = \kappa^{-3}2\eta_k f^{ik}, \quad F^{\lambda\lambda} = \kappa^{-4}4\eta_i\eta_k f^{ik},\\ &F^{i\kappa} = F^{\kappa i} = F^{\kappa\kappa} = F^{\lambda\kappa} = F^{\kappa\lambda} = 0.\end{aligned} \tag{34}$$

This can be derived from relation (33) and from the properties (28).

Of special interest for us are the so-called skew-symmetric tensors and tensor fields which we want to discuss next.

We have seen that every tensor of rank 2 on M_c^4 can be represented as a class of tensors of rank 2 on Q_0^5. From now on we make the identification

$$T_2^*(M_c^4) = \bar{T}_2^*(M_c^4) = \{[(q, F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu)]\} \tag{35}$$

Then every $F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu$ can be written as

$$\begin{aligned}F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu &= 2^{-1}F^{\mu\nu}(d\eta_\mu \otimes d\eta_\nu + d\eta_\nu \otimes d\eta_\mu)\\ &\quad + 2^{-1}F^{\mu\nu}(d\eta_\mu \otimes d\eta_\nu - d\eta_\nu \otimes d\eta_\mu)\end{aligned} \tag{36}$$

One can see immediately that only the symmetric part of $F^{\mu\nu}$ contributes to the first term and only the antisymmetric part to the second one. For the antisymmetric part we write, as is common,

$$d\eta_\mu \wedge d\eta_\nu := 2^{-1}(d\eta_\mu \otimes d\eta_\nu - d\eta_\nu \otimes d\eta_\mu). \tag{37}$$

The antisymmetric tensors of rank 2 which we denote by $F^{\mu\nu}d\eta_\mu \wedge d\eta_\nu$ are therefore exactly the tensors $F^{\mu\nu}d\eta_\mu \otimes d\eta_\nu$ where $F^{\mu\nu} = -F^{\nu\mu}$. Whereas the condition (28) is still valid, two antisymmetric tensors, $(q, F^{\mu\nu}d\eta_\mu \wedge d\eta_\nu)$ and $(q', F^{\mu\nu\prime}d\eta_\mu \wedge d\eta_\nu)$, are equivalent iff

$$\begin{aligned}&F^{\mu\nu\prime} = \rho^{-2}F^{\mu\nu} + b^\mu\eta^\nu - b^\nu\eta^\mu\\ &\quad \text{for } q' = \rho q \text{ and some } b = (b^\mu) \text{ with } \eta^\mu b_\mu = 0.\end{aligned} \tag{38}$$

In local coordinates the antisymmetric tensor of rank 2 can be expressed as $S^{ij}dx_i \wedge dx_j$, where $S^{ij} = -S^{ji}$. Given an antisymmetric tensor $(q, F^{\mu\nu}d\eta_\mu \wedge d\eta_\nu)$ in η-coordinates, the corresponding tensor in x-space reads as follows [see (33)]:

$$S^{ij}dx_i \wedge dx_j, \quad \text{where } S^{ij} = \kappa^2F^{ij} - \kappa^2F^{i\kappa}x^j - \kappa^2F^{\kappa j}x^i. \tag{39}$$

Inserting $F^{\mu\nu\prime}$ from (38) gives again the same S^{ij} for all b^μ with $\eta^\mu b_\mu = 0$.

The inverse problem given S^{ij} to find $F^{\mu\nu}$ is already solved in formula (34). For $S^{ij} = -S^{ji}$ we get

$$\begin{aligned}&F^{ij} = \kappa^{-2}S^{ij}, \quad F^{\lambda j} = \kappa^{-3}2\eta_i S^{ij} = -\kappa^{-3}2\eta_i S^{ji} = -F^{j\lambda},\\ &F^{\kappa\kappa} = F^{\lambda\lambda} = F^{\lambda\kappa} = F^{\kappa\lambda} = F^{i\kappa} = F^{\kappa i} = 0.\end{aligned} \tag{40}$$

III. TENSOR FIELDS ON M_c^4

After the discussion of the different tangent, cotangent, and tensor spaces in the last sections, we consider next tensor fields on the manifold M_c^4. Generally these are defined as differentiable sections of the correspond-

ing tensor bundles. As a special case we have already discussed in Sec. I the sections of the tangent bundle of M_c^4, the so-called vector fields. This procedure will be generalized now to tensor fields of rank 2 on the manifold M_c^4.

Let be $T_2^*(\mathring{\mathbb{R}}_2^6)$ the set of all tensor fields ω of rank 2 in $\mathring{\mathbb{R}}_2^6$, where

$$\omega = F^{\mu\nu}(\cdot)d\eta_\mu \otimes d\eta_\nu, F^{\mu\nu}(\cdot): \mathring{\mathbb{R}}_2^6 \to \mathbb{R} \tag{41}$$

with the following properties:

(1) $F^{\mu\nu}(\cdot) \in C^\infty(Q_0^5)$,

(2) $F^{\mu\nu}(\rho q) = \rho^{-2} F^{\mu\nu}(q) \; \forall \, q \in \mathring{\mathbb{R}}_2^6 \; \forall \rho \in \mathbb{R}_0$,

(3) $F^{\mu\nu}(\eta)\eta_\mu = F^{\mu\nu}(\eta)\eta_\nu = 0 \; \forall \, (\eta) \in Q_0^5$.

We introduce an equivalence relation $\overset{t}{\sim}$ as follows:

If $\omega_1 = F^{\mu\nu}(\cdot)d\eta_\mu \otimes d\eta_\nu$ and $\omega_2 = G^{\mu\nu}(\cdot)d\eta_\mu \otimes d\eta_\nu$, then

$$\omega_1 \overset{t}{\sim} \omega_2 \text{ iff } G^{\mu\nu}(q) = F^{\mu\nu}(q) + b^\mu(q)\eta^\nu + c^\nu(q)\eta^\mu,$$
$$b^\mu(\cdot), c^\nu(\cdot) \in C^\infty(Q_0^5)$$
$$\text{homogeneous of degree } -3 \text{ in } q. \tag{42}$$

Denoting

$$\bar{T}_2^*(M_c^4) := \{[\omega]\} = T_2^*(\mathring{\mathbb{R}}_2^6)/\overset{t}{\sim} \tag{43}$$

we show that $\bar{T}_2^*(M_c^4)$ can be identified with $T_2^*(M_c^4)$, the set of all differentiable tensor fields of rank 2 on the manifold M_c^4.

This can be seen immediately: Take $q, q' \in [q]$, $q' = \rho q$ and $F^{\mu\nu}(\cdot)d\eta_\mu \otimes d\eta_\nu$, $G^{\mu\nu}(\cdot)d\eta_\mu \otimes d\eta_\nu$; then

$$[\omega]([q]) = [(q, F^{\mu\nu}(q)d\eta_\mu \otimes d\eta_\nu)] =$$
$$= [(q', G^{\mu\nu}(q')d\eta_\mu \otimes d\eta_\nu)]. \tag{44}$$

This is true because

$$G^{\mu\nu}(q') = F^{\mu\nu}(q') + b^\mu(q')\eta^{\nu\prime} + c^\nu(q')\eta^{\mu\prime}$$
$$= \rho^{-2}F^{\mu\nu}(q) + \rho^{-2}(b^\mu(q)\eta^\nu + c^\nu(q)\eta^\mu)$$

and therefore $(q, F^{\mu\nu}(q)d\eta_\mu \otimes d\eta_\nu)$ and $(q', G^{\mu\nu}(q')d\eta_\mu \otimes d\eta_\nu)$ are representatives of the same class in $\bar{T}_{2\,[q]}^*(M_c^4)$.

On the other side it is clear that every differentiable tensor field $\omega \in T_2^*(M_c^4)$ determines one class of $T_2^*(\mathring{\mathbb{R}}_2^6)/\overset{t}{\sim}$.

The same arguments as above show us also that the set of all C^∞-antisymmetric tensor fields of rank 2 which are also called differential 2-forms is isomorphic to the set $T_2^a(\mathring{\mathbb{R}}_2^6)/\overset{a}{\sim}$, where the equivalence relation $\overset{a}{\sim}$ according to (38) is given by

$$\omega_1^a \overset{a}{\sim} \omega_2^a \text{ iff } G^{\mu\nu}(q) = F^{\mu\nu}(q) + b^\mu(q)\eta^\nu - b^\nu(q)\eta^\mu$$
$$\text{with } b^\mu(q) \in C^\infty(Q_0^5) \text{ homogeneous of degree } -3 \text{ in } q$$
$$\text{for all } \mu \text{ and } \eta^\mu b_\mu(q) = 0 \text{ on } Q_0^5. \tag{45}$$

The set $T_2^a(\mathring{\mathbb{R}}_2^6)$ is the set of all tensor fields from $T_2^*(\mathring{\mathbb{R}}_2^6)$ which are antisymmetric.

IV. MAXWELL EQUATIONS FOR THE VECTOR POTENTIAL

In Minkowski space Maxwell's equations for the antisymmetric Maxwell tensor field $f^{ij}(x)dx_i \wedge dx_j$ in the presence of an external current $c(x) = (c_j(x))$ are

$$\partial^j f_{ij}(x) = -c_i(x). \tag{46}$$

To solve these equations, it is convenient to introduce the so-called vector potential field $A^j(x)$, $j = 0, 1, \cdots, 3$, in terms of which the Maxwell field $f^{ij}(x)$ reads

$$f^{ij}(x) = \partial^i A^j(x) - \partial^j A^i(x). \tag{47}$$

Equations (46) then become

$$\partial^i \partial_j A^j(x) - \Box A^i(x) = -c^i(x), \quad i = 0, \cdots, 3, \tag{48}$$

or, if we introduce the function $\chi(x)$,

$$\chi(x) = \partial_j A^j(x), \tag{49}$$

Eqs. (48) are

$$\Box A^i(x) = \partial^i \chi(x) + c^i(x). \tag{50}$$

The set of equations (49) and (50) is equivalent to Maxwell's equations (46). The potential $A^j(x)$ is not uniquely determined because any gauge transformation

$$A^j(x) \to A^j(x) + \partial^j \Lambda(x), \quad \Lambda(\cdot) \in C^1(M_4), \tag{51}$$

keeps the tensor field $f^{ij}(x)$ invariant, a fact which is known as gauge invariance of electrodynamics. Working in Minkowski space with the Lorentz group as the relevant invariance group, one chooses the so-called Lorentz gauge which is defined by the function

$$\chi(x) = 0. \tag{52}$$

To arrive at a Lorentz covariant procedure, one must then demand that the gauge function $\Lambda(x)$ fulfill the equation

$$\Box \Lambda(x) = 0. \tag{53}$$

If one does not specialize the function $\chi(x)$, then under a general gauge transformation (51) the function $\chi(x)$ is transformed in the following form:

$$\chi(x) \to \chi(x) + \Box \Lambda(x) \tag{54}$$

and the potential $A^{j\prime}(x) = A^j(x) + \partial^j \Lambda(x)$ therefore fulfills the equation

$$\Box A^{j\prime}(x) = \partial^j \chi'(x) + c^j(x), \tag{55}$$

where $\chi'(x)$ is given by (54) and $\Lambda(x)$ is any differentiable function in M_4.

It has been known already for a long time[4] that Maxwell's equations are covariant with respect to the full conformal group. We want to show how this conformal covariance results when working on the manifold M_c^4. This we shall do in two ways: First we investigate the set of equations (49) and (50) for the vector potential on M_c^4 and show that there is a natural generalization of these equations on the compact manifold which are manifestly conformal covariant. In the second treatment we extend Maxwell's tensor f^{ij} to a conformal tensor $F^{\mu\nu}$ on M_c^4 which fulfills also manifestly conformal covariant equations on M_c^4. (See also Refs. 7 and 16.)

Consider now the equations

$$\Box A^j(x) = \partial^j \chi(x) + c^j(x), \tag{56}$$

$$\chi(x) = \partial^j A_j(x). \tag{57}$$

Discussing the vector fields on M_c^4, we have seen that a

vector field $[X]=a^\mu(\cdot)\partial_\mu$ on M_c^4 can be written locally as

$$A^j(x)\partial_j, \quad \text{where } A^j(x)=\kappa^{-1}a^j(\eta)-\kappa^{-2}\eta^j a^\kappa(\eta). \tag{58}$$

On the chart U_κ therefore we can express every vector field $A^j(x)\partial_j$ in terms of the coordinates η as we did in (8). In general the functions $a^\mu(\eta)$ are not well defined on the whole manifold Q_0^5; this depends on the behavior of the functions $A^j(x)$ at infinity. For the forthcoming discussion we shall assume that the functions $a^\mu(\eta)$ are even $C^\infty(\mathbb{R}^6)$.

We mention the fact that the choice of the function $a^\kappa(\eta)$ in the relations (8) is competely free because we have a whole class of vector fields $a^\mu(\cdot)\partial_\mu$ which locally have exactly the given form $A^j(x)\partial_j$. To describe the vector potential $A^j(x)$ in terms of a field $a^\mu(\eta)$, we have therefore the degree of freedom of a function. The question now is what function $a^\kappa(\eta)$ shall we take. The answer to this is given to us if we look at the set of equations (56), (57). There appears a function $\chi(x)$ for which we also assume to be extendable to the whole manifold M_c^4 and to belong to the class $C^\infty(\mathbb{R}^6)$ in the variables η. As the representative $a^\mu(\cdot)\partial_\mu$ of the class $[a^\mu(\cdot)\partial_\mu]$ therefore we take the following:

$$\begin{aligned} &a^\kappa(\eta)=-2^{-1}\kappa\chi(\eta), \quad a^j(\eta)=\kappa A^j(\eta/\kappa)-2^{-1}\eta^j\chi(\eta/\kappa), \\ &a^\lambda(\eta)=2\eta^j A_j(\eta/\kappa)-\kappa^{-1}\eta^j\eta_j\chi(\eta/\kappa)+2^{-1}\lambda\chi(\eta/\kappa). \end{aligned} \tag{59}$$

The function $a^\lambda(\eta)$ is determined by the requirement

$$\eta^\mu a_\mu(\eta)=0. \tag{60}$$

It would be enough for $a^\mu(\cdot)\partial_\mu$ to be the representative of a vector field on M_c^4 if the equality (60) holds on Q_0^5 as we have seen earlier. Now we demand (60) to hold on the whole space $\mathring{\mathbb{R}}_2^6$. This is of importance for the proof of the following Theorem:

Theorem: Let $[X]$ and $[C]\in X(M_c^4)$ be C^∞ vector fields on M_c^4 and let $a^\mu(\cdot)\partial_\mu$, $c^\mu(\cdot)\partial_\mu$ be representatives of $[X]$ and $[C]$ with $a^\mu(\cdot)$ and $c^\mu(\cdot)\in C^\infty(\mathbb{R}^6)$ and $\eta^\mu a_\mu(\eta)=\eta^\mu c_\mu(\eta)=0$ on $\mathbb{R}^6$. Let $A^j(x)\partial_j$ and $C^j(x)\partial_j$ be the local representatives of $[X]$ and $[C]$ in the coordinates $x\in M_4$. Then the following two sets of equations are equivalent:

$$\left.\begin{aligned} &P_\square a^\mu(\eta)=c^\mu(\eta) \\ &\forall\ \mu \end{aligned}\right\}$$

$$\begin{aligned} &\square A_j(x)=-2\partial_j a^\kappa(x)+C_j(x), \\ &\text{iff} \quad \partial^j A_j(x)=-2a^\kappa(x), \\ &\square a^\kappa(x)=C^\kappa(x) \quad \text{where } a^\kappa(x)=\kappa^{-1}a^\kappa(\eta) \\ &\qquad\qquad \text{and} \quad C^\kappa(x)=\kappa^{-1}c^\kappa(\eta). \end{aligned}$$

$P_\square=\kappa^2\square_6+4\kappa\partial_\lambda(\eta^\mu\partial_\mu+1)$ is the Klein–Gordon operator on M_c^4.[10]

Proof: In the already mentioned paper[10] we have shown that the Klein–Gordon equation $\square\varphi(x)=0$ on the manifold M_c^4 reads $P_\square\phi([\eta])=0$ with $P_\square=\kappa^2\square_6+4\kappa\partial_\lambda(\eta^\mu\partial_\mu+1)$ and $\phi([\eta])=\varphi(\eta/\kappa)$. A simple calculation gives the following important property of the differential operator $P_\square$: Let $\varphi(\eta)$ be any $C^\infty(\mathbb{R}^6)$ function homogeneous of degree n in η. Then for any $m\in\mathbb{Z}$

$$P_\square\kappa^m\varphi(\eta)=\kappa^m P_\square\varphi(\eta) \tag{61}$$

as long as $\kappa^m\varphi(\eta)$ is still a $C^2(\mathbb{R}^6)$ function. Therefore,

$$P_\square\kappa^{-1}a^\kappa(\eta)=\kappa^{-1}P_\square a^\kappa(\eta). \tag{62}$$

On the other hand we have shown in Ref. 10 that

$$P_\square\kappa^{-1}a^\kappa(\eta)=c^\kappa(\eta)\kappa^{-1} \quad \text{iff} \quad \square a^\kappa(x)=C^\kappa(x)$$

$$\text{where} \quad a^\kappa(x)=\kappa^{-1}a^\kappa(\eta), \quad C^\kappa(x)=\kappa^{-1}c^\kappa(\eta). \tag{63}$$

Next let us calculate the action of the operator $P_\square$ on the expression $\kappa^{-1}a^j(\eta)-\kappa^{-2}\eta^j a^\kappa(\eta)=A^j(x)$ for $\kappa\neq 0$:

$$\begin{aligned} &P_\square(\kappa^{-1}a^j(\eta)-\kappa^{-2}\eta^j a^\kappa(\eta)) \\ &\quad=\kappa^{-1}P_\square a^j(\eta)-\kappa^{-2}(\eta^j P_\square a^\kappa(\eta)+2\kappa(\kappa\partial^j+2\eta^j\partial_\lambda)a^\kappa(\eta). \end{aligned} \tag{64}$$

In local coordinates x on M_4 we get

$$\square A^j(x)=\kappa^{-1}P_\square a^j(\eta)-x^j\square a^\kappa(x)-2\frac{\partial}{\partial x_j}a^\kappa(x). \tag{65}$$

Therefore, the two equations

$$\square A^j(x)=-2\partial^j a^\kappa(x)+C^j(x), \tag{66}$$

$$\square a^\kappa(x)=C^\kappa(x) \tag{67}$$

are equivalent to the two equations

$$P_\square a^j(\eta)=c^j(\eta), \tag{68}$$

$$P_\square a^\kappa(\eta)=c^\kappa(\eta). \tag{69}$$

Let us next calculate $P_\square a^\lambda(\eta)$ where $a^\lambda(\eta)=\kappa^{-1}(2\eta^j a_j(\eta)-\lambda a^\kappa(\eta))$ for $\kappa\neq 0$ everywhere in $\mathbb{R}^6$. An easy calculation gives

$$\begin{aligned} P_\square a^\lambda(\eta)=\kappa^{-1}&(2\eta^j P_\square a_j(\eta)-\lambda P_\square a^\kappa(\eta)+4\kappa^2(\kappa\partial^j+2\eta^j\partial_\lambda) \\ &\times\kappa^{-1}(a_j(\eta)-\kappa^{-1}\eta_j a^\kappa(\eta))+8\kappa a^\kappa(\eta)). \end{aligned} \tag{70}$$

In local coordinates this reads

$$\begin{aligned} P_\square\kappa^{-1}a^\lambda(\eta)=\kappa^{-2}&2\eta^j P_\square a_j(\eta)-\kappa^{-2}\lambda P_\square a^\kappa(\eta) \\ &+4\frac{\partial}{\partial x_j}A^j(x)+8a^\kappa(x). \end{aligned} \tag{71}$$

Therefore, under the condition $P_\square a^j(\eta)=c^j(\eta)$ and $P_\square a^\kappa(\eta)=c^\kappa(\eta)$ the relations

$$P_\square a^\lambda(\eta)=c^\lambda(\eta) \quad \text{and} \quad \partial_j A^j(x)=-2a^\kappa(x) \tag{72}$$

are equivalent.

The set of equations

$$P_\square a^\mu(\eta)=c^\mu(\eta), \quad \mu=0,\cdots,5, \tag{73}$$

are Maxwell's equations for the vector potential field on M_c^4. Let us add a corollary to the above theorem which shows explicitly the conformal covariance of Maxwell's equations on the manifold M_c^4.

Corollary: Let be $[X]$ and $[C]\in X(M_c^4)$ and $a^\mu(\cdot)\partial_\mu$, $c^\mu(\cdot)\partial_\mu$ representatives of $[X]$ and $[C]$ with the following properties: $a^\mu(\eta)=\kappa^2\tilde{a}^\mu(\eta)$, $c^\mu(\eta)=\kappa^4\tilde{c}^\mu(\eta)$, where $\tilde{a}^\mu(\eta)$ and $\tilde{c}^\mu(\eta)$ are $C^\infty(\mathbb{R}^6)$ functions homogeneous of degree -1 and -3 respectively. Then Maxwell's equations for the vector field $A^j(x)$ in Minkowski space

$$\square A^j(x)=-2\partial^j a^\kappa(x)+C^j(x),$$

$$\partial^j A_j(x)=-2a^\kappa(x), \quad \square a^\kappa(x)=C^\kappa(x)$$

are equivalent to Maxwell's equations in M_c^4:

$$\square_6\tilde{a}^\mu(\eta)=\tilde{c}^\mu(\eta), \quad \mu=0,\cdots,5 \text{ with } \square_6=\partial^\mu\partial_\mu.$$

Proof: $P_{\Box}\kappa^2\tilde{a}^\mu(\eta)=P_{\Box}a^\mu(\eta)=\kappa^2P_{\Box}\tilde{a}^\mu(\eta)$. But for any function $f(\eta)$ homogeneous of degree -1 in η the differential operator $P_{\Box}$ is exactly the operator $\kappa^2\Box_6$. This and the theorem proves, therefore, the corollary.

The corollary gives us in a manifest way the conformal covariance of Maxwell's equations: If $[X]$ and $[C]\in X(M_c^4)$ are vector fields with representatives $a^\mu(\circ)\partial_\mu$, $c^\mu(\circ)\partial_\mu$, where $a^\mu(\eta)=\kappa^2\tilde{a}^\mu(\eta)$ and $c^\mu(\eta)=\kappa^4\tilde{c}^\mu(\eta)$ for all μ, such that Eqs. (73) are fulfilled, the for every $w\in SO(2,4)/Z_2$ the vector fields $[X]_w$ and $[C]_w$ are also solutions of Eqs. (73), where the generating representatives $a_w^\mu(\cdot)\partial_\mu$ and $c_w^\mu(\circ)\partial_\mu$ of $[X]_w$ and $[C]_w$ are defined as follows:

$$a_w^\mu(\eta)=\kappa^2w^\mu{}_\nu\tilde{a}^\nu(w^{-1}\eta),\quad c_w^\mu(\eta)=\kappa^4w^\mu{}_\nu\tilde{c}^\nu(w^{-1}\eta). \tag{74}$$

The components $\tilde{a}_w^\mu(\eta)$ and $\tilde{c}_w^\mu(\eta)$ indeed fulfill the equations $\Box_6\tilde{a}_w^\mu(\eta)=\tilde{c}_w^\mu(\eta)$ for all μ and therefore $P_{\Box}\kappa^2\tilde{a}_w^\mu(\eta)=c_w^\mu(\eta)$.

We want to add the following remark: The transformation (74) is not the transformation which is induced by the mapping w_* (see Ref. 14). We can now say that the system of differential equations for the vector fields $A^j(x)$ as they are written down in the theorem is a system of conformal covariant equations. The important fact is that the Lorentz gauge $\chi(x)=0$ is not a conformal covariant gauge. One has indeed to take a whole class of functions $\chi(x)$ with $\Box\chi(x)=0$.

The conformal covariant equations $\Box_6\tilde{a}^\mu(\eta)=\tilde{c}^\mu(\eta)$ has been used already by some people some years ago. Mack and Salam take one further supplementary condition for the fields $\tilde{a}^\mu(\eta)$, namely,

$$\partial^\mu\tilde{a}_\mu(\eta)=0. \tag{75}$$

We want to show that this condition follows already from the set of equations $\Box_6\tilde{a}_\mu(\eta)=\tilde{c}_\mu(\eta)$. To see this, let us consider the following expression:

$$\begin{aligned}(\kappa\partial_j+2\eta_j\partial_\lambda)(\kappa^{-1}a^j-\kappa^{-2}\eta^ja^\kappa)&=\partial_ja^j+2\kappa^{-1}\partial_\lambda 2^{-1}(a^\lambda\kappa+a^\kappa\lambda)-4a^\kappa\kappa^{-1}\\&\quad-\kappa^{-1}(1-\kappa\partial_\kappa-\lambda\partial_\lambda)a^\kappa-2\lambda\kappa^{-1}\partial_\lambda a^\kappa,\end{aligned}$$

where we have used the identity

$$\partial_\lambda\eta_ja^j=\partial_\lambda 2^{-1}(\kappa a^\lambda+\lambda a^\kappa), \tag{76}$$

which follows from the condition

$$\eta^\mu a_\mu=0. \tag{77}$$

The identity (76) is only true if the relation (77) is valid for the whole space $\mathbb{R}_2^6$. If the relation (77) is true only on Q_0^5, which is enough for $a^\mu(\cdot)\partial_\mu$ to be an element of $X(Q_0^5)$, then we cannot use (76), and what follows must be modified.

The right-hand side of the identity preceding (76) can be written as

$$\partial_ja^j+\partial_\lambda a^\lambda+\partial_\kappa a^\kappa-4\kappa^{-1}a^\kappa=\partial_\mu a^\mu-4\kappa^{-1}a^\kappa. \tag{78}$$

In local coordinates, then, we get

$$\partial_jA^j(x)=\partial_\mu a^\mu(\eta)-4a^\kappa(x). \tag{79}$$

But $\partial_jA^j(x)=-2a^\kappa(x)$, and therefore the relation (79) says

$$\partial_\mu a^\mu(\eta)=2\kappa^{-1}a^\kappa(\eta). \tag{80}$$

If we further have $a^\mu(\eta)=\kappa^2\tilde{a}^\mu(\eta)$ for all μ, then

$$\partial_\mu a^\mu(\eta)=\kappa^2\partial_\mu\tilde{a}^\mu(\eta)+2\kappa\tilde{a}^\kappa(\eta)=2\kappa\tilde{a}^\kappa(\eta), \tag{81}$$

and therefore

$$\partial_\mu\tilde{a}^\mu(\eta)=0. \tag{82}$$

We have therefore shown that the relation (82) follows already from the equations $\Box_6\tilde{a}^\mu(\eta)=\tilde{c}^\mu(\eta)$ if the condition (77) holds on the whole space $\mathbb{R}_2^6$. For vector fields $a^\mu(\cdot)\partial_\mu$ with $a^\mu(\eta)=\kappa^2\tilde{a}^\mu(\eta)$ and the condition (77) holding only on Q_0^5 the relation (75) is in contradiction to the set of equations $\Box_6\tilde{a}^\mu(\eta)=\tilde{c}^\mu(\eta)\ \forall\ \mu$.

V. GAUGE TRANSFORMATIONS ON M_c^4

It is quite natural to generalize the concept of gauge transformations to the manifold M_c^4. Let $[X]\in X(M_c^4)$ be a vector field with a representative $a^\mu(\eta)\partial_\mu=\kappa^2\tilde{a}^\mu(\eta)\partial_\mu$ which fulfill Maxwell's equations

$$\Box_6\tilde{a}^\mu(\eta)=\tilde{c}^\mu(\eta). \tag{83}$$

Then we can introduce the transformation

$$\tilde{a}^\mu(\eta)\to\tilde{a}^\mu(\eta)+\partial^\mu\phi(\eta), \tag{84}$$

where $\phi(\eta)$ is any $C^\infty(\mathbb{R}^6)$ function with

$$\Box_6\phi(\eta)=0 \tag{85}$$

and homogeneous of degree 0 in the variables η.

The vector field $a^{\mu\prime}(\eta)\partial_\mu$ with

$$a^{\mu\prime}(\eta)=\kappa^2(\tilde{a}^\mu(\eta)+\partial^\mu\phi(\eta)) \tag{86}$$

has the property $\eta^\mu a_\mu'(\eta)=0$ everywhere on $\mathbb{R}^6$ and is therefore the generator of a vector field $[X']\in X(M_c^4)$. Furthermore, it fulfills Eqs. (83) because of (85) and is therefore a solution of Maxwell's equations on M_c^4. Let us next see how the transformation (84) acts in local coordinates. From (85) and the theorem of the last section it follows that the vector field $\varphi^j(x)\partial_j$, which is the vector field $[\kappa^2\partial^\mu\phi(\eta)\partial_\mu]$ in local coordinates x, fulfills Maxwell's equations

$$\begin{aligned}&\Box\varphi^j(x)=-2\partial^j\varphi^\kappa(x),\\&\partial^j\varphi_j(x)=-2\varphi^\kappa(x),\quad\Box\varphi^\kappa(x)=0.\end{aligned} \tag{87}$$

In terms of the function $\phi(\eta)$ the components $\varphi^j(x)$ read as

$$\begin{aligned}&\varphi^j(x)=\kappa\partial^j\phi(\eta)+2\eta^j\partial_\lambda\phi(\eta)=\frac{\partial}{\partial x_j}\phi(x),\\&\varphi^\kappa(x)=-2\kappa\partial_\lambda\phi(\eta)\big|_{\substack{\eta^j=\kappa x^j\\ \lambda=\kappa x^2}}.\end{aligned} \tag{88}$$

These expressions have to be interpreted in the sense that we first perform the differentiations and then replace the variables η by $\eta^j=\kappa x^j$ and $\lambda=\kappa x^kx_k$. Inserting (88) into (87) gives

$$\begin{aligned}&\Box\partial^j\phi(x)=2\partial^j\varphi^\kappa(x)=2\partial^j(-2\kappa\partial_\lambda\phi(\eta))\big|_{\substack{\eta^j=\kappa x^j\\ \lambda=\kappa x^2}},\\&\partial^j\partial_j\phi(x)=4\kappa\partial_\lambda\phi(\eta)\big|_{\substack{\eta^j=\kappa x^j\\ \lambda=\kappa x^kx_k}},\\&\Box(-2\kappa\partial_\lambda\phi(\eta))\big|_{\substack{\eta^j=\kappa x^j\\ \lambda=\kappa x^kx_k}}=0,\end{aligned} \tag{89}$$

and therefore

$$\Box\Box\phi(x)=0. \tag{90}$$

The transformation (84) $[X]\to[X']$ induces, therefore, in local coordinates the transformation

$$A^j(x)\to A^j(x)+\partial^j\phi(x),$$
$$\chi(x)\to\chi'(x)=\chi(x)+\Box\phi(x), \tag{91}$$

with

$$\Box\chi'(x)=\Box\chi(x)+\Box\Box\phi(x)=0,$$

where the function $\phi(x)$ fulfills

$$\Box\phi(x)=4\kappa\partial_\lambda\phi(\eta)\Big|_{\substack{\eta^j=\kappa x^j\\ \lambda=\kappa x^2}}. \tag{92}$$

Equation (92) means the following: Take the function $\phi(x)$ then this defines a function $\phi(\eta)=\phi(\eta/\kappa)$, $\eta=(\eta^0,\eta^1,\eta^2,\eta^3)$ on $\mathbb{R}^6$. On this function the operator ∂_λ acts, and afterwards we replace the η again by the x coordinates in the known way.

It is trivial to go the other way round: We start with a transformation $A^j(x)\to A^j(x)+\partial^j\phi(x)$, where $\phi(x)$ fulfills Eqs. (89); this determines a $C^\infty(\mathbb{R}^6)$ function $\phi(\eta)$ and a vector field $[\varphi^\mu(\eta)\partial_\mu]$, where

$$\varphi^\kappa(\eta)=-2\kappa^2\partial_\lambda\phi(\eta),\quad \varphi^j(\eta)=\kappa^2\partial^j\phi(\eta),$$
$$\varphi^\delta(\eta)=-2\kappa^2\partial_\lambda\phi(\eta).$$

Therefore, we can write

$$\varphi^\mu(\eta)=\kappa^2\partial^\mu\phi(\eta). \tag{93}$$

Since $P_\Box\varphi^\mu(\eta)=P_\Box\kappa^2\partial^\mu\phi(\eta)=0$ it follows that $\Box_6\phi(\eta)=0$. Therefore, the transformations (91) and (92), on the one hand, and the transformations (84) and (85) are completely equivalent.

As is known, the transformation $A^j(x)\to A^j(x)+\partial^j\phi(x)$ keeps the Maxwell tensor $f^{ij}(x)\,dx_i\wedge dx_j$ fixed. The equivalence of the gauge transformation in M_4 and M_c^4 as disucssed above suggests that the transformation $\tilde a^\mu(\eta)\to\tilde a^\mu(\eta)+\partial^\mu\phi(\eta)$ also keeps a similar antisymmetric tensor field $f^{\mu\nu}d\eta_\mu\wedge d\eta_\nu$ invariant. That this is indeed the case we want to show next.

VI. THE MAXWELL TENSOR IN M_c^4

In this section we use the results of our discussion of tensor fields on M_c^4. As we have shown in Sec. III the antisymmetric tensor fields of rank 2 on M_c^4 can be written as a class of tensor fields on Q_0^5:

$$[F^{\mu\nu}d\eta_\mu\wedge d\eta_\nu],$$

where the equivalence relation defining the different classes was given in (45). For the local coordinate representation we got the expression (39). Let us therefore calculate in the η coordinates

$$\frac{\partial}{\partial x^j}S^{ij}(x)=(\kappa\partial_j+2\eta_j\partial_\lambda)$$
$$\times(\kappa^2F^{ij}(\eta)-\kappa^2F^{i\kappa}(\eta)\kappa^{-1}\eta^j-\kappa^2F^{\kappa j}(\eta)\kappa^{-1}\eta^i).$$

A rather trivial calculation gives

$$\frac{\partial}{\partial x^j}S^{ij}(x)=\kappa^3\partial_\mu F^{i\mu}(\eta)-\kappa^2\eta^i\partial_\mu F^{\kappa\mu}(\eta), \tag{94}$$

where we have used the relations (28) on the whole space $\mathbb{R}^6$. If now $\partial_jS^{ij}(x)=C^i(x)$, then from (94) it follows that

$$\kappa^3\partial_\mu F^{i\mu}(\eta)-\kappa^2\eta^i\partial_\mu F^{\kappa\mu}(\eta)=\kappa^{-1}c^i(\eta)-\kappa^{-2}\eta^ic^\kappa(\eta). \tag{95}$$

For given $S^{ij}(x)$ in Minkowski space we have determined in (40) a representative of the corresponding class $[F^{\mu\nu}d\eta_\mu\wedge d\eta_\nu]$ on M_c^4. Because of the fact that the functions $F^{\kappa\mu}(\eta)$ can be chosen always such that they satisfy the equation

$$\partial_\mu F^{\kappa\mu}(\eta)=\kappa^{-4}c^\kappa(\eta), \tag{96}$$

we have the result

$$\kappa^3\partial_\mu F^{i\mu}(\eta)=\kappa^{-1}c^i(\eta) \tag{97}$$

and therefore

$$\partial_\mu F^{i\mu}(\eta)=\kappa^{-4}c^i(\eta)\quad\text{for } i=0,\cdots,3. \tag{98}$$

If, as we have assumed, the $F^{\mu\nu}$ fulfill on the whole space $\mathbb{R}^6$ the conditions (28), then the relations (96) and (98) give that the equation

$$\partial_\mu F^{\lambda\mu}(\eta)=\kappa^{-4}c^\lambda(\eta)$$

also holds on M_c^4, where we have used the relation $\eta^\mu c_\mu(\eta)=0$.

If, on the other hand, there is given an antisymmetric tensor field $[F^{\mu\nu}d\eta_\mu\wedge d\eta_\nu]$ on M_c^4 of rank 2 which has a representative $F^{\mu\nu}d\eta_\mu\wedge d\eta_\nu$ that fulfills the equations

$$\partial_\mu F^{\nu\mu}(\eta)=\tilde c^\nu(\eta),\quad c^\nu(\eta)=\kappa^4\tilde c^\nu(\eta) \tag{99}$$

and $\eta_\mu F^{\mu\nu}(\eta)=0$ on the whole space $\mathbb{R}^6$, then the antisymmetric tensor field $S^{ij}(x)dx_i\wedge dx_j$, which is the tensor field $[F^{\mu\nu}d\eta_\mu\wedge d\eta_\nu]$ in local coordinates x of Minkowski space, satisfies Maxwell's equations $\partial_jS^{ij}(x)=C^i(x)$ for all $i=0,\cdots,3$, where $C^i(x)=\kappa^{-1}c^i(\eta)-\kappa^{-2}\eta^ic^\kappa(\eta)$.

Equations (99) can be solved by the standard procedure of introducing a vector potential $\tilde a^\mu(\eta)$ such that

$$F^{\mu\nu}(\eta)=\partial^\mu\tilde a^\nu(\eta)-\partial^\mu\tilde a^\nu(\eta) \tag{100}$$

The functions $\tilde a^\mu(\eta)$ must thereby satisfy the conditions

$$\tilde a^\mu(\rho\eta)=\rho^{-1}\tilde a^\mu(\eta),\quad \eta^\mu\tilde a_\mu(\eta)=0,$$
$$\Box_6\tilde a^\mu(\eta)=c^\mu(\eta)\text{on }\mathring{\mathbb{R}}_2^6\quad\forall\mu. \tag{101}$$

Our discussion in Sec. IV shows that these are exactly the conditions a vector field $a^\mu(\cdot)\partial_\mu$ with $a^\mu(\eta)=\kappa^2\tilde a^\mu(\eta)$ must fulfill to be a solution of the set of Maxwell equations on M_c^4. The gauge transformation $\tilde a^\mu(\eta)\to\tilde a^\mu(\eta)+\partial^\mu\phi(\eta)$ therefore keeps the antisymmetric tensor field $F^{\mu\nu}(\eta)d\eta_\mu\wedge d\eta_\nu$ with $F^{\mu\nu}=\partial^\mu\tilde a^\nu-\partial^\nu\tilde a^\mu$ invariant so that we have a complete analogy to the local situation in Minkowski space.

The formulation of Maxwell's equations as the set of equations (83) for the potential or as the set of equations (99) for the components of the tensor field shows manifestly the conformal covariance of these equations:

If $\tilde a^\mu(\eta)\partial_\mu$ and $\tilde c^\mu(\eta)\partial_\mu$ fulfill (83), then $w^\mu_\nu\tilde a^\nu(w^{-1}\eta)$ and $w^\mu_\nu\tilde c^\nu(w^{-1}\eta)$ do also for all $w\in SO(2,4)$, and, if $F^{\mu\nu}(\eta)d\eta_\mu\wedge d\eta_\nu$ and $\tilde c^\mu(\eta)\partial_\mu$ satisfy (99), then $w^\mu_\rho w^\nu_\sigma F^{\rho\sigma}(w^{-1}\eta)$ and $w^\mu_\sigma\tilde c^\sigma(w^{-1}\eta)$ also do the same.

Equations (8) and (33) allow us to write these transformations also in the local coordinates x in Minkowski space, which we shall do in the next section.

VII. TRANSFORMATION PROPERTIES OF FIELDS UNDER CONFORMAL TRANSFORMATIONS

Let $\varphi(x)$ be a classical scalar field on M_4 that means a mapping $\varphi: M_4 \to C$. Under certain conditions which we have investigated in a recent paper[10] this function $\varphi(x)$ can be extended to the whole compactified Minkowski space M_c^4. The resulting function we denote by $\phi([\eta])$. The function $\phi([\eta])$ therefore has the property

$$\phi \cdot \varphi_\kappa^{-1}(x) = \varphi(x), \tag{102}$$

where $\varphi_\kappa: M_c^4 \supset U_\kappa \to \varphi_\kappa(U) = M_4$ is the local chart $\varphi_\kappa([\eta]) = (\eta^0/\kappa, \cdots, \eta^3/\kappa)$.

We can now define what we mean by the dimension d of the scalar field $\phi([\eta])$.

Definition: A field $\phi([\eta])$ has the dimension d if it transforms under the conformal group in the following way: If $\phi([\eta]) = \kappa^d \tilde{\phi}(\eta)$, then $\phi'([\eta]) = \kappa^d \tilde{\phi}'(\eta)$, where $\tilde{\phi}'(\eta) = \tilde{\phi}(w^{-1}\eta)$ for any w an element of the conformal group $SO(2,4)$.

We see from the discussion of the free scalar field in Ref. 10 that the free scalar field has dimension 1, because only then a solution of the Klein–Gordon operator will be mapped under any conformal transformation onto another solution of this equation. For any $d \neq 1$ this is not the case. It is quite straightforward to write the transformation law locally in the coordinates x: For a Poincaré transformation (Λ, a) we get

$$\varphi'(x) = \varphi(\Lambda^{-1}(x-a)), \tag{103}$$

for a dilatation $D(\rho)$

$$\varphi'(x) = \rho^{-d}\varphi(\rho^{-1}x), \tag{104}$$

and finally for a special conformal transformation $C(c)$ the result is

$$\varphi'(x) = (1 + c^2x^2 - 2c\circ x)^{-d}\varphi\left(\frac{x + cx^2}{1 + c^2x^2 + 2c\circ x}\right). \tag{105}$$

For infinitesimal c and $\rho = 1 + \epsilon$ we get just the transformation properties of a scalar field which many authors[17] have already postulated. The transformation property of a scalar field under any global conformal transformation as we have written down it in (103) to (105) has also been postulated by Todorov.[13]

Let us next consider the case of vector fields $[X]$ in M_c^4. Take any representative $a^\mu(\eta)\partial_\mu$ of this field. The dimension d of $[X]$ is then defined as follows: If $a^\mu(\eta) = \kappa^{1+d}\tilde{a}^\mu(\eta)$, then $a^\mu(\eta)$ should transform under any conformal transformation w as

$$\tilde{a}^\mu(\eta) \to a^{\mu\prime}(\eta) = \kappa^{1+d}\tilde{a}^{\mu\prime}(\eta), \tag{106}$$

where $\tilde{a}^{\mu\prime}(\eta) = w^\mu_\nu \tilde{a}^\nu(w^{-1}\eta)$.

From our discussion of the free Maxwell equations in Sec. IV we see again that the dimension d of the free Maxwell field is equal to 1 since then a solution of Maxwell's equations is transformed under (106) into another one.

The transformations (106) in local coordinates x are the following ones: Under a Poincaré transformation (Λ, a),

$$A^{j\prime}(x) = \Lambda^j{}_k A^k(\Lambda^{-1}(x-a)), \tag{107}$$

under a dilatation $D(\rho)$

$$A^{j\prime}(x) = \rho^{-d}A^j(\rho^{-1}x), \tag{108}$$

and under a special conformal transformation $C(c)$,

$$\begin{aligned} A^{j\prime}(x') = {} & (1 - 2c\circ x + c^2x^2)^d A^j(x) + 2x^j(1 - 2c\circ x + c^2x^2)^{d-1} \\ & \times c^k A_k(x) - 2x^j(1 - 2c\circ x + c^2x^2)^{d-1} \\ & \times c^2x^k A_k(x) - 2c^j(1 - 2c\circ x + c^2x^2)^d x^k A_k(x) \\ & - 2c^j x^2(1 - 2c\circ x + x^2c^2)^{d-1}c^k A_k(x) \\ & + 2c^j x^2 c^2(1 - 2c\circ x + c^2x^2)^{d-1}x^k A_k(x), \end{aligned}$$

with $x' = (x - cx^2)/(1 + c^2x^2 - 2cx)$. (109)

For the special case of canonical dimension $d = 1$ this gives

$$\begin{aligned} A^{j\prime}(x') = {} & (1 - 2c\circ x + c^2x^2)A^j(x) + 2x^j c^k A_k(x) \\ & - 2c^j x^k A_k(x) + 2c^j c\circ x x^k A_k(x) - 2c^2 x^j x^k A_k(x) \\ & + 2c^j c\circ x x^k A_k(x) - 2c^j x\circ x c^k A_k(x). \end{aligned} \tag{110}$$

If we further restrict our attention to infinitesimal special conformal transformations, then the result is

$$\begin{aligned} A^{j\prime}(x') = {} & A^j(x) - 2c\circ x A^j(x) + 2x^j c^k A_k(x) \\ & - 2c^j x^k A_k(x). \end{aligned}$$

This is exactly what other authors like such as those of Refs. 12 and 17 have also postulated.

Finally for the transformation properties of the antisymmetric tensor field $S^{ij}(x)dx_i \wedge dx_j$ we get: Under Poincare transformations (Λ, a),

$$S^{ij\prime}(x) = \Lambda^i_k \Lambda^j{}_l S^{kl}(\Lambda^{-1}(x-a)). \tag{111}$$

Under a dilatation $D(\rho)$,

$$S^{ij\prime}(x) = \rho^{-2}S^{ij}(\rho^{-1}x),$$

and under a special conformal transformation $C(c)$,

$$\begin{aligned} S^{ij\prime}(x) = {} & \sigma(x,c)^{-1}S^{ij}(x') + \sigma(x,c)^{-3}S^{ik}(x') \\ & (-2x^j x_k c^2 - 2c^j x_k + 2x^j c_k(1 + 2x\circ c) \\ & - 2c^j c_k x^2) + \sigma(x,c)^{-3}S^{kj}(x') \\ & \times (-2x^i x_k c^2 - 2c^i x_k + 2x^i c_k(1 + 2c\circ x) \\ & - 2c^i c_k x^2) + 4\sigma(x,c)^{-3}(x^2)^{-1}S^{lk}(x') \\ & \times (x_k x_l(x^j c^i - x^i c^j) + x_k c_l(x^j c^i - x^i c^j)x^2), \end{aligned}$$

with $x' = \sigma(x,c)^{-1}(x + cx^2)$ and $\sigma(x,c) = 1 + x^2c^2 + 2c\circ x$.

ACKNOWLEDGMENTS

I am indebted to Dr. H.A. Kastrup, Dr. T.H. Go, and and Dr. Q. Shafi for helpful discussions and critical comments. I thank the Bundesminsterium für Bildung und Wissenschaft for financial support. I also thank the referee for bringing to my attention the work of Flato *et al.* and of Rosen.

*Work supported by the Bundesministerium für Bildung und Wissenschaft.

[1] R. Penrose *et al.*, Phys. Rep. 6, No. 4 (1972).
[2] I. Segal, Astron. Astrophys. 18, 143 (1972); Proc. Nat. Acad. Sci. USA 71, 765 (1974).

[3]M. Gell-Mann *et al.*, Phys. Rev. **95**, 1300 (1954).
[4]H. Bateman, Proc. Lond. Math. Soc. **8**, 223 (1910); E. Cunningham, Proc. Lond. Math. Soc. **8**, 77 (1910).
[5]M. Flato *et al.*, Ann. Phys. (N.Y.) **61**, 78 (1970).
[6]G. Rosen, Ann. Phys. (N.Y.) **77**, 452 (1973).
[7]P. Dirac, Ann. Math. **37**, 657 (1936).
[8]R. Penrose, Proc. Roy. Soc. Lond. A **284**, 159 (1965).
[9]W. Kopczynski *et al.*, Rep. Math. Phys. **2**, 35 (1971).
[10]T. Go *et al.*, Rep. Math. Phys. **5**, 43 (1974).
[11]G. Mack *et al.*, Phys. Rev. D **8**, 1764 (1973).
[12]G. Mack *et al.*, Ann. Phys. (N.Y.) **53**, 174 (1969).
[13]I. Todorov, "Lectures at the XII. Internationale Universitatswochen für Kernphysik, Schladming 1973," in Acta Phys. Austriaca, Suppl. XI (1973).
[14]T. Go *et al.*, "Properties of dilatations and conformal transformations in Minkowski space," TH-Aachen Preprint 1973, to appear in Rep. Math. Phys. (1974).
[15]S. Helgason, *Differential Geometry and Symmetric Spaces* (Academic, New York, 1962).
[16]A. Barut *et al.*, Ann. Phys. (N.Y.) **71**, 519 (1972).
[17]D. Gross *et al.*, Phys. Rev. D **2**, 753 (1970).

Systems of differential inequalities and stochastic differential equations. II

G. S. Ladde*

Department of Mathematics, The State University of New York at Potsdam, Potsdam, New York 13676
(Received 18 June 1974)

By employing vector Lyapunov-like functions and the theory of systems of differential inequalities, a very general comparison theorem for Itô type stochastic differential systems is developed. Furthermore, sufficient conditions are given for conditional stability and conditional boundedness of solutions in the mean.

I. INTRODUCTION

Stochastic differential systems provide a mathematical formulation for sophisticated dynamical systems in physical and life sciences. In many circumstances, it is difficult to solve such stochastic differential systems (especially nonlinear systems) explicitly, in order to study qualitative and quantitative behavior of systems. Many cases, it is enough to know the behavior of the system rather than its explicit realization of solutions.

By assuming just the existence of solutions, qualitative and quantitative properties of the system can be studied by emplying the second method of Lyapunov. This method has been successfully employed to study a variety of problems, in a unified way, of ordinary differential equations, functional differential equations (deterministic and stochastic), and parabolic differential equations.[1-4] This extension is based on the use of a single Lyapunov function. It is natural to ask whether it might be more advantageous, in some situations to use vector Lyapunov function. The answer is positive. In fact, Lakshmikantham and others[2,3] have exhibited the fruitfulness of such a vector Lyapunov function for the deterministic case. So, it is natural to except such an important extension to stochastic differential systems.

In this paper, we wish to exploit the above idea for Itô type stochastic differential systems. In Sec. 2, we define various notions of conditional stability and conditional boundedness of the solutions in the mean. These notions, include as special cases the usual notions of stability and boundedness of solutions in the mean. In Sec. 3, we develop a very general comparison theorem for Itô type stochastic differential systems based on the vector Lyapunov function and the theory of systems of differential inequalities. In Sec. 4, we give sufficient conditions for conditional stability and conditional boundedness of solutions in the mean. These results are direct extensions of the Theorems 5.1, 5.2 of Ladde, Lakshmikantham, and Liu,[1] and are analogous to deterministic results of Lakshmikantham.[2,3] Finally, examples are worked out to illustrate the fruitfulness of our results. Furthermore, an example is given in order to show the advantage of a vector Lyapunov function over a single Lyapunov function.

2. NOTATIONS AND DEFINITIONS

Let R^n denote the n-dimensional Euclidean space with a convenient norm $\|\cdot\|$. We also denote by the same symbol $\|\cdot\|$ the corresponding norm of a matrix. Let R_+ and R denote the nonnegative real and real line respectively. Let $(\Omega, \mathcal{J}, P)$ be a complete probability space. By the symbol $E[x|\mathcal{K}]$, we mean the conditional mean of x, where $\mathcal{K} \subset \mathcal{J}$ is a sub σ-algebra of $\mathcal{J}$. Let $(\cdot)^T$ stand for the transpose of a vector or a matrix and let I denote the identity matrix. Let $M_{(n-k)}$ denote a manifold of $(n-k)$ dimensions containing the origin.

Consider the stochastic differential system of Itô type

$$dx = f(t,x)\,dx + \sigma(t,x)\,dz(t), \quad x(t_0) = x_0, \tag{2.1}$$

where dx is a stochastic increment in the sense of Itô,[5,6] x, $f \in R^n$, $\sigma(t,x)$ is an $n \times m$ matrix and $z(t)$ is a normalized m-vector Wiener process with

$$E[(z(t) - z(s)) \cdot (z(t) - z(s))^T] = I\,|t - s|.$$

Assume that the functions f and σ satisfy the following assumptions:

(a_1) The m column vectors of σ and f belong to $C[R_+ \times R^n, R^n]$;

(a_2) for $(t,x) \in R_+ \times R^n$,
$\|f(t,x)\| + \|\sigma(t,x)\| \leq L(1 + \|x\|)$;

(a_3) for (t,x), $(t,y) \in R_+ \times R^n$,
$\|f(t,x) - f(t,y)\| + \|\sigma(t,x) - \sigma(t,y)\| \leq L\|x - y\|$.

Under these hypotheses, it is known[6] that the solution $x(t) = x(t, t_0, x_0)$ of the Itô system (2.1) is:

(I) a strong Markov process with killing time equal to infinity;

(II) continuous with probability one, separable and for any $0 \leq t_0 \leq b < \infty$,

$$E\left(\max_{t_0 \leq t \leq b} \|x(t)\|^2 / x_0\right) < \infty;$$

(III) independent of $z(s) - z(r)$ for all $s > r \geq t$;

(IV) uniformly stochastically continuous in any compact set;

(V) continuous in probability with respect to the initial data.

We shall now formulate the definitions of conditional stability and boundedness in the mean.

Definition 2.1: The trivial solution $x \equiv 0$ of (2.1) is said to be:

(CSM_1) *conditionally equi-stable in the mean* if, for each $\epsilon > 0$, $t_0 \in R_+$, there exists positive function $\delta = \delta(t_0, \epsilon)$ that is continuous in t_0 for each $\epsilon > 0$ such that $x_0 \in M_{(n-k)}$ and the inequality $\|x_0\| \leq \delta$ implies

$$E[\|x(t, t_0, x_0)\| / x_0] < \epsilon, \quad \text{for } t \geq t_0;$$

(CSM_2) *conditionally uniformly stable in the mean* if the δ in (CSM_1) is independent of t_0;

(CSM_3) *conditionally quasi-equi-asymptotically stable*

in the mean if, given $\epsilon > 0$, $\alpha > 0$, $t_0 \in R_+$, there exists a positive number $T = t(t_0, \epsilon, \alpha)$ such that $x_0 \in M_{(n-k)}$ and the inequality $\|x_0\| \leq \alpha$ implies

$$E[\|x(t, t_0, x_0)\|/x_0] < \epsilon, \quad \text{for } t \geq t_0 + T;$$

(CSM_4) *conditionally quasi-uniformly asymptotically stable in the mean* if the T in (CSM_3) is independent of t_0;

(CSM_5) *conditionally equi-asymptotically stable in the mean* if (CSM_1) and (CSM_3) hold simultaneously;

(CSM_6) *conditionally uniformly stable in the mean* if (CSM_2) and (CSM_4) hold at the same time.

Definition 2.2: The stochastic differential system (2.1) is said to be:

(CBM_1) *conditionally equi-bounded in the mean* if, given $\alpha \geq 0$, $t_0 \in R_+$, there exists a positive function $\beta = \beta(t_0, \alpha)$ that is continuous in t_0 for each α such that $x_0 \in M_{(n-k)}$ and the inequality $\|x_0\| \leq \alpha$ implies

$$E[\|x(t, t_0, x_0)\|/x_0] < \beta, \quad t \geq t_0;$$

(CBM_2) *conditionally uniformly bounded in the mean* if the β in (CBM_1) is independent of t_0;

(CBM_3) *conditionally quasi-equi-ultimately bounded in the mean* if, given $\alpha \geq 0$, $t_0 \in R_+$, there exist positive numbers N and $T = T(t_0, \alpha)$ such that $x_0 \in M_{(n-k)}$ and the inequality $\|x_0\| \leq \alpha$ implies

$$E[\|x(t, t_0, x_0)\|/x_0] < N, \quad t \geq t_0 + T;$$

(CBM_4) *conditionally quasi-uniformly-ultimately bounded in the mean* if (CBM_1) and (CBM_3) hold at the same time;

(CBM_6) *conditionally uniformly-ultimately bounded in the mean* if (CBM_2) and (CBM_4) hold simultaneously.

Remark 2.1: Note that if $k = 0$ so that $M_{(n-k)} = R^n$, our definitions reduce to the usual definitions of stability and boundedness of solutions of (2.1) with respect to the origin and we denote by (SM_1)–(SM_6) and (BM_1)–(BM_6).

Consider now the auxiliary differential system

$$u' = g(t, u), \quad u(t_0) = u_0, \tag{2.2}$$

where $g \in C[R_+ \times R_+^m, R^m]$ and $g(t, u)$ is quasimonotone nondecreasing in u, for fixed $t \in R_+$. Let $u(t, t_0, u_0)$ be any solution of (2.2).

Relative to auxiliary differential system (2.2), we need the corresponding definitions (CS_1^*)–(CS_6^*) and (CB_1^*)–(CB_6^*) in our discussion that may be defined analogously. For example, the definition of conditional equi-stability (CS_1^*) runs as follows:

Definition 2.3: The trivial solution $u \equiv 0$ of (2.2) is said to be *conditionally equi-stable* if, given $\epsilon > 0$, $t_0 \in R_+$, there exists a positive function $\delta = \delta(t_0, \epsilon)$ that is continuous in t_0 for each ϵ such that

$$\sum_{i=1}^{m} u_{i0} \leq \delta \quad \text{and} \quad u_{i0} = 0, \quad \text{for } 1 \leq i \leq k,$$

implies

$$\sum_{i=1}^{m} u_i(t, t_0, u_0) < \epsilon, \quad t \geq t_0.$$

Definition 2.4: A function $b(r)$ is said to belong to the class $V\mathcal{K}$, if $b \in C[R_+, R_+]$, $b(0) = 0$ and $b(r)$ is a convex and strictly increasing in r.

Definition 2.5: A function $a(t, r)$ is said to belong to the $C\mathcal{K}$, if $a \in C[R_+ \times R_+, R_+]$, $a(t, 0) \equiv 0$ and $a(t, r)$ is a concave and increasing in r for each fixed $t \in R^+$.

Definition 2.6: Let G be a function on R^n into R^m. The function G is said to be covex if each component G_i, for $1 \leq i \leq m$ is convex, and G is said to be concave if $-G_i$ is convex. For more about convex functions, see Ref. 7.

3. COMPARISON THEOREMS

In this section, we shall develop some results which furnish a very general comparison theorem. This is achieved by employing the concept of vector Lyapunov function and the theory of system of differential inequalities.

Let the function $V \in C[R_+ \times R^n, R_+^m]$, V_t, V_x, V_{xx} exist and are continuous for $(t, x) \in R_+ \times R^n$, the calculus introduced by Itô[6] shows that

$$dV(t, x) = LV(t, x)\, dt + \frac{\partial V}{\partial x} \cdot \sigma(t, x)\, dz(t), \tag{3.1}$$

where

$$LV(t, x) = \frac{\partial V}{\partial t} + \frac{\partial V}{\partial x} \cdot f(t, x) + \frac{1}{2} \sum_{i,j=1}^{n} \frac{\partial^2 V}{\partial x_i \partial x_j} b_{ij}(t, x), \tag{3.2}$$

and $(b_{ij}(t, x)) = \sigma(t, x) \cdot \sigma(t, x)^T$.

Here and after, we shall assume that Eq. (2.2) and the function V satisfy the following hypotheses:

(H_1) $g \in C[R_+ \times R_+^m, R^m]$, $g(t, u)$ is concave and quasimonotone nondecreasing in u, for each fixed $t \in R_+$.

(H_2) Let $r(t, t_0, u_0)$ be the maximal solution of the auxiliary equation (2.2) existing for $t \geq t_0$, $t_0 \in R_+$.

(H_3) Assume that $g(t, 0) \equiv 0$.

(H_4) $V \in C[R_+ \times R^n, R_+^m]$, $\partial V/\partial t$, $\partial V/\partial x$, $\partial^2 V/\partial x^2$ exist and are continuous for $(t, x) \in R_+ \times R^n$. Furthermore, for $(t, x) \in R_+ \times R^n$,

$$LV(t, x) \leq g(t, V(t, x)), \tag{3.3}$$

where L is the operator as defined in (3.2).

(H_5) Assume that the hypothesis (H_4) holds except that the inequality (3.3) is strengthened to

$$A(t)LV(t, x) + A'(t)V(t, x) \leq g(t, A(t)V(t, x)), \tag{3.4}$$

where $A(t)$ is continuously differentiable positive matrix function such that $A^{-1}(t)$ continuous and positive matrix for $t \in R_+$.

(H_6) $V_i(t, x) \equiv 0$, for $1 \leq i < k < n$, if $x \in M_{(n-k)}$, where $M_{(n-k)}$ is an $(n-k)$-dimensional manifold containing the origin.

(H_7) For $(t, x) \in R_+ \times R^n$,

$$b(\|x\|) < \sum_{i=1}^{m} V_i(t, x) \leq a(t, \|x\|),$$

where $b \in V\mathcal{K}$, $a \in C\mathcal{K}$.

(H_8) For $(t, x) \in R_+ \times R^n$

$$b(\|x\|) \leq \sum_{i=1}^{m} V_i(t, x) \leq a(t, \|x\|),$$

where $a \in C\mathcal{K}$, $b \in V\mathcal{K}$, and $b(r) \to \infty$, as $r \to \infty$.

(H_9) In addition to the hypothesis (H_7), we assume that $a(t, r) = a(r)$.

(H_{10}) Assume that (H_8) holds and further assume that $a(t, r) = a(r)$.

We shall state and prove the following comparison theorem.

Theorem 3.1: Let the hypotheses (H_1), (H_2), and (H_4) be satisfied. Assume that for the solution process $x(t) = x(t, t_0, x_0)$ of (2.1), $E[V(t, x(t))/x_0]$ exists, with probability one, for $t \geq t_0$, $t_0 \in R_+$ and

$$V(t_0, x_0) \leq u_0. \tag{3.5}$$

Then, we have

$$E[V(t, x(t)/x_0] \leq r(t, t_0, u_0), \quad t \geq t_0. \tag{3.6}$$

Proof: Set

$$m(t) = E[V(t, x(t))/x_0], \quad m(t_0) = V(t_0, x_0).$$

The existence of $E[V(t, x(t))/x_0]$ together with the continuity of $V(t, x)$ and $x(t)$ implies that $m(t)$ is continuous[8] for $t \geq t_0$. For small $h > 0$, we have

$$\begin{aligned} &m(t+h) - m(t) \\ &\quad = E[V(t+h, x(t+h))/x_0] - E[V(t, x(t))/x_0] \\ &\quad = E[E[V(t+h, x(t+h))/x = x(t)] - V(t, x(t))/x_0]. \end{aligned} \tag{3.7}$$

Note that the system (2.1) and the process $x(t)$ satisfy the following properties, namely,

$$E[(x(t+h) - x(t))/x = x(t)] = f(t, x(t))h + o(h), \tag{3.8}$$

and

$$\begin{aligned} &E[(x(t+h) - x(t)) \cdot (x(t+h) - x(t))^T/x = x(t)] \\ &\quad = \sigma(t, x(t))\sigma^T(t, x(t))h + o(h), \end{aligned} \tag{3.9}$$

and the fact that

$$o[(x(t+h) - x(t)) \cdot (x(t+h) - x(t))^T] \sim o(h). \tag{3.10}$$

For more details about these properties, see Refs. 5, 6. From the hypothesis (H_4), we have

$$\begin{aligned} &V(t+h, x(t+h)) - V(t, x(t)) \\ &\quad = V_t(t, x(t))h + V_x(t, x(t))[x(t+h) - x(t)] \\ &\quad + \tfrac{1}{2} \sum_{i,j=1}^{m} V_{x_i x_j}(t, x(t))[x_i(t+h) - x_i(t)] \\ &\quad \times [x_j(t+h) - x_j(t)] + o(h). \end{aligned} \tag{3.11}$$

From (3.8), (3.9), (3.10), and (3.11), the relation (3.7) reduces to

$$m(t+h) - m(t) = E[LV(t, x(t))/x_0]h + o(h).$$

This together with the hypotheses (H_1) and (H_4) gives the inequality

$$m(t+h) - m(t) \leq g(t, m(t))h + o(h),$$

which yields the system of differential inequalities

$$D^+ m(t) \leq g(t, m(t)). \tag{3.12}$$

Moreover, $m(t_0) \leq u_0$. Hence, by Corollary 1.7.1 in Ref. 3, we obtain

$$m(t) \leq r(t, t_0, u_0), \quad \text{for } t \geq t_0.$$

The proof is complete.

The following variant of Theorem 3.1 is often more useful in applications.

Theorem 3.2: Let the hypotheses of Theorem 3.1 hold except (H_4) is replaced by (H_5). Then, $V(t_0, x_0) \leq u_0$ implies

$$E[V(t, x(t))/x_0] \leq R(t, t_0, v_0), \tag{3.13}$$

where $R(t, t_0, v_0)$ is the maximal solution of the auxiliary differential system

$$v' = A^{-1}(t)[-A'(t)v + g(t, A(t)v)], \quad v(t_0) = v_0 \tag{3.14}$$

existing for $t \geq t_0$.

Proof: Setting $W(t, x) = A(t)V(t, x)$. Because of (3.4), we have

$$\begin{aligned} LW(t, x) &= A(t)LV(t, x) + A'(t)V(t, x) \\ &\leq g(t, W(t, x)). \end{aligned}$$

This together with the hypotheses of the theorem, one can easily verify that $W(t, x)$ satisfies all the hypotheses of Theorem 3.1 and consequently, we have

$$E[W(t, x(t))/x_0] \leq r(t, t_0, u_0), \quad t \geq t_0, \tag{3.15}$$

whenever

$$W(t_0, x_0) \leq u_0.$$

Here $r(t, t_0, u_0)$ is the maximal solution of (2.2). In view of the properties of $A(t)$, it is easy to see that

$$A(t)R(t, t_0, v_0) = r(t, t_0, u_0) \tag{3.16}$$

with $A(t_0)v_0 = u_0$.

From (3.15), (3.16), properties of conditional mean E, the definition of $W(t, x)$ and the properties of $A(t)$, we have

$$E[V(t, x(t))/x_0] \leq R(t, t_0, v_0).$$

Thus the proof is complete.

Remark 3.1: Note that the comparison Theorems in Ref. 4 are derived by using single Lyapunov function and the theory of functional differential and integral inequalities and sufficient conditions are given for stability in the mean. In this respect, our present comparison theorems differ and give a wide range applicability for stability analysis of hierarchial stochastic models.

Remark 3.2: Theorems 3.1 and 3.2 are direct extensions to systems of the corresponding Theorems 3.4 and 3.5 in Ref. 1 respectively. Furthermore Theorem 3.1 is analogous to deterministic Theorem 4.1.1 in Ref. 3, and Theorem 3.2 has no analogy in deterministic theory.

Remark 3.3: Note that the assumption that $E[V(t, x(t))/x_0]$ exists can be dropped. Under certain conditions, one could show that this assumption holds.

For example, let

$$\sum_{i=1}^{m} V_i(t, x) \leq a(t, \|x\|), \quad \text{where } a \in C[R_+ \times R_+, R_+]$$

and $a(t, r)$ is concave in r for fixed $t \in R_+$. Then we would have

$$0 \leq \sum_{i=1}^{m} E[V_i(t, x(t))/x_0] \leq a(t, E[\|x(t)\|/x_0]),$$

which establishes the existence of $E[V(t, x(t))/x_0]$, in

view of the property (II) of $x(t)$ and the additive property of mean.

4. CONDITIONAL STABILITY AND BOUNDEDNESS IN THE MEAN

Employing the comparison theorems developed in the preceding section, we shall present various results giving sufficient conditions for conditonal stability and conditional boundedness of solutions of (2.1). Some of our results may be viewed as stochastic analogs of the corresponding basic results in deterministic case [2, 3].

Theorem 4.1: Let the hypotheses (H_1), (H_2), (H_3), (H_4), (H_6), and (H_7) be satisfied. Assume that $f(t,0)\equiv 0$ and $\sigma(t,0)\equiv 0$. Then,

(i) (CS_1^*) implies (CSM_1),
(ii) (CS_3^*) implies (CSM_3),
(iii) (CS_5^*) implies (CSM_6).

Proof: Let $x(t)$ be the solution process associated with (2.1). From (H_7) and Remark 3.3, the existence of $E[V(t,x(t))/x_0]$ is assured. Hence by Theorem 3.1, the inequality

$$E[V(t,x(t))/x_0] \le r(t,t_0,u_0) \tag{4.1}$$

is valid for $t \ge t_0$, provided that

$$V(t_0,x_0) \le u_0. \tag{4.2}$$

It is obvious that the relation (4.1) yields the estimate

$$\sum_{i=1}^{m} E[V_i(t,x(t))/x_0] \le \sum_{i=1}^{m} r_i(t,t_0,u_0), \quad t \ge t_0. \tag{4.3}$$

Let us first prove the statement (i). Let $\epsilon > 0$ and $t_0 \in R_+$ be given. Assume that (CS_1^*) holds. Then, given $b(\epsilon)$, $t_0 \in R_+$, there exists a positive function $\delta_1 = \delta_1(t_0,\epsilon)$ that is continuous in t_0 for each ϵ, so that

$$\sum_{i=1}^{m} u_i(t,t_0,u_0) < b(\epsilon), \quad t \ge t_0, \tag{4.4}$$

provided

$$\sum_{i=1}^{m} u_{i0} \le \delta_1, \quad u_{i0} = 0, \quad \text{for } 1 \le i \le k. \tag{4.5}$$

Let us choose $u_0 = (u_{10}, u_{20}, \ldots, u_{i0}, \ldots, u_{m0})$ so that $u_{i0} = 0$, for $1 \le i \le k$, $V(t_0,x_0) \le u_0$, and

$$\sum_{i=1}^{m} u_{i0} = a(t_0, \|x_0\|), \quad \text{for } x_0 \in M_{(n-k)}. \tag{4.6}$$

Note that this choice of u_0 in (4.6) was possible because of (H_6). Since $a \in CK$, we can find a $\delta = \delta(t_0,\epsilon) > 0$ that is continuous in t_0 for each $\epsilon > 0$ such that

$$\|x_0\| \le \delta \quad \text{implies} \quad a(t_0,\|x_0\|) \le \delta_1. \tag{4.7}$$

Now, we claim that (CSM_1) holds. Suppose that this claim is false. Then there would exist a solution process $x(t)$ of (2.1) with $x_0 \in M_{(n-k)}$, $\|x_0\| \le \delta$, and $t_1 > t_0$ such that

$$E[\|x(t_1,t_0,x_0)\|/x_0] = \epsilon. \tag{4.8}$$

From (H_7), we have

$$b(E[\|x(t)\|/x_0]) \le \sum_{i=1}^{m} E[V_i(t,x(t))/x_0], \quad t \ge t_0. \tag{4.9}$$

The relations (4.3), (4.4), (4.8), and (4.9) lead us to the contradiction

$$b(\epsilon) \le \sum_{i=1}^{m} E[V_i(t_1,x(t_1))/x_0] \le \sum_{i=1}^{m} r_i(t_1,t_0,u_0) < b(\epsilon),$$

thus proving the statement (i).

Now, we shall give the proof of the statement (ii). Let $\epsilon > 0$, $\alpha > 0$, $t_0 \in R_+$ given and let $x_0 \in M_{(n-k)}$ and $\|x_0\| \le \alpha$. From (H_7), we can find a number of $\alpha_1 = \alpha_1(t_0,\alpha)$ such that

$$\|x_0\| \le \alpha, \quad a(t_0,\|x_0\|) \le \alpha_1 \tag{4.10}$$

hold simultaneously. As before, we choose u_0 so that (4.6) holds and one can obtain the estimate (4.3). Suppose that (CS_3^*) holds. Then given $b(\epsilon) > 0$, $\alpha_1 > 0$, $t_0 \in R_+$, there exists a number $T = T(t_0,\alpha,\epsilon)$ such that

$$\sum_{i=1}^{m} u_i(t,t_0,u_0) < b(\epsilon), \quad t \ge t_0 + T, \tag{4.11}$$

whenever

$$\sum_{i=1}^{m} u_{i0} \le \alpha_1, \quad u_{i0} = 0, \quad 1 \le i \le k.$$

We claim that (CSM_3) holds. Otherwise, there exists a sequence $\{t_n\}$, $t_n \ge t_0 + T$, $t_n \to \infty$ as $n \to \infty$ such that for some solution process $x(t)$ of (2.1) satisfying $\|x_0\| \le \alpha$ and $x_0 \in M_{(n-k)}$ will satisfy the relation

$$E[\|x(t_n,t_0,x_0)\|/x_0] \ge \epsilon, \quad t_n \ge t_0 + T. \tag{4.12}$$

From (4.3), (4.9), (4.11), and (4.12), we have the contradiction

$$b(\epsilon) \le \sum_{i=1}^{m} E[V_i(t_n,x(t_n))/x_0] \le \sum_{i=1}^{m} r_i(t_n,t_0,u_0) < b(\epsilon),$$

which establishes the statement (ii).

The proof of the statement (iii) follows from the proof of (i) and (ii), thus proving the theorem.

Theorem 4.2: Let the hypotheses (H_1), (H_2), (H_4), (H_6), and (H_8) be satisfied. Then,

(i) (CB_1^*) implies (CBM_1),
(ii) (CB_3^*) implies (CBM_3^*),
(iii) (CB_5^*) implies (CBM_5^*).

Proof: Let $\alpha > 0$, $t_0 \in R_+$ be given. By following the argument in the proof of Theorem 4.1, we conclude that every solution process $x(t)$ of (2.1) satisfies the relation (4.3), whenever $\|x_0\| \le \alpha$ and $x_0 \in M_{(n-k)}$. Assume that (CB_1^*) holds. Then, $\alpha_1 > 0$ that is obtained in (4.10) and $t_0 \in R_+$, there exists a $\beta_1 = \beta_1(t_0,\alpha_1)$ that is continuous in t_0 for each α_1 such that

$$\sum_{u=1}^{m} u_i(t,t_0,u_0) < \beta_1, \quad t \ge t_0, \tag{4.13}$$

whenever

$$\sum_{i=1}^{m} u_{i0} \le \alpha_1.$$

Since $b(r) \to \infty$ as $r \to \infty$, there exists $\beta = \beta(t_0,\alpha)$ such that

$$\beta_1(t_0,\alpha_1) \le b(\beta). \tag{4.14}$$

To prove the statement (i), we assume that there is a solution process $x(t)$ of (2.1) such that $\|x_0\| \le \alpha$, $x_0 \in$

$M_{(n-k)}$, and $t_1 > t_0$ such that

$$E[\|x(t_1)\|/x_0] = \beta. \tag{4.15}$$

The relations (4.3), (4.13), (4.14), (4.15), and the hypothesis (H_8) lead us to the contradiction

$$b(\beta) \leq \sum_{i=1}^{m} E[V_i(t_1, x(t_1))/x_0] \leq \sum_{i=1}^{m} r_i(t_1, t_0, u_0) < b(\beta),$$

which proves the statement.

The proofs of (ii) and (iii) can be given by following the proof of Theorem 4.1 and that given above.

In general, we may not be able to find the auxiliary differential system (2.2) whose trivial solution has (CS_1^*)—(CS_6^*) properties. In such cases, the following result, which is based on the comparison Theorem 3.2, is useful in discussing (CSM_1)—(CSM_6) properties of (2.1). We simply state the result whose proof can be formulated on the basis of the proofs of the Theorems 3.2 and 4.1.

Theorem 4.3: Assume that the hypotheses of the Theorem 4.1 hold except that (H_4) is replaced by (H_5) with $\|A(t)\| \to \infty$ as $t \to \infty$. Then, (CS_1^*) and (CS_5^*) properties of the trivial solution of (3.14) implies (CSM_1) and (CSM_5) respectively.

In the following, we shall indicate some modifications necessary in order to obtain the usual stability in the mean and boundedness in the mean results, using vector Lyapunov function and a system of differential inequalities. We denote (CS_1^{**})—(CS_6^{**}) and (CB_1^{**})—(CB_6^{**}) by dropping the conditional character in (CS_1^*)—(CS_6^*) and (CB_1^*)—(CB_6^*) respectively. For example the definition (CS_1^{**}) would run as follows: For each $\epsilon > 0$ and $t_0 \in R_+$, there exists a positive function $\delta = \delta(t_0, \epsilon)$ that is continuous in t_0 for each ϵ such that the inequality

$$\sum_{i=1}^{m} u_{i0} \leq \delta$$

implies

$$\sum_{i=1}^{m} u_i(t, t_0, u_0) < \epsilon, \quad t \geq t_0.$$

In the following, we shall state a theorem that gives sufficient conditions, in terms vector Lyapunov function and a system of differential inequalities, for stability in the mean of the trivial solution of (2.1).

Theorem 4.4: Assume that hypotheses (H_1), (H_2), (H_3), (H_4), and (H_7) hold. Further, assume that $f(t, 0) \equiv 0$ and $\sigma(t, 0) \equiv 0$. Then

(i) (CS_1^{**}) implies (SM_1),

(ii) (CS_3^{**}) implies (SM_3),

(iii) (CS_5^{**}) implies (SM_5).

Proof: The proof of the theorem can be formulated with the help of the proof of the Theorem 4.1. We omit the details.

Remark 4.1: Note that one could formulate the results corresponding to uniform notions under the hypotheses of the previous theorems except that (H_7) and (H_8) are replaced by (H_9) and (H_{10}) respectively and the corresponding notions relative to auxiliary equation (2.2) are uniform.

Remark 4.2: Note that all these results are natural extensions of deterministic results due to Lakshmikantham[2,3] for Itô type stochastic differential system. Further, note that these results include the usual results on stability and boundedness in the mean[1] as special cases.

Remark 4.3: Observe that the concavity of $a(t, r)$ is used only to show that $E[V(t, x(t))/x_0]$ exists. However, if one knows the existence of $E[V(t, x(t))/x_0]$, then the concavity of $a(t, r)$ can be dropped.

5. EXAMPLES

In this section, we shall present some examples in order to illustrate the fruitfulness of our results. Furthermore, we also give an example to show the advantage of a vector Lyapunov function and system of differential inequalities over a single Lyapunov function and a scalar differential inequality.

Example 5.1: Consider the system of stochastic differential equation

$$dx = A(t)x\,dt + \sigma(t, x)\,dz(t), \tag{5.1}$$

where

$$A(t) = \begin{bmatrix} 1+\cos t & 1-\cos t & \cos t - 1 \\ -e^{-t}+1 & 1+e^{-t} & e^{-t}-1 \\ \cos t - e^{-t} & e^{-t} - \cos t\, e^{-t} + \cos t \end{bmatrix},$$

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad \sigma(t, x) = \begin{bmatrix} \sigma_1(t, x) \\ \sigma_2(t, x) \\ \sigma_3(t, x) \end{bmatrix},$$

$z(t)$ is a normalized scalar Wiener process and $\sigma(t, x)$ satisfies the hypotheses (a_1)—(a_3). Further, assume that $\sigma(t, 0) = 0$ and

$$[\sigma_1(t, x) + \sigma_2(t, x) - \sigma_3(t, x)]^2 \leq \lambda(t)(x_1 + x_2 - x_3)^2,$$

$$[\sigma_2(t, x) - \sigma_2(t, x) + \sigma_3(t, x)]^2 \leq \lambda(t)(x_1 - x_2 + x_3)^2,$$

and

$$[-\sigma_1(t, x) + \sigma_2(t, x) + \sigma_3(t, x)]^2 \leq \lambda(t)(-x_1 + x_2 + x_3)^2, \tag{5.2}$$

where $\lambda \in C[R_+, R_+] \cap L_1[0, \infty]$.

Take $m = 3$ and

$$V(t, x) = \begin{bmatrix} (x_1 + x_2 - x_3)^2 \\ (x_1 - x_2 + x_3)^2 \\ (-x_1 + x_2 + x_3)^2 \end{bmatrix}.$$

Since

$$\sum_{i=1}^{3} V_i(t, x) = [x_1^2 + x_2^2 + x_3^2 + (x_2 - x_3)^2 + (x_3 - x_1)^2 + (x_1 - x_2)^2],$$

hence

$$(x_1^2 + x_2^2 + x_3^2) \leq \sum_{i=1}^{3} V_i(t, x) \leq 5(x_1^2 + x_2^2 + x_3^2),$$

Further, we deduce the vectorial inequality

$$LV(t,x) \leq g(t, V(t,x))$$

with

$$g(t,u) = \begin{bmatrix} [4+\lambda(t)]u_1 \\ [4\cos t + \lambda(t)]u_2 \\ [4e^{-t} + \lambda(t)]u_3 \end{bmatrix},$$

whenever (5.2) holds.

Now, one can easily see that $g(t,u)$ is concave and quasimonotone nondecreasing in u for fixed $t \in R_+$. Choose $k=1$. Then the solution of (2.2) satisfying $u_{10}=0$ is

$$r(t,t_0,u_0) = \begin{bmatrix} 0 \\ u_{20}\exp\{\int_{t_0}^{t}[4\cos u + \lambda(u)]\,du\} \\ u_{30}\exp\{\int_{t_0}^{t}[e^{-u} + \lambda(u)]\,du\} \end{bmatrix}.$$

One can easily observe that the trivial solution of (2.2) is conditionally uniformly stable. In this case, $M_{(n-k)} = M_{(2)} = \{(x_1,x_2,x_3) \in R^3 : x_1 + x_2 = x_3\}$. Thus all the hypotheses of Theorem 4.1 and Remark 4.1 are satisfied. Hence, we conclude that the trivial solution of the system (5.1) is conditionally uniformly stable in the mean.

Example 5.2: Consider the system of differential equations

$$dx = F(t)x\,dt + \sigma(x)\,dz(t), \tag{5.3}$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad F(t) = \begin{bmatrix} -f_1(t) & 0 \\ 0 & -f_2(t) \end{bmatrix},$$

$$f_i \in C[R_+, R_+], \quad i=1,2, \quad \sigma(x) = \begin{bmatrix} \sigma_1(x) \\ \sigma_2(x) \end{bmatrix}$$

and σ satisfies the Lipschitz condition with Lipschitz constant C and $\sigma(0)=0$. Furthermore, assume that

$$\liminf_{t\to\infty}\left(\frac{1}{t-t_0}\int_0^t f(s)\,ds\right) > C^2, \tag{5.4}$$

where $f = \min\{f_1, f_2\}$.

Take $m=2$ and

$$V(t,x) = \begin{bmatrix} x_1^2 \\ x_2^2 \end{bmatrix}, \quad A(t) = \exp[2\textstyle\int_{t_0}^{t} f(s)\,ds]I,$$

where I is 2×2 identity matrix. In view of the assumptions on (5.3), we obtain that

$$A(t)LV(t,x) + A'(t)V(t,x) \leq BA(t)V(t,x), \tag{5.5}$$

where

$$B = \begin{bmatrix} C^2 & C^2 \\ C^2 & C^2 \end{bmatrix}.$$

The auxiliary system is $u' = -2f(t)u + Bu$. Because of (5.4), $u \equiv 0$ is asymptotically stable. Hence by Theorem 4.3 and Theorem 4.4, it follows that the trivial solution of (5.3) is asymptotically stable in the mean.

Now, we shall present an example that shows the advantage of vector Lyapunov function over a single Lyapunov function.

Example 5.3: Consider the stochastic differential system

$$dx = F(t,x)x\,dt + \sigma(t,x)\,dz(t), \tag{5.6}$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad F(t,x) = \begin{bmatrix} e^{-t} - f_1(t,x) & \sin t \\ \sin t & e^{-t} - f_1(t,x) \end{bmatrix},$$

$f_1 \in C[R_+ \times R^2, R_+]$, $f_1(t,0) = 0$,

$z(t)$ is a normalized scalar process, and $\sigma \in C[R^+ \times R^2, R^2]$, it also satisfies the hypotheses (a_1)—(a_3), $\sigma(t,0)=0$ and

$$[\sigma_1(t,x) + \sigma_2(t,x)]^2 \leq (x_1+x_2)^2\lambda(t),$$
$$[\sigma_1(t,x) - \sigma_2(t,x)]^2 \leq (x_1-x_2)^2\lambda(t), \tag{5.7}$$

and $\lambda \in C[R_+, R_+] \cap L_1[0,\infty)$.

First, we choose a single Lyapunov function $V(t,x)$ given by $V(t,x) = x_1^2 + x_2^2$. Then, it is evident that

$$LV(t,x) \leq [2e^{-t} + 2|\sin t| + \lambda(t)]V(t,x),$$

using the inequalities (5.7),

$$2|ab| \leq a^2 + b^2 \quad \text{and} \quad f_1(t,x) \geq 0, \quad \text{for} \quad (t,x) \in R_+ \times R^2.$$

Clearly, the trivial solution of the comparison equation

$$u' = [2e^{-t} + 2|\sin t| + \lambda(t)]u$$

is not stable. Hence, we can not deduce any information about the stability in the mean of (5.6) from the Theorem 5.1 in Ref. 1, even though it is stable.

Now, we attempt to seek the stability information of (5.6) by employing vector Lyapunov function. We choose

$$V(t,x) = \begin{bmatrix} (x_1+x_2)^2 \\ (x_1-x_2)^2 \end{bmatrix}.$$

Note that the components of V, V_1, and V_2 are not positive definite and hence do not satisfy the hypotheses of Theorem 5.1 in Ref. 1. However, they do satisfy all the hypotheses of Theorem 4.4. In fact,

$$(x_1^2 + x_2^2) \leq \sum_{i=1}^{2} V_i(t,x) \leq 2(x_1^2 + x_2^2)$$

and the vectorial inequality

$$LV(t,x) \leq g(t, V(t,x))$$

are satisfied, with

$$g(t,u) = \begin{bmatrix} [2e^{-t} + 2\sin t + \lambda(t)]u_1 \\ [2e^{-t} - 2\sin t + \lambda(t)]u_2 \end{bmatrix}.$$

It is easy to observe that $g(t,u)$ is concave and quasi-monotone nondecreasing in u, for fixed t, and the trivial solution of (2.2) is uniformly stable. Consequently, the trivial solution of (5.6) is stable in the mean.

*The author acknowledges the support of faculty fellowship from the Research Foundation of State University of New York.

[1]G.S. Ladde, V. Lakshmikantham, and P.T. Liu, *Differential Inequalties and Itô Type Stochastic Differential Equations*, Proc. of the Intern. Conf. on Nonlinear and Functional Equations, Bruxelles and Louvian, Belgium (Hermann, Paris, 1973), pp. 611—40.
[2]V. Lakshmikantham, J. Math. Anal. Appl. **10**, 368 (1965).
[3]V. Lakshmikantham and S. Leela, *Differential and Integral Inequalities, Theory and Applications* (Academic, New York, 1969), Vols. I and II.
[4]G.S. Ladde, J. Math. Phys. **15**, 738 (1974).
[5]J.L. Doob, *Stochastic Processes* (Wiley, New York, 1953).
[6]I.I. Gikhman and A.V. Skorohod, *Introduction to the Theory of Random Processes* (Saunders, Philadelphia, 1969).
[7]A.W. Roberts and D.E. Varberg, *Convex Functions* (Academic, New York, 1973).
[8]H.L. Royden, *Real Analysis* (Macmillan, New York, 1968), 2nd ed.

Generalized free fields and the representations of Weyl group. II. Reducible representations

J. Lukierski and W. Sienkiewicz

Institute of Theoretical Physics, University of Wrocław, Wrocław, Poland
(Received 22 April 1974)

The multiplets of generalized free fields, transforming according to triangle indecomposable representation of dilatation group are studied. Further, using the technique of Mellin transform, we represent an arbitrary generalized free field as a continuous superposition of fields with definite dimensionality.

1. INTRODUCTION

There are well-known[1] transformation properties of massless fields under the action of Weyl group, defined as

$$W = T \otimes DL_4, \quad DL_4 = L_4 \times S \tag{1.1}$$

where T denotes the group of translations, L_4 the homogeneous Lorentz group, and S the one-parameter dilatation group

$$S: x_\mu \to x'_\mu = l x_\mu. \tag{1.2}$$

We define the dimensionality parameter δ of the field operator $\Phi_\delta(x)$ by means of the relation

$$U(l)\Phi_\delta(x)U^{-1}(l) = l^\delta \Phi(l^{-1}x) \tag{1.3}$$

where $U(l)$ is the unitary representation of S in the Hilbert space $\mathcal{H}$

$$U^+(l) = U^{-1}(l) = U(l^{-1}). \tag{1.3'}$$

Further, we assume the absence of spontaneous breaking of dilatational invariance, i.e.,

$$U(l)|0\rangle = |0\rangle. \tag{1.3''}$$

For massless fields we obtain

$\delta = 1$ for bosons (helicity even),

$\delta = \frac{3}{2}$ for fermions (helicity odd).

In our previous paper[2] which we shall refer to as I, it has been shown that the relation (1.3) with *any value* of $\delta > 1$ can be obtained if[3]

$$\Phi_\delta(x) = \int_0^\infty (\mathcal{H}^2)^{\delta/2}\Phi(x;\mathcal{H}^2)\frac{d\mathcal{H}^2}{\mathcal{H}^2} \tag{1.4}$$

where $\Phi(x;\mathcal{H}^2)$ is defined as

$$(\Box - \mathcal{H}^2)\Phi(x;\mathcal{H}^2) = 0, \tag{1.5a}$$

$$[\Phi(x;\mathcal{H}^2), \Phi(x';\mathcal{H}'^2)] = i\Delta(x-x';\mathcal{H}^2)\delta(\mathcal{H}^2 - \mathcal{H}'^2) \tag{1.5b}$$

and has the dimensionality d equal to zero,

$$U(l)\varphi(x;\mathcal{H}^2)U^{-1}(l) = \varphi\left(lx, \frac{\mathcal{H}^2}{l^2}\right), \tag{1.5c}$$

consistent with the canonical E. T. limit

$$[\dot{\varphi}(\mathbf{x}, t;\mathcal{H}^2), \varphi(x', t;\mathcal{H}'^2)] = i\delta^3(\mathbf{x}-\mathbf{x}')\delta(\mathcal{H}^2 - \mathcal{H}'^2). \tag{1.5d}$$

By using (1.5c) the proof of (1.3) for the field operator (1.4) is reduced to the change of variables $\mathcal{H}^2 \to \mathcal{H}'^2 = \mathcal{H}^2/l^2$. The field operator (1.4) is a generalized free field with the following commutator function[4]:

$$[\Phi_\delta(x), \Phi_\delta(x')] = i\Delta(x;\{\delta\}) = i\int d\mathcal{H}^2(\mathcal{H}^2)^{d-2}\Delta(x;\mathcal{H}^2)$$

$$= \frac{1}{(2\pi)^3}\int_{V^+} d^4p\epsilon(p_0)(p^2)^{d-2}\exp(ipx) = \frac{2^{2d-3}}{\pi}\frac{\Gamma(d-1)}{\Gamma(1-d)}\epsilon(x_0)(x^2)_+^{-d}. \tag{1.6}$$

The restriction $\delta > 1$ follows from the requirement that the Kallen–Lehman spectral function should be positive definite.[5]

The field operator $\Phi_\delta(x)$ generates from the dilatation-invariant vacuum state (1.3'), the linear irreducible representation space $R_2^{(0,\delta)}$ of the Weyl group, related with orbit O_2 (see I). Introducing $\Phi_\delta[f]$,

$$\Phi_\delta[f] = \int d^4x f(x)\Phi_d(x) \tag{1.7a}$$

where $\mathrm{supp}\tilde{f}(p) \in V^+$, $\tilde{f}(p) \in S$ and using (1.4)–(1.5) one can write the vectors belonging to $R_2^{(0,\delta)}$ as follows:

$$|f\rangle_\delta = \Phi_\delta[f]|0\rangle. \tag{1.7b}$$

In $R_2^{(0,\delta)}$ one can introduce various scalar products. The conventional choice

$${}_\delta\langle f|f'\rangle_\delta = \int \frac{d^4p}{(p^2)^2}(p^2)^\delta f^*(p)f'(p) \tag{1.8}$$

is only invariant under (1.3) if $\delta = 0$. In order to define the representation space $\mathcal{H}_2^{(0,\delta)}$ with invariant scalar product ${}_\delta\langle\langle f|f'\rangle\rangle_\delta$, we should put into the definition of ${}_\delta\langle\langle f|f'\rangle\rangle_\delta$ the weight function $(p^2)^{-\delta}$, or define

$${}_\delta\langle\langle f|f'\rangle\rangle_\delta \equiv {}_{-\delta}\langle f|f\rangle_\delta. \tag{1.8'}$$

The change $\delta \to -\delta$ defines the so-called shadow operator.[6] One can say, therefore, that the dual space to (1.7) is generated from the vacuum by shadow operator.

The representation spaces $\mathcal{H}_2^{(s,\delta)}$ where s denotes the spin value of irreducible representation can be introduced in analogous way. The assignment of spin for the orbit O_2 is the same for the Wigner representations of Poincaré group with positive mass square, and for simplicity we shall consider here only the spinless case ($s = 0$).[7]

Following I we can write that the generator $\hat{D}$ of dilatations as the sum of two operators

$$\hat{D} = \hat{D}_{\mathrm{geom}}(t) + \hat{D}_{\mathrm{mass}}(t) \tag{1.9}$$

where

$$\hat{D}_{\mathrm{geom}}(t) = \int d^3x T_{0\nu}(x)x^\nu \tag{1.9'}$$

and[8]

$$\hat{D}_{\mathrm{mass}}(t) = -2\int d^3x \int_0^\infty d\mathcal{H}^2\mathcal{H}^2 : \partial_0\Phi(x;\mathcal{H}^2)\frac{\partial}{\partial\mathcal{H}^2}\Phi(x;\mathcal{H}^2): \tag{1.9''}$$

Any generalized free field

$$\Phi_{[\xi]}(x) = \int_0^\infty \xi(\mathcal{H}^2)\Phi_0(x;\mathcal{H}^2)\,d\mathcal{H}^2 \tag{1.10}$$

commutes with (1.9) as follows:

$$\frac{1}{i}[\hat{D}, \Phi_{[\xi]}(x)] = (x_\mu \partial^\mu + \hat{d})\Phi_{[\xi]}(x) \tag{1.11}$$

where $\hat{d}$ denotes *dimensionality operator*

$$\hat{d}\Phi_{[\xi]}(0) = \frac{1}{i}[\hat{D}_{\text{mass}}, \Phi_{[\xi]}(0)]. \tag{1.12}$$

In particular, $\Phi_\delta(x)$ satisfies the equation

$$(\hat{d} - \delta)\Phi_\delta(0) = 0. \tag{1.13}$$

In this paper we shall introduce in Sec. 2 the multiplets of generalized free fields $\Phi_\delta^{(N;i)}(x)$ $(i = 1, 2, \ldots, N)$, transforming under the generator (1.8) of the dilatation transformations as partly reducible indecomposable unitary representation. [9]

Further, in Sec. 3 we shall discuss fully reducible representations of Weyl group. We shall introduce the Mellin transform of the generalized free field with respect to the invariant mass square parameter. Such spectral decomposition of the generalized free field leads to the replacement of Kallen—Lehman representation, describing mass spectrum by the spectral representation introducing the measure characterizing the dimensionality spectrum.

2. MULTIDIMENSIONAL PARTLY REDUCIBLE REPRESENTATIONS OF DILATATION GROUP AND GENERALIZED FREE FIELDS

Recently[9–11] the following generalization of the formula (1.3) was considered:

$$U(l)\Phi_{\delta;n}U^{-1}(l) = T^{(N;\delta)}_{nn'}(l)\Phi_{\delta;n'}(l^{-1}x)$$
$$= l^\delta \sum_{k=0}^{n-1} \frac{(\ln l)^k}{k!}\,\Phi^{(N)}_{\delta;n-k}(l^{-1}x). \tag{2.1}$$

The representation matrix[12]

$$T^{(N;\delta)}(l) = l^\delta \begin{pmatrix} 1 & & & \\ \ln l & & 0 & \\ \cdot & \cdot & & \\ \cdot & & \cdot & \\ \cdot & & & \cdot \\ \dfrac{\ln l^{N-1} l}{(N-1)!} & \cdots & \ln l & 1 \end{pmatrix} \tag{2.2}$$

defines N-dimensional reducible indecomposable realization of the dilatation group. If $N=1$ we obtain to the case of irreducible representation, discussed in I. If $N>1$, the representation is reducible, but not completely reducible. [13] It appears that the multiplets (2.2) have some importance if one tries to reconcile the scale invariance with perturbation expansion or with the so-called "naive" canonical manipulations. [10]

In order to construct the field operator occuring in the multiplet (2.1) with $n=2$ we should perform the following limit:

$$\Phi_{\delta;2} = \lim_{\Delta\delta\to 0} \frac{1}{\Delta\delta}[\Phi_{\delta+\Delta\delta;1}(x) - \Phi_{\delta;1}(x)]$$
$$= \frac{d}{d\lambda}\Phi_{\lambda,1}(x)\Big|_{\lambda=\delta}. \tag{2.3}$$

The triangular representation (2.2) one obtains simply by differentiating the Eq. (1.13). One gets the set of two equations

$$(\hat{d} - \delta)\frac{d}{d\delta}\Phi_{\delta,1}(x) = \Phi_{\delta,1}(x), \tag{2.4a}$$

$$(\hat{d} - \delta)\Phi_{\delta,1}(x) = 0 \tag{2.4b}$$

describing in infinitesimal form the transformation (2.1) for $N=2$.

It is easy to show the following *statement*:

The components of the multiplet defined by the formula

$$\Phi_{\delta;k}(x) = \frac{1}{(k-1)!}\left(\frac{\partial}{\partial\lambda}\right)^{k-1}\Phi_\lambda(x)\Big|_{\lambda=\delta} \tag{2.5}$$

transform under the dilatations in accordance with (2.1)

Proof: Let us differentiate the formula (1.3). We have

$$U(l)\left[\left(\frac{\partial}{\partial\lambda}\right)^{n-1}\Phi_\lambda(x)\right]U^{-1}(l)$$
$$= \sum_{k=0}^{n-1}\binom{n-1}{k}\left[\left(\frac{\partial}{\partial\lambda}\right)^k l^\lambda\right]\left(\frac{\partial}{\partial\lambda}\right)^{n-k-1}\Phi_\lambda(x). \tag{2.6}$$

Because $\binom{n-1}{k} = (n-1)!/k!\,(n-k-1)!$, putting $\lambda=\delta$ in (2.6), and substituting (2.5), one gets the formula (2.1). QED

The explicit formula for the field operator (2.5) looks as follows:

$$\Phi_{\delta;k}(x) = \frac{1}{(k-1)!}\int_0^\infty d\mathcal{H}^2\,\frac{(\ln\mathcal{H}^2)^{k-1}}{2^{k-1}}\,(\mathcal{H}^2)^{\delta/2-1}\Phi(x;\mathcal{H}^2). \tag{2.7}$$

The formula (2.7) introduces a definite set of field operators, satisfying the transformation law (2.1). The infinitesimal form of (2.1) has, however, the form

$$\begin{aligned}
&(\hat{d} - \delta)\Phi_{\delta;N}(x) = \Phi_{\delta;N-1}(x),\\
&(\hat{d} - \delta)\Phi_{\delta;N-1}(x) = \Phi_{\delta;N-2}(x),\\
&(\hat{d} - \delta)\Phi_{\delta;2}(x) = \Phi_{\delta;1}(x),\\
&(\hat{d} - \delta)\Phi_{\delta;1}(x) = 0.
\end{aligned} \tag{2.8}$$

The general solution of the set (2.8) has the form

$$\begin{aligned}
&\Phi_{\delta;1}(x) = \Phi_\delta(x),\\
&\Phi_{\delta;2}(x) = \frac{\partial}{\partial\delta}\Phi_\delta(x) + c_1\Phi_\delta(x),\\
&\quad\cdot\\
&\quad\cdot\\
&\quad\cdot\\
&\Phi_{\delta;N}(x) = \frac{\partial}{\partial\delta}\Phi_{\delta;N-1}(x) + c_{N-1}\Phi_\delta(x),
\end{aligned} \tag{2.9}$$

or

$$\Phi_{\delta;k}(x) = (2.7) + \sum_{i=0}^{k-2} c_i\left(\frac{\partial}{\partial\delta}\right)^i\Phi_\delta(x). \tag{2.10}$$

The arbitrary coefficients c_i can be obtained if we

look for the solutions of the following set of N^2 equations $(n, n' \leq N)$:

$$W_{\delta;n,n'}(x) = (l^2)^{\delta} \sum_{k=0}^{n-1} \sum_{l=0}^{n'-1} \frac{(\ln l)^{k+l}}{k!\,l!} W_{\delta;n-k,n'-l}(l^{-1}x), \tag{2.11}$$

generalizing the conventional condition of scale invariance for the Wightman function $(N-1)$

$$W_{\delta}(x) = (l^2)^{\delta} W_{\delta}(l^{-1}x) \tag{2.12}$$

to the case of Dell'Antonio multiplet.[14]

Remark 1: The introduction of Dell'Antonio multiplets does not lead to the appearance of indefinite metric. Indeed, the field operator (2.7), as well as (2.10), has positive definite spectral function. This nice property is not valid if we introduce multidimensional indecomposable representations for the Poincaré group by means of the formulas [compare with (2.8)]

$$\begin{aligned} &(\hat{p}^2 - M^2)\psi_N(x) = \psi_{N-1}(x) \\ &\cdot \\ &\cdot \\ &\cdot \\ &(\hat{p}^2 - M^2)\psi_1(x) = 0, \end{aligned} \tag{2.13}$$

where $\hat{p}^2 \equiv \Box$ and M^2 real. It can be shown that the field operators $\psi_1(x) \cdots \psi_N(x)$ generate the space of states necessarily with indefinite matric.[14–18] A similar conclusion can be reached if we assume that the multiplet (2.1) describes a conformally-invariant theory.[19]

Remark 2: The multidimensional representations, described in this section, can be constructed for the orbits O_2, O_3, and O_4 of the Weyl group, but they do not exist for orbits O_5 and O_6, localized on the light cone. In particular (see Ref. 4), it does not exist for $N > 1$ the limit $\delta \to 1$.

Remark 3: There exists a four-dimensional integral kernel $k_n(x)$ which allows us to express the field operators $\Phi_{\delta;n}$ $(n > 1)$ as the convolution of k_n and Φ_{δ}. We have

$$\tilde{k}_n(p) = \frac{1}{2^{n-1}} \frac{1}{(n-1)!} (\ln p_+^2)^{n-1}. \tag{2.14}$$

3. MELLIN TRANSFORM OF THE GENERALIZED FREE FIELDS AND REDUCIBLE REPRESENTATIONS

Let us write positive-frequency part of an arbitrary generalized free field Φ

$$\Phi^{(+)}(x) = \int_0^{\infty} \xi(\mathcal{H}^2)\Phi^{(+)}(x;\mathcal{H}^2)\frac{d\mathcal{H}^2}{\mathcal{H}^2} \tag{3.1}$$

with the spectral function $\xi(\mathcal{H}^2)$ satisfying the condition for some $k > 0$

$$\int_0^{\infty} (\mathcal{H}^2)^k \,|\, \xi(\mathcal{H}^2) \,|\, d\mathcal{H}^2 < \infty. \tag{3.2}$$

Then one can write, if $c < k$,

$$\xi(\mathcal{H}^2) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} G(\Delta)(\mathcal{H}^2)^{-\Delta} d\Delta \tag{3.3}$$

where

$$G(\Delta) = \int_0^{\infty} (\mathcal{H}^2)^{\Delta} \xi(\mathcal{H}^2) \frac{d\mathcal{H}^2}{\mathcal{H}^2} \tag{3.4}$$

or

$$\Phi^{(+)}(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} G(\Delta)\Phi_{-2\Delta}^{(+)}(x)\, d\Delta. \tag{3.5}$$

We see that any generalized free field with spectral function satisfying the condition (3.2) can be written as a superposition of the fields $\Phi_{-2c+i\alpha}^{(+)}(x)$ $(-\infty < \alpha < \infty)$, generating from the vacuum irreducible representation spaces $R_2^{(O_1 - 2c + i\alpha)}$ of the Weyl group. It is easy to see that all these representations are unitary with respect to the scalar product (1.8′) with δ replaced by $-2c$, i.e., $\mathcal{H}_2^{(O_1 - 2c)}$.

The fact that irreducible fields with respect to the Poincaré group and with respect to Weyl group are related by Mellin transform follows from the commutation relations of the generator of dilatations $\hat{D}$ and the mass operator $\hat{M}^2$:

$$[\hat{D}, \hat{M}^2] = 2i\hat{M}^2. \tag{3.6}$$

The relation (3.6) leads to

$$[\hat{D}, \tfrac{1}{2}\ln\hat{M}^2] = i \tag{3.7}$$

and the eigenvectors

$$\hat{D}\,|\,\Delta\rangle = \Delta\,|\,\Delta\rangle \tag{3.8a}$$

$$\tfrac{1}{2}\ln\hat{M}^2\,|\,\mathcal{H}^2\rangle = \tfrac{1}{2}\ln\mathcal{H}^2\,|\,\mathcal{H}^2\rangle \tag{3.8b}$$

are related by Fourier transform

$$|\,\Delta\rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d(\tfrac{1}{2}\ln\mathcal{H}^2) \exp(\tfrac{1}{2}i \ln\mathcal{H}^2 \cdot \Delta)\,|\,\mathcal{H}^2\rangle \tag{3.9}$$

which, as it is easily seen, is equivalent to Mellin transform.

The formula (3.5) describes as a special case the Dell'Antonio multiplet (2.5), which can be obtained if we choose $c = \delta$ and

$$G_k(\delta + i\alpha) = \frac{(-i)^{k-1}}{(k-1)!} \delta^{(k-1)}(\alpha). \tag{3.10}$$

In the general case, however, $G(\Delta)$ is not localized in one point. In order to study the general case let us observe that the commutator of the field

$$\Phi(x) = \Phi^{(+)}(x) + \text{H. C.}, \tag{3.11}$$

where $\Phi^{(+)}(x)$ is given by (3.1), can be written as

$$[\Phi(x), \Phi(0)] = \frac{1}{4\pi^2 i} \int_{-\infty}^{+\infty} d\alpha \int_{-\infty}^{+\infty} d\alpha' G^*(c - i\alpha) \times G(c + i\alpha') \int_0^{\infty} (\mathcal{H}^2)^{i(\alpha - \alpha') - 2c} \Delta(x;\mathcal{H}^2) \frac{d\mathcal{H}^2}{\mathcal{H}^2}. \tag{3.12}$$

Introducing

$$g(c + i\beta, c - i\beta) = \int_{-\infty}^{+\infty} G^*(c - i(\beta' + \beta))G(c + i(\beta' - \beta)), \tag{3.13}$$

we obtain

$$[\Phi(x), \Phi(0)] = \frac{1}{\pi^2 i} \int_{-\infty}^{+\infty} d\beta\, g(c + i\beta, c - i\beta) \times \int_0^{\infty} (\mathcal{H}^2)^{i\beta - 2c} \Delta(x;\mathcal{H}^2) \frac{d\mathcal{H}^2}{\mathcal{H}^2}$$

$$= \frac{1}{\pi^2 i} \int_{-\infty}^{+\infty} d\beta g(c + i\beta, c - i\beta)$$
$$\times \frac{-i2^{i\beta-2c}\Gamma(1 + (i\beta - 2c)/2)\Gamma(2 + (i\beta - 2c)/2)}{\pi^2(-x^2 + ix_0 O)^{2+(i\beta-2c)/2}} . \quad (3.14)$$

The formula (3.14) describes the Mellin transform of the commutator function, with the spectral function which is a bilinear form (3.13) in the Mellin transform $G(\Delta)$ of the field operator [see (3.5)].

The aim of this section was to show that the basic notion in the dimensional analysis of generalized free field is the Mellin transform of the field operator, and the Mellin transform of the two-point functions is its consequence.[20]

[1]See, for example, G. Mack and I. Todorov, J. Math. Phys. **10**, 2078 (1969).
[2]J. Lukierski and W. Sienkiewicz, J. Math. Phys. **15**, 344 (1974).
[3]We shall restrict in Secs. 1, 2 our considerations to the case of the real dimensionality parameter δ. However, in Sec. 3 we also discuss extensively the case of complex δ ($\mathrm{Re}\delta > 1$).
[4]W. Güttinger, Forsch. Physik **14**, 483 (1966).
[5]One can also reach the value $\delta = 1$ provided we introduce vanishing normalization factor. The following limit exists
$$\varphi(x) = \lim_{\delta \to 0} \left(\frac{1}{\Gamma(1-\delta)} \right)^{1/2} \Phi_6(x) .$$
By performing such a limit we contract the orbit O_2 of the Weyl group into orbit O_5. This problem in the framework of suitably chosen representation space has been discussed thoroughly in W. Rühl, "The Canonical Dimensions of Field as the Limit of Noncanonical Dimensions," Trier-Kaiserslautern University preprint, March 1973.
[6]S. Ferrara, R. Gatto, A.F. Grillo, and G. Parisi, Lett. Nuovo Cim. **4**, 115 (1972).
[7]The representation spaces $\mathcal{H}^{(S,5)}$, where S denotes arbitrary physical spin value ($S = 0, \frac{1}{2}, 1, \ldots$), have been considered by W. Rühl, Commun. Math. Phys. **30**, 287 (1973).
[8]It should be mentioned that in the derivation of (1.9″) we omit the term related with the boundaries of $\mathcal{H}^2$ integration at $\mathcal{H}^2 = \infty$. Besides, in comparison with I, we introduce in (1.9″) Wick normal products.
[9]Such multidimensional representations have been discussed recently by G.F. Del'Antonio, Nuovo Cimento **12 A**, 756 (1972).
[10]R.A. Brandt and Wing-Chiu Ng, Nuovo Cimento **13 A**, 1025 (1973).
[11]J. Łopuszański, Wroclaw University preprint No. 257, February 1973.
[12]We changed the definition in 8 of multidimensional representation matrix $T^{(N;\delta)}$ by reflection with respect to the diagonal. Such definition leads further to simple formula (2.5).
[13]The extensive study of such triangle representations for general Lie group has been presented by I.C. Philips, Jr., Ph.D. Thesis, University of Colorado, 1971.
[14]The most general solution of the functional equation (2.11) for $N = 2$ has been given in Ref. 10.
[15]M. Froissart, Nuovo Cim. Suppl. **14**, 197 (1959).
[16]J. Lukierski, Acta Phys. Polon. **32**, 551, 771 (1967).
[17]N. Nakanishi, Brookhaven preprint, BL 14425.
[18]E. Iacopini, Trieste preprint IC/73/27.
[19]S. Ferrara, R. Gatto, and A.F. Grillo, Phys. Lett. **42 B**, 264 (1972).
[20]The Mellin transform of the two-point function has been studied recently extensively by Bo Andersson, Nucl. Phys. **B 55**, 195 (1973).

Electrostatic or gravitational interaction energy of coaxial ellipsoids*

H. Schultheis and R. Schultheis

Institut für Theoretische Physik, D-74 Tübingen, West Germany
(Received 17 June 1974; revised manuscript received 29 July 1974)

An expression, which is appropriate for high-precision calculations, is derived for the interaction energy of two coaxial ellipsoidal distributions of charge or mass. By starting from Dirichlet's expression for the potential it is shown that the (in general) sixfold integration can be considerably reduced by integrating over equipotential surfaces and introducing elliptic integrals. The evaluation of the final expression requires only a double numerical integration.

1. INTRODUCTION

The study of nuclear deformations requires the calculation of electrostatic self- and interaction energies of homogeneous distributions of charge. (Inhomogeneities at the nuclear surface can be treated by corrections.[1]) The self-energy is essential for determining nuclear equilibrium shapes and related data, such as masses, binding energies, quadrupole moments, and rotational bands; the interaction energy is important for the motion of the fragments in nuclear fission as well as the collision of projectile and target in heavy-ion scattering experiments.

The determination of electrostatic energies in such cases requires high numerical accuracy since the total energy of a nuclear configuration is determined by a balance of electrostatic and nuclear forces, such that the electrostatic and other contributions to the deformation energy almost cancel one another. On the other hand one often has to compute the deformation energy for many different deformations of the nucleus (e.g., several hundred in fission theory). Therefore, great effort has been expended in order to evaluate the energy of different distributions of charge in an analytical way or to reduce multiple numerical integrations as much as possible.

For general solids of revolution the electrostatic energy can be calculated after the integration methods[2–4] given by Hill and Wheeler, Beringer, Cohen and Swiatecki, Lawrence, Nix,[3] and more recently by Davies and Sierk.[4] These methods, of course, can also be used to compute the interaction energy between two solids which are arbitrarily deformed but have a common axis of symmetry.

Spheroidal shapes are commonly used in those cases in which computational difficulties prevent the study of more complicated shapes. For these the self-energy is available as an elementary function. It was derived by Flügge[5] in 1951 employing the explicit expression for the electrostatic potential given by Dirichlet[6] in 1839. Moreover, expressions in terms of elliptic integrals are available for the self-energy of ellipsoids. The homogeneous case has been treated by Rosenkilde,[7] Pal, Götz *et al.*, and Leander.[8] Carlson[9] has also determined the self-energy of inhomogeneous distributions with ellipsoidal surfaces of constant density.

Series expansions around spherical or spheroidal shapes have been given by Bohr and Wheeler,[10] Swiatecki,[11] Present *et al.*,[12] and by Businaro and Gallone.[13] However, these expansions are applicable only to small deformations. Highly distorted nonellipsoidal shapes in general require multiple numerical integrations or multipole expansions. This is extensively studied in the work of Nix,[3] where also the application to spheroidal shapes together with a survey of the relevant literature is given.

Up to now rapidly converging expressions are not available for the interaction energy between general nonaxial distributions of charge or mass even if they are homogeneous. However, if the distributions are well separated, Nix's fivefold multipole summation[3] is applicable. In Ref. 3 explicit formulas for the case of arbitrarily oriented homogeneous spheroids are also given.

In connection with gravitation, Darwin[14] has developed an implicit formula for the interaction energy of homogeneous ellipsoids. It consists of a twofold infinite summation over increasing orders of mixed partial derivatives of $(x^2+y^2+z^2)^{-1/2}$. In the case of coaxial spheroids these derivatives generate Legendre polynomials. Thus an explicit twofold multipole summation can be obtained[15] for the axial case.

The present paper deals with the electrostatic interaction energy between two homogeneously charged ellipsoids with parallel axes, which are in contact or separated. Though originally carried out for nuclear fission theory,[16] the results are applicable to any distribution of charge or mass of this kind. Therefore, the calculation is given without reference to nuclear physics.

Starting from Dirichlet's[6] expression for the potential, the (in general) sixfold integration for the interaction energy is given in Sec. 2. By integrating over equipotential surfaces this expression can be reduced to a threefold integral and further to a twofold integration over elliptic integrals. In practice only two integrations have to be performed numerically for the evaluation of the final expression, since elliptic integrals can easily be obtained from standard routines.[17] The results are summarized in Sec. 3, so that the reader can refer directly to this section without going through the calculations of Sec. 2.

2. METHOD

The electrostatic[18] energy E of a system of two distributions of charge with densities $\rho_1(\mathbf{r})$ and $\rho_2(\mathbf{r})$ which

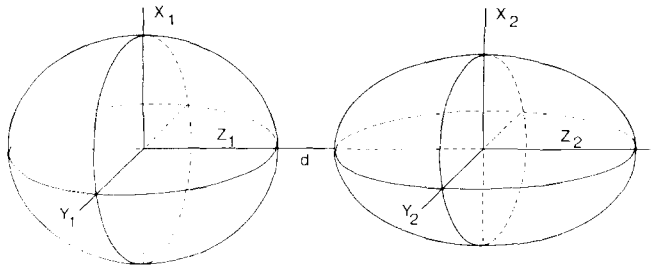

FIG. 1. Diagram of the distribution of charge or mass. In general all axes of the ellipsoids have different lengths. Note that the common axis, z, is not an axis of symmetry.

are separated or in contact can be split up into self-energies E_{ii} $(i=1, 2)$ and interaction energies E_{ij} $(i, j=1, 2; i\neq j)$ due to the repulsion or attraction between them, i.e.,

$$E = E_{11} + E_{22} + E_{12} + E_{21}, \tag{2.1}$$

where

$$E_{ij} = \frac{1}{2}\int \frac{\rho_i(\mathbf{r})\rho_j(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}' \quad (i, j=1, 2) \tag{2.2}$$

involves in general a sixfold integration. By use of the electrostatic potentials

$$\varphi_i(\mathbf{r}) = \int \frac{\rho_i(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}' \quad (i=1, 2) \tag{2.3}$$

equation (2.2) can be rewritten as

$$E_{ij} = \tfrac{1}{2}\int \rho_i(\mathbf{r})\, \varphi_j(\mathbf{r})\, d\mathbf{r} \quad (i, j=1, 2). \tag{2.4}$$

Since the interaction energies are equal,

$$E_{12} = E_{21}, \tag{2.5}$$

the total Coulomb interaction energy E_{CI} is given by

$$E_{CI} = E_{12} + E_{21} = 2E_{12} = 2E_{21}. \tag{2.6}$$

The present paper deals with two homogeneously charged ellipsoids with semiaxes x_i, y_i, and z_i $(i=1, 2)$ respectively, which are coaxial but may be separated by a distance d (see Fig. 1). For the self-energies E_{ii} of (2.1) one can evaluate Eq. (2.4) with the potential (2.15) given below. The result

$$E_{ii} = \tfrac{2}{75}\pi^2 x_i^2 y_i^2 z_i^2 \rho_i^2 \int_0^\infty \left(5 - \frac{x_i^2}{x_i^2+\lambda} - \frac{y_i^2}{y_i^2+\lambda} - \frac{z_i^2}{z_i^2+\lambda}\right) \frac{d\lambda}{D_i(\lambda)} \tag{2.7}$$

[for $D_i(\lambda)$ see (2.16)] can be transformed into an expression which involves an elliptic integral of the first kind but no numerical integration, see Refs. 7–9. For the axial symmetric case $(x_i = y_i)$ explicit formulas have been derived by Flügge,[5]

$$E_{ii} = \tfrac{2}{15} E_{CO} \frac{(1-\epsilon_i^2)^{1/3}}{\epsilon_i} \cdot \ln\left(\frac{1+\epsilon_i}{1-\epsilon_i}\right) \tag{2.8}$$

with

$$\epsilon_i^2 = 1 - x_i^2/z_i^2 \tag{2.9}$$

and the self-energy E_{CO} is that of a sphere of the same charge and volume.

The interaction energies E_{ij} in Eq. (2.1) are available only for coaxial homogeneously charged spheroids $(x_i = y_i)$. If the charges of the spheroids are denoted with Q_i, the total Coulomb interaction energy E_{CI} reads[3]

$$E_{CI} = \frac{Q_1 Q_2}{z_1 + z_2 + d}\, [s(\lambda_1) + s(\lambda_2) - 1 + S(\lambda_1, \lambda_2)], \tag{2.10}$$

where

$$\lambda_i^2 = \frac{z_i^2 - x_i^2}{(z_1 + z_2 + d)^2}, \tag{2.11}$$

and $S(\lambda_1, \lambda_2)$ can be represented in the form of a twofold summation

$$S(\lambda_1, \lambda_2) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \frac{3}{(2j+1)(2j+3)} \frac{3}{(2k+1)(2k+3)} \frac{(2j+2k)!}{(2j)!\,(2k)!} \times \lambda_1^{2j}\lambda_2^{2k}. \tag{2.12}$$

The summands $s(\lambda_i)$ are different for prolate $(x_i < z_i)$ and oblate $(x_i > z_i)$ shapes:

$$s(\lambda) = \begin{cases} \frac{3}{4}\left(\frac{1}{\lambda} - \frac{1}{\lambda^3}\right) \ln\frac{1+\lambda}{1-\lambda} + \frac{3}{2}\frac{1}{\lambda^2}, & \text{prolate}, \quad (2.13a) \\ \frac{3}{2}\left(\frac{1}{\omega} + \frac{1}{\omega^3}\right) \tan^{-1}\omega - \frac{3}{2}\frac{1}{\omega^2}, & \text{oblate } (\omega^2 = -\lambda^2). \quad (2.13b) \end{cases}$$

For the general case without rotational symmetry the Coulomb interaction energy E_{CI} shall be derived in the following:

The two ellipsoidal surfaces sketched in Fig. 1 obey the following relations in Cartesian coordinates:

$$\frac{x^2}{x_1^2} + \frac{y^2}{y_1^2} + \frac{z^2}{z_1^2} = 1 \tag{2.14a}$$

and

$$\frac{x^2}{x_2^2} + \frac{y^2}{y_2^2} + \frac{(z - z_1 - z_2 - d)^2}{z_2^2} = 1. \tag{2.14b}$$

Following Eq. (2.6) the total interaction energy can be determined either from E_{12} or from E_{21}. To be definite, we calculate E_{21} in the following. The potential $\varphi_1(\mathbf{r})$ in a point $\mathbf{r}$ outside the ellipsoid (2.14a) has been derived by Dirichlet[6]:

$$\varphi_1(x, y, z) = \pi x_1 y_1 z_1 \rho_1 \times \int_u^\infty \left(1 - \frac{x^2}{x_1^2+\lambda} - \frac{y^2}{y_1^2+\lambda} - \frac{z^2}{z_1^2+\lambda}\right) \frac{d\lambda}{D_1(\lambda)}, \tag{2.15}$$

where $D_1(\lambda)$ is given by

$$D_i(\lambda) = [(x_i^2+\lambda)(y_i^2+\lambda)(z_i^2+\lambda)]^{1/2}. \tag{2.16}$$

The lower limit u of the integral in (2.15) is defined as the largest positive solution of the equation

$$\frac{x^2}{x_1^2+u} + \frac{y^2}{y_1^2+u} + \frac{z^2}{z_1^2+u} = 1. \tag{2.17}$$

Thus the sixfold integration in (2.2) is reduced to a fourfold integral and E_{21} can be written

$$E_{21} = 2\pi\rho_1\rho_2 x_1 y_1 z_1 \int_{\tilde{z}_{min}}^{\tilde{z}_{max}} dz \int_0^{\tilde{y}_{max}} dy \int_0^{\tilde{x}_{max}} dx \times \int_u^\infty \frac{d\lambda}{D_1(\lambda)} \left(1 - \frac{x^2}{x_1^2+\lambda} - \frac{y^2}{y_1^2+\lambda} - \frac{z^2}{z_1^2+\lambda}\right) \tag{2.18}$$

with the limits of integration

$$\tilde{z}_{\min} = z_1 + d, \tag{2.19a}$$

$$\tilde{z}_{\max} = z_1 + 2z_2 + d, \tag{2.19b}$$

$$\tilde{y}_{\max} = y_2 \left(1 - \frac{(z - z_1 - z_2 - d)^2}{z_2^2}\right)^{1/2}, \tag{2.20}$$

$$\tilde{x}_{\max} = x_2 \left(1 - \frac{y^2}{y_2^2} - \frac{(z - z_1 - z_2 - d)^2}{z_2^2}\right)^{1/2}. \tag{2.21}$$

One further integration can be performed analytically by first integrating over equipotentials (with constant integrant) and then summing up the shares of all equipotentials, which can be parametrized by the above-mentioned variable u [(2.17)]. Since the equipotentials of an ellipsoid are confocal ellipsoids, this procedure mainly consists in integrating the Jacobian of x, y, z with respect to x, y, u over the area of the end section of an ellipsoid. Explicitly one has to transform the set of variables (x, y, z) to the new set (x, y, u). Thus the volume element $dx\,dy\,dz$ becomes

$$dx\,dy\,du \left| \frac{\partial(x, y, z)}{\partial(x, y, u)} \right| = dx\,dy\,du \left| \frac{\partial z}{\partial u} \right| \tag{2.22}$$

with

$$\frac{\partial z}{\partial u} = \frac{1}{2} \left[1 + \frac{x^2}{x_1^2 + u} \left(\frac{z_1^2 + u}{x_1^2 + u} - 1\right) + \frac{y^2}{y_1^2 + u} \left(\frac{z_1^2 + u}{y_1^2 + u} - 1\right)\right] \times \left[\left(1 - \frac{x^2}{x_1^2 + u} - \frac{y^2}{y_1^2 + u}\right)^{1/2} (z_1^2 + u)^{1/2}\right]^{-1}. \tag{2.23}$$

Consequently, formula (2.18) goes over into

$$E_{21} = 2\pi\rho_1\rho_2 x_1 y_1 z_1 \int_{u_{\min}}^{u_{\max}} du \int_0^{y_{\max}} dy \int_u^{\infty} \frac{d\lambda}{D_1(\lambda)} \times \int_0^{x_{\max}} dx \left[1 - \frac{z_1^2 + u}{z_1^2 + \lambda} - x^2 \left(\frac{1}{x_1^2 + \lambda} - \frac{z_1^2 + u}{x_1^2 + u} \frac{1}{z_1^2 + \lambda}\right) - y^2 \left(\frac{1}{y_1^2 + \lambda} - \frac{z_1^2 + u}{y_1^2 + u} \frac{1}{z_1^2 + \lambda}\right)\right] \left| \frac{\partial z}{\partial u} \right|. \tag{2.24}$$

The integration over x can be evaluated analytically. One arrives at the threefold integral

$$E_{21} = \pi\rho_1\rho_2 x_1 y_1 z_1 \int_{u_{\min}}^{u_{\max}} du (z_1^2 + u)^{-1/2} \int_0^{y_{\max}} dy \int_u^{\infty} \frac{d\lambda}{D_1(\lambda)} \times [A(\lambda, y, u) I_1(y, u) + B(\lambda, y, u) I_2(y, u) + C(\lambda, u) I_3(y, u)]. \tag{2.25}$$

The limits $u_{\min}$, $u_{\max}$, and $y_{\max}$ in (2.25) are given by

$$u_{\min} = d(2z_1 + d), \tag{2.26a}$$

$$u_{\max} = 4z_2(z_1 + z_2) + 2d(z_1 + 2z_2) + d^2, \tag{2.26b}$$

and by the solution $y_{\max}$ of

$$\beta_4 y_{\max}^4 + \beta_2 y^2{}_{\max} + \beta_0 = 0 \tag{2.27}$$

with

$$\beta_4 = \left(\frac{1}{y_2^2} - \frac{z_1^2 + u}{y_1^2 + u} \frac{1}{z_2^2}\right)^2, \tag{2.28a}$$

$$\beta_2 = 2 \left(\frac{2(z_1 + z_2)(z_1 + d) + u + d^2}{y_2^2 z_2^2} + \frac{z_1^2 + u}{y_1^2 + u} \frac{2(z_1 + z_2)(z_2 + d) - u + d^2}{z_2^4}\right), \tag{2.28b}$$

$$\beta_0 = \frac{d^4 + 4d^3(z_1 + z_2) + 2d^2(2z_1^2 + 2z_2^2 + 6z_1 z_2 - u)}{z_2^4} + \frac{4d(z_1 + z_2)(2z_1 z_2 - u) + u^2 - 4uz_2(z_1 + z_2)}{z_2^4}. \tag{2.28c}$$

The expressions $I_1(y, u)$, $I_2(y, u)$, and $I_3(y, u)$ of (2.25) are given by

$$I_1(y, u) = \int_0^{x_{\max}} f^{-1/2}(x, y, u)\, dx, \tag{2.29a}$$

$$I_2(y, u) = \int_0^{x_{\max}} x^2 f^{-1/2}(x, y, u)\, dx, \tag{2.29b}$$

$$I_3(y, u) = \int_0^{x_{\max}} x^4 f^{-1/2}(x, y, u)\, dx, \tag{2.29c}$$

$$f(x, y, u) = 1 - \frac{x^2}{x_1^2 + u} - \frac{y^2}{y_1^2 + u}, \tag{2.30}$$

where the upper limit $x_{\max}$ is the solution of

$$\gamma_4 x_{\max}^4 + \gamma_2 x_{\max}^2 + \gamma_0 = 0 \tag{2.31}$$

with the coefficients γ_4, γ_2, and γ_0

$$\gamma_4 = \left(\frac{1}{x_2^2} - \frac{z_1^2 + u}{x_1^2 + u} \frac{1}{z_2^2}\right)^2, \tag{2.32a}$$

$$\gamma_2 = 2 \left[y^2 \left(\frac{1}{y_2^2} - \frac{z_1^2 + u}{y_1^2 + u} \frac{1}{z_2^2}\right) \left(\frac{1}{x_2^2} - \frac{z_1^2 + u}{x_1^2 + u} \frac{1}{z_2^2}\right) + \frac{2(z_1 + z_2)(z_1 + d) + u + d^2}{x_2^2 z_2^2} + \frac{z_1^2 + u}{x_1^2 + u} \frac{2(z_1 + z_2)(z_2 + d) - u + d^2}{z_2^4}\right], \tag{2.32b}$$

$$\gamma_0 = \beta_4 y^4 + \beta_2 y^2 + \beta_0. \tag{2.32c}$$

The integrals I_1, I_2, and I_3 can be determined analytically.[19] The result is given in the next section [formulas (3.1)–(3.6)].

In the following paragraphs it shall be shown how the numerical integrations in the Coulomb interaction energy can be further reduced by introducing elliptic integrals, for which excellent routines[17] are standard in many computer systems.

According to (2.15), (2.16), (2.23), and (2.24) the expression (2.25) for E_{21} is a sum of integrals over functions of $(x_1^2 + \lambda)^{-1/2}$, $(y_1^2 + \lambda)^{-1/2}$, and $(z_1^2 + \lambda)^{-1/2}$ or powers of these up to the third degree:

$$E_{21} = \pi\rho_1\rho_2 x_1 y_1 z_1 \int_{u_{\min}}^{u_{\max}} du (z_1 + u)^{-1/2} \times \Big(\int_u^{\infty} d\lambda [(x_1^2 + \lambda)(y_1^2 + \lambda)(z_1^2 + \lambda)]^{-1/2} \int_0^{y_{\max}} dy\, G_0(y, u) + \int_u^{\infty} d\lambda [(x_1^2 + \lambda)^3 (y_1^2 + \lambda)(z_1^2 + \lambda)]^{-1/2} \int_0^{y_{\max}} dy\, G_1(y, u) + \int_u^{\infty} d\lambda [(x_1^2 + \lambda)(y_1^2 + \lambda)^3 (z_1^2 + \lambda)]^{-1/2} \int_0^{y_{\max}} dy\, G_2(y, u) + \int_u^{\infty} d\lambda [(x_1^2 + \lambda)(y_1^2 + \lambda)(z_1^2 + \lambda)^3]^{-1/2} \int_0^{y_{\max}} dy\, G_3(y, u) \Big). \tag{2.33}$$

In (2.33) the improper integrals over λ can be replaced by expressions, which are free of (numerical) integrations but employ elliptical integrals of the first and

TABLE I. Transformations for the standard form of the interaction energy (3.1) in the axial asymmetric case. If ellipsoid (1) is triaxial the required permutations of semiaxes $P(x_1, y_1, z_1)$ and the corresponding sequence of indices j, k, l are given in entries 2 and 3.

semiaxes	$P(x_1, y_1, z_1)$	$j\ k\ l$
$x_1 > y_1 > z_1$	(x_1, y_1, z_1)	1 2 3
$x_1 > z_1 > y_1$	(x_1, z_1, y_1)	1 3 2
$z_1 > x_1 > y_1$	(z_1, x_1, y_1)	3 1 2

second kind $F(\alpha, p)$ and $E(\alpha, p)$.[20] If $x_1 > y_1 > z_1$, the first one is equal[19] to

$$\Lambda_0(x_1, y_1, z_1; u) = \frac{2}{(x_1^2 - z_1^2)^{1/2}} F(\alpha, p), \tag{2.34a}$$

the second to

$$\Lambda_1(x_1, y_1, z_1; u) = \frac{2}{(x_1^2 - y_1^2)(x_1^2 - z_1^2)^{1/2}} [F(\alpha, p) - E(\alpha, p)], \tag{2.34b}$$

the third to

$$\Lambda_2(x_1, y_1, z_1; u) = \frac{2(x_1^2 - z_1^2)^{1/2}}{(x_1^2 - y_1^2)(y_1^2 - z_1^2)} E(\alpha, p) - \frac{2}{(x_1^2 - y_1^2)(x_1^2 - z_1^2)^{1/2}} F(\alpha, p) - \frac{2}{y_1^2 - z_1^2} \left(\frac{z_1^2 + u}{(x_1^2 + u)(y_1^2 + u)}\right)^{1/2}, \tag{2.34c}$$

and the last one to

$$\Lambda_3(x_1, y_1, z_1; u) = \frac{2}{(z_1^2 - y_1^2)(x_1^2 - z_1^2)^{1/2}} E(\alpha, p) + \frac{2}{y_1^2 - z_1^2} \left(\frac{y_1^2 + u}{(x_1^2 + u)(z_1^2 + u)}\right)^{1/2}. \tag{2.34d}$$

Here α and p are defined as

$$\alpha = \arcsin \left(\frac{x_1^2 - z_1^2}{x_1^2 + u}\right)^{1/2} \tag{2.35a}$$

$$p = \left(\frac{x_1^2 - y_1^2}{x_1^2 - z_1^2}\right)^{1/2}. \tag{2.35b}$$

For cases other than $x_1 > y_1 > z_1$ some reordering of the variables and indices in Λ_i is necessary. This will be discussed for the final expression in the next section.

3. RESULTS

In the following section we give the final expression for the electrostatic interaction energy E_{CI} of two ellipsoids—which have constant charge densities ρ_i $(i = 1, 2)$ and parallel semiaxes x_i, y_i, z_i $(i = 1, 2)$, are coaxial with common z axes and are in contact or separated by a distance d (see Fig. 1). To be definite, $x_1 > y_1$ is assumed in the following [if $x_1 = y_1$ and $x_2 = y_2$ see (2.10)]. Then—apart from a particular case treated below—the interaction energy is given by

$$E_{CI} = 2\pi\rho_1\rho_2 x_1 y_1 z_1 \int_{u_{min}}^{u_{max}} du (z_1^2 + u)^{-1/2} \times (\Lambda_0(P(x_1, y_1, z_1); u) \int_0^{y_{max}} dy\, G_0(y, u) + \Lambda_j(P(x_1, y_1, z_1); u) \int_0^{y_{max}} dy\, G_1(y, u) + \Lambda_k(P(x_1, y_1, z_1); u) \int_0^{y_{max}} dy\, G_2(y, u) + \Lambda_l(P(x_1, y_1, z_1); u) \int_0^{y_{max}} dy\, G_3(y, u)). \tag{3.1}$$

Here $P(a_1, a_2, a_3)$ is a permutation of real numbers (a_1, a_2, a_3) which orders these with decreasing magnitude; (j, k, l) is the resulting order of indices, i.e.,

$$P(x_1, x_2, x_3) = (x_j, x_k, x_l) \quad \text{with } x_j > x_k > x_l. \tag{3.2}$$

The factors Λ_i $(i = 0, 1, 2, 3)$ are defined in (2.34), their indices j, k, l and the actual values of $P(x_1, y_1, z_1)$ can be obtained from Table I.

The integrants G_0, G_1, G_2, and G_3 in (3.1) are defined by

$$G_0(y, u) = \tfrac{1}{2}(x_1^2 + u)^{1/2} \left[1 + \frac{z_1^2 + u}{x_1^2 + u} - \frac{y^2}{y_1^2 + u} \times \left(1 + \frac{z_1^2 + u}{x_1^2 + u} - 2\frac{z_1^2 + u}{y_1^2 + u}\right)\right] \times \arcsin x_{max} \left[(x_1^2 + u)\left(1 - \frac{y^2}{y_1^2 + u}\right)\right]^{-1/2} + \frac{1}{2} x_{max} \frac{x_1^2 - z_1^2}{x_1^2 + u} \left(1 - \frac{y^2}{y_1^2 + u} - \frac{x_{max}^2}{x_1^2 + u}\right)^{1/2}, \tag{3.3a}$$

$$G_1(y, u) = \tfrac{1}{2}(x_1^2 + u) \left\{\frac{1}{4} + \frac{3}{4}\frac{z_1^2 + u}{x_1^2 + u} - \frac{y^2}{y_1^2 + u} \times \left(\frac{1}{4} - \frac{z_1^2 + u}{y_1^2 + u} + \frac{3}{4}\frac{z_1^2 + u}{x_1^2 + u}\right)\right\} \times \left\{x_{max} \left(1 - \frac{y^2}{y_1^2 + u} - \frac{x_{max}^2}{x_1^2 + u}\right)^{1/2} - (x_1^2 + u)^{1/2} \left(1 - \frac{y^2}{y_1^2 + u}\right) \times \arcsin x_{max} \left[(x_1^2 + u)\left(1 - \frac{y^2}{y_1^2 + u}\right)\right]^{-1/2}\right\} + \frac{1}{4} x_{max}^3 \left(1 - \frac{y^2}{y_1^2 + u} - \frac{x_{max}^2}{x_1^2 + u}\right)^{1/2} \frac{z_1^2 - x_1^2}{x_1^2 + u}, \tag{3.3b}$$

$$G_2(y, u) = \tfrac{1}{2} x_{max} y^2 \frac{z_1^2 - x_1^2}{x_1^2 + u} \left(1 - \frac{y^2}{y_1^2 + u} - \frac{x_{max}^2}{x_1^2 + u}\right)^{1/2} - (x_1^2 + u)^{1/2} y^2 \left[\frac{1}{2} + \frac{1}{2}\frac{z_1^2 + u}{x_1^2 + u} - \frac{y^2}{y_1^2 + u}\left(\frac{1}{2} - \frac{z_1^2 + u}{y_1^2 + u} + \frac{1}{2}\frac{z_1^2 + u}{x_1^2 + u}\right)\right] \times \arcsin x_{max} \left[(x_1^2 + u)\left(1 - \frac{y^2}{y_1^2 + u}\right)\right]^{-1/2}, \tag{3.3c}$$

and

$$G_3(y, u) = \tfrac{1}{2}(x_1^2 + u)^{1/2}(z_1^2 + u) \left\{-\frac{3}{4} - \frac{1}{4}\frac{z_1^2 + u}{x_1^2 + u}\right.$$

$$+\frac{y^2}{y_1^2+u}\left[\frac{3}{2}+\frac{1}{2}\frac{z_1^2+u}{x_1^2+u}-\frac{z_1^2+u}{y_1^2+u}+\frac{y^2}{y_1^2+u}\left(-\frac{3}{4}-\frac{1}{4}\frac{z_1^2+u}{x_1^2+u}+\frac{z_1^2+u}{y_1^2+u}\right)\right]\Bigg\}$$
$$\times\arcsin x_{\max}\left[(x_1^2+u)\left(1-\frac{y^2}{y_1^2+u}\right)\right]^{-1/2}$$
$$-\frac{1}{2}x_{\max}(z_1^2+u)\left(1-\frac{y^2}{y_1^2+u}-\frac{x_{\max}^2}{x_1^2+u}\right)^{1/2}$$
$$\times\left[\frac{5}{4}-\frac{1}{4}\frac{z_1^2+u}{x_1^2+u}+\frac{1}{2}\frac{x_{\max}^2}{x_1^2+u}\frac{z_1^2-x_1^2}{x_1^2+u}+\frac{y^2}{y_1^2+u}-\frac{5}{4}+\frac{z_1^2+u}{y_1^2+u}+\frac{1}{4}\frac{z_1^2+u}{x_1^2+u}\right)\Bigg]. \tag{3.3d}$$

The limits $u_{\min}$ and $u_{\max}$ in (3.1) are defined in (2.26).

$$y_{\max}=\begin{cases}\{[-\beta_2+(\beta_2^2-4\beta_4\beta_0)^{1/2}]/2\beta_4\}^{1/2} & \\ \qquad \text{if } \beta_0\le 0,\ \beta_4\neq 0, & (3.4a)\\ (-\beta_0/\beta_2)^{1/2} \text{ if } \beta_0\le 0,\ \beta_4=0,\ \beta_2\neq 0, & (3.4b)\\ 0 \qquad \text{if } \beta_0=0,\ \beta_4=0,\ \beta_2=0, & (3.4c)\\ 0 \qquad \text{if } \beta_0>0, & (3.4d)\end{cases}$$

with β_i $(i=0,2,4)$ from (2.28), and $x_{\max}$ is analogous to that if one replaces β with γ from (2.32).

The expression (3.1) cannot be applied to ellipsoids which are solids of revolution with symmetry axes perpendicular to z. In this case the factors Λ_i in (3.1) have to be replaced in the following manner. If $x_1=z_1$:

$$\Lambda_0=\frac{2}{(x_1^2-y_1^2)^{1/2}}\left(\frac{\pi}{2}-\arctan\frac{(y_1^2+u)^{1/2}}{(x_1^2+u)^{1/2}}\right), \tag{3.5a}$$

$$\Lambda_j=\Lambda_i=\frac{(y_1^2+u)^{1/2}}{(y_1^2-x_1^2)(x_1^2+u)}+\frac{1}{2(x_1^2-y_1^2)}\Lambda_0, \tag{3.5b}$$

$$\Lambda_k=-\frac{2}{(y_1^2-x_1^2)(y_1^2+u)^{1/2}}+\frac{1}{y_1^2-x_1^2}\Lambda_0. \tag{3.5c}$$

If $y_1=z_1$:

$$\Lambda_0=-\frac{1}{(x_1^2-y_1^2)^{1/2}}\ln\left|\frac{(x_1^2+u)^{1/2}-(x_1^2-y_1^2)^{1/2}}{(x_1^2+u)^{1/2}+(x_1^2-y_1^2)^{1/2}}\right|. \tag{3.6a}$$

The other factors Λ are analogous to (3.5b, c) if one exchanges the axes x_1 and y_1 and the indices j and k.

ACKNOWLEDGMENT

The authors are grateful to Dr. J.D. Immele for reading the English manuscript.

*Supported in part by the Bundesministerium für Forschung und Technologie.

[1]W.D. Myers and W.J. Swiatecki, Nucl. Phys. **81**, 1 (1966).
[2]D.L. Hill and J.A. Wheeler, Phys. Rev. **89**, 1102 (1953); D.L. Hill, *Proceedings Second International Conference on Peaceful Uses of Atomic Energy, Geneva*, 1958 (United Nations, New York, 1958), Paper P/660; R. Beringer, Phys. Rev. **131**, 1402 (1963); S. Cohen and W.J. Swiatecki, Ann. Phys. (N.Y.) **22**, 406 (1963); J.N.P. Lawrence, Phys. Rev. **139**, B 1227 (1965).
[3]J.R. Nix, University of California, UCRL-11338 (1964).
[4]K.T.R. Davies and A.J. Sierk, Los Alamos Preprint LA-UR-74-790 (1974). The results of this recent work seem to be more accurate than those of Refs. 2 and 3. We are grateful to the referee for drawing our attention to this point.
[5]S. Flügge, Z. Physik **130**, 159 (1951).
[6]P.G.L. Dirichlet, *Über eine neue Methode zur Bestimmung vielfacher Integrale, Abh. der Berliner Akademie*, 1839; R. Becker and F. Sauter, *Theorie der Elektrizität* (Teubner, Stuttgart, 18. Auflage, 1964), Vol. 1, p. 77.
[7]C.E. Rosenkilde, J. Math. Phys. **8**, 88, 98 (1967).
[8]M.K. Pal, Nucl. Phys. A **183**, 545 (1972); U. Götz, H.C. Pauli, K. Alder, and K. Junker, Nucl. Phys. A **192**, 1 (1972); G. Leander, Nucl. Phys. A **219**, 245 (1974).
[9]B.C. Carlson, J. Math. Phys. **2**, 441 (1961).
[10]N. Bohr and J.A. Wheeler, Phys. Rev. **56**, 426 (1939).
[11]W.J. Swiatecki, Phys. Rev. **104**, 993 (1956); W.J. Swiatecki, *Proceedings Second International Conference on Peaceful Uses of Atomic Energy, Geneva*, 1958 (United Nations, New York, 1958), Paper P/651.
[12]R.D. Present and J.K. Knipp, Phys. Rev. **57**, 571, 1188 (1940); R.D. Present, F. Reines, and J.K. Knipp, Phys. Rev. **70**, 557 (1946).
[13]U.L. Businaro and S. Gallone, Nuovo Cimento **1**, 629, 1277 (1955).
[14]G.H. Darwin, *Scientific Papers. III* (Cambridge U.P., Cambridge, 1910) (Cf. Ref. 15, p. 154), p. 462
[15]S. Cohen and W.J. Swiatecki, Ann. Phys. (N.Y.) **19**, 67 (1962).
[16]H. Schultheis and R. Schultheis, Lett. Nuovo Cimento **6**, 169 (1973); H. Schultheis and R. Schultheis, Nucl. Phys. A **215**, 329 (1973).
[17]Scientific Subroutine Package (IBM Corporation, Fifth ed. GH20-0205-4, 1970).
[18]To be definite, only the electric case is treated here as the gravitational one is analogous.
[19]I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, London, 1971), 5th printing.
[20]For the notation of $F(\alpha,p)$ and $E(\alpha,p)$ see, e.g., F. Bowman, *Introduction to Elliptic Functions* (Dover, New York, 1961).

Space–time symmetries and nonunitary representations of the Poincaré semigroup: Description of unstable particles

M. Comi, L. Lanz*, L. A. Lugiato*, and G. Ramella

Istituto di Fisica dell'Università di Milano, Milan, Italy

**Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Milan, Italy*

(Received 24 June 1974; revised manuscript received 30 July 1974)

In this paper we justify the use of nonunitary representations of the space–time symmetry group to describe physical systems, as, e.g., unstable particles. It is shown that such a generalization of the standard theory of symmetries is possible inside the approach to quantum mechanics recently developed by Ludwig. The Poincaré semigroup turns out to be the fundamental symmetry group and only Lorentz transformations must be unitary.

1. INTRODUCTION

The problem of characterizing the kinematical behavior of a particle by space–time symmetry considerations treating stable and unstable particles on the same footing has been recently considered by several authors.[1–3]

More specifically, one can describe a relativistic (nonrelativistic) particle by an irreducible linear contractive up to a factor representation on a Hilbert space $\mathfrak{H}$ of the restricted Poincaré semigroup[2] (resp. Galilei semigroup); in particular stable particles correspond to unitary representations which can be immediately extended to the whole group. In the nonrelativistic case one gets in such a way a quite natural and well-known description of the unstable particle in which the wavefunction decays exponentially; the description of the relativistic particle is more involved and has been investigated recently. However, both cases present a basic difficulty with respect to the axiomatics of quantum mechanics which allows only unitary representations of the symmetry group. Furthermore, in the relativistic case one meets some difficulties in the physical interpretation:

(1) Spacelike translations are not contained in the Poincaré semigroup and can be represented *a posteriori* only on a proper subset of $\mathfrak{H}$.[2]

(2) The kinematics of the particle leads to define the following probability amplitude:

$$\psi_\xi(x)=\frac{1}{(2\pi\hbar)^{3/2}}\int\frac{d_3\underline{p}}{\sqrt{p_0}}\exp[-i(1-i\gamma)(p_0x_0-\underline{p}\,\underline{x})/\hbar]\varphi_\xi(\underline{p}) \tag{1.1}$$

with

$$p_0=(\underline{p}^2+m^2c^2)^{1/2},\quad \int\frac{d_3\underline{p}}{p_0}|\varphi(\underline{p})|^2=1,$$

$$\gamma=\frac{1}{2}\frac{\lambda}{c\tau_0},\quad \xi=1,2,\ldots,2j+1,$$

m being the mass, j the spin, λ the Compton wavelength, τ_0 the mean lifetime of the particle. The integral in the rhs of Eq. (1.1) converges for all $\varphi(\underline{p})$ only for timelike x. Furthermore, the wavefunction (1.1) is not linked to a self-adjoint "position" operator. All these difficulties seem to be intimately connected; therefore, one expects that in a framework in which the use of a nonunitary representation of the Poincaré semigroup is well motivated, also the difficulties (1), (2) can be overcome.

Such a framework can be found inside the approach to quantum mechanics recently given by Ludwig.[4] An important feature of such an approach is the introduction of the so-called "effects" aside the usual "properties" of quantum mechanics. Such a generalization of quantum mechanics proves to be essential to our purpose. For a nonrelativistic particle the present analysis provides a more fundamental motivation of the treatment of Ref. 5.

In this paper we shall use the metric

$$a\cdot b=a_\mu b^\mu=a_0b_0-\underline{a}\cdot\underline{b}$$

and the following symbols: $\mathcal{L}_+^\uparrow$, $\mathcal{P}_+^\uparrow$ are the proper orthochronous Lorentz and Poincaré groups respectively, i.e.,

$$\mathcal{L}_+^\uparrow=:\{\Lambda: x^\mu\to x'^\mu=\Lambda^\mu{}_\nu x^\nu\,|\,\det\Lambda=1,\ \Lambda^0_0\geq 1,\ \Lambda^\mu{}_\nu\Lambda_\sigma{}^\nu=g^\mu{}_\sigma\},$$

$$\mathcal{P}_+^\uparrow=:\{(a,\Lambda): x^\mu\to x'^\mu=\Lambda^\mu{}_\nu x^\nu+a^\mu\,|\,\Lambda\in\mathcal{L}_+^\uparrow,\ a\in\mathbb{R}_4\}.$$

We indicate by $\mathcal{P}_{+s_+}^\uparrow$ the Poincaré semigroup

$$\mathcal{P}_{+s_+}^\uparrow=:\{(a,\Lambda)\in\mathcal{P}_+^\uparrow\,|\,a^2=a_0^2-\underline{a}^2\geq 0,\ a_0\geq 0\},$$

and by $\mathcal{P}_{+s_-}^\uparrow$ the Poincaré "antisemigroup"

$$\mathcal{P}_{+s_-}^\uparrow=:\{(a,\Lambda)\in\mathcal{P}_+^\uparrow\,|\,a^2=a_0^2-\underline{a}^2\geq 0,\ a_0\leq 0\},$$

$\mathcal{G}_+^\uparrow$ is the Galilei group

$$\mathcal{G}_+^\uparrow=:\{(b,\underline{a},\underline{v}R): \underline{x}\to\underline{x}'=R\underline{x}+\underline{v}t+\underline{a},\ t\to t'=t+b\,|\ b\in\mathbb{R},\ \underline{a}\in\mathbb{R}_3,\ \underline{v}\in\mathbb{R}_3,\ R\in O_3,\ \det R=1\},$$

and $\mathcal{G}_{+s_\pm}^\uparrow$ the Galilei semigroups

$$\mathcal{G}_{+s_\pm}^\uparrow=\{(b,\underline{a},\underline{v},R)\in\mathcal{G}_+^\uparrow\,|\ b\gtrless 0\}.$$

The subgroup of $\mathcal{G}_+^\uparrow\{(0,\underline{a},\underline{v},R)\}$ is called $\mathcal{G}_G$.

Let $\mathfrak{H}$ be a Hilbert space and $\mathcal{L}(\mathfrak{H})$ the set of the linear operators on $\mathfrak{H}$ to $\mathfrak{H}$; $\tau c(\mathfrak{H})$ is the Banach space of the "trace-class" operators on $\mathfrak{H}$:

$$\tau c(\mathfrak{H})=:\{A\in\mathcal{L}(\mathfrak{H})\,|\,\mathrm{Tr}((A^*A)^{1/2})<\infty\};$$

$\tau c(\mathfrak{H})$ is a base-norm space[6] with base K:

$$K=\{W\in\tau c(\mathfrak{H})\,|\,W\geq 0,\ \mathrm{Tr}(W)=1\}.$$

$\mathbb{B}(\mathfrak{H})$ is the Banach space of bounded operators on $\mathfrak{H}$; $\mathbb{B}(\mathfrak{H})$ is an order-unit space[6] and its $[0,1]$ order interval L is

$$L=\{F\in\mathbb{B}(\mathfrak{H})\,|\,0\leq F\leq 1\}.$$

2. SPACE-TIME SYMMETRIES IN THE APPROACH OF LUDWIG TO QUANTUM MECHANICS

Let us give first a very sketchy account of the approach of Ludwig,[4] emphasizing some points which are relevant for the discussion of space–time symmetries.

Let us consider the set $\underline{\underline{M}}$ of experiments which should provide evidence for the physics of a microobject. Each experiment can be abalyzed into two parts: a preparation part $\underline{V}$ and an effect part $\underline{F}$. $\underline{V}$ if a certain macroscopic process by which the microobject is produced, $\underline{F}$ consists of a certain macroscopic process which can be suitably modified by the microobject and of such a modification to the process. Let $\underline{L}$ be the set of all $\underline{F}$ and $\underline{K}$ the set of all $\underline{V}$. One has that $\underline{\underline{M}}$ is contained in the Cartesian product of $\underline{K}$ and $\underline{L}$:

$$\underline{\underline{M}} \subset \underline{K} \times \underline{L}. \tag{2.1}$$

On the set $\underline{\underline{M}}$ a real function $\mu(\underline{V},\underline{F})$, $0 \leq \mu(\underline{V},\underline{F}) \leq 1$, is defined with the following interpretation: $\mu(\underline{V},\underline{F})$ gives, in physical approximation, the frequency of occurrence, in the experiment $(\underline{V},\underline{F})$, of the modification associated with $\underline{F}$. One assumes further that

$$\forall\, \underline{V} \in \underline{K},\ \exists\, \underline{F}_{\underline{V}} \in \underline{L}:\ \mu(\underline{V},\underline{F}_{\underline{V}}) = 1; \tag{2.2}$$

$$\exists\, \underline{Q} \in \underline{L}:\ \mu(\underline{V},\underline{Q}) = 0,\ \forall\, \underline{V} \in \underline{K}. \tag{2.2'}$$

Let us consider the following relation between $\underline{V}$ and $\underline{V}'$, $\underline{V}$, $\underline{V}' \in \underline{K}$: $\underline{V} \sim \underline{V}'$, if $\mu(\underline{V},\underline{F}) = \mu(\underline{V}',\underline{F})$, $\forall\, \underline{F}$ such that $(\underline{V},\underline{F})$, $(\underline{V}',\underline{F}) \in \underline{\underline{M}}$. Such a relation is assumed to be an equivalence relation (it is an assumption since $\underline{\underline{M}} \neq \underline{K} \times \underline{L}$). Let $\underline{K}$ be the set of equivalence classes $\underline{V}$. Let us consider the subset $\underline{M} \subset \underline{K} \times \underline{L}$:

$$\underline{M} =: \{(\underline{V},\underline{F}) \mid \exists\, \underline{V} \in \underline{V} \text{ such that } (\underline{V},\underline{F}) \in \underline{\underline{M}}\};$$

on $\underline{M}$ one defines

$$\mu(\underline{V},\underline{F}) = \mu(\underline{V},\underline{F}).$$

The the following axiom is formulated:

$$\underline{M} = \underline{K} \times \underline{L}. \tag{2.3}$$

As a consequence, the relation

$$\underline{F} \sim \underline{F}':\ \mu(\underline{V},\underline{F}) = \mu(\underline{V}\underline{F}')\ \forall\ \underline{V} \in \underline{K}$$

is an equivalence relation. Let $\underline{L}$ be the set of equivalence classes $\underline{F}$; on $\underline{K} \times \underline{L}$ one defines

$$\mu(\underline{V},\underline{F}) = \mu(\underline{V},\underline{F}),\quad \underline{F} \in \underline{F}.$$

Building up from this basis, introducing physically relevant axioms on the sets $\underline{K}$ and $\underline{L}$ and mathematical hypotheses on the structures which are successively specified, Ludwig and co-workers prove a sequence of theorems leading to the following statement: A Hilbert space $\underline{\mathfrak{H}}$ can be found such that $\underline{K}$ is norm dense in the basis K of the Banach space $\tau c(\underline{\mathfrak{H}})$ and $\underline{L}$ is dense in the so-called weak* topology[7] in the $[0,1]$ order interval L of the dual space $\mathbb{B}(\underline{\mathfrak{H}})$; the function $\mu(\underline{V},\underline{F})$ is given by

$$\mu(\underline{V},\underline{F}) = \mathrm{Tr}(\underline{V}\underline{F}). \tag{2.4}$$

To discuss the problem of space–time symmetries within this theory, let us give the space time characterization of effect and of preparation parts. We shall consider three different characterizations.

A. Characterization I

The usual treatment of symmetries in quantum mechanics is based on the following description of the experiments in terms of preparation and effect parts. Each preparation part (effect part) $\underline{V}(\underline{F})$ is defined as a production process (a modification of a given macroscopic process) referred to a fixed reference frame R. The experiment $(\underline{V},\underline{F})$ consists in the determination of the frequency of occurrence of the effect $\underline{F}$ in the frame R, as a consequence of the preparation $\underline{V}$. The invariance of macroscopic physics under $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$ implies that $\underline{K}$ and $\underline{L}$ are the spaces of two representations of $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$ $\mathcal{U}_{\underline{K}}(g)$, $\mathcal{U}_{\underline{L}}(g)$ defined in the following way: Let us consider a concrete realization of $\underline{V}(\underline{F})$ in R and a transformed reference frame $R' = gR$; the realization of $\underline{V}(\underline{F})$ is described in R' as a new preparation (effect) which is defined as $\mathcal{U}_{\underline{K}}(g)\underline{V}$ $(\mathcal{U}_{\underline{L}}(g)\underline{F})$.

The symmetry of the theory implies that

$$\mu(\underline{V},\underline{F}) = \mu(\mathcal{U}_{\underline{K}}(g)\underline{V}, \mathcal{U}_{\underline{L}}(g)\underline{F}),\qquad \forall\, g \in \mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+}),\ \forall\, (\underline{V},\underline{F}) \in \underline{\underline{M}}, \tag{2.5}$$

from which it easily follows that $\mathcal{U}_{\underline{K}}(g)$, $\mathcal{U}_{\underline{L}}(g)$ preserve the equivalence classes so that, defining

$$\mathcal{U}_{\underline{K}}(g)\underline{V} =: \{\mathcal{U}_{\underline{K}}(g)\underline{V},\ \underline{V} \in \underline{V}\},\ \mathcal{U}_{\underline{L}}(g)\underline{F} =: \{\mathcal{U}_{\underline{L}}(g)\underline{F},\ \underline{F} \in \underline{F}\},\qquad \mu(\underline{V},\underline{F}) = \mu(\mathcal{U}_{\underline{K}}(g)\underline{V}, \mathcal{U}_{\underline{L}}(g)\underline{F}), \tag{2.6}$$

where $\mathcal{U}_{\underline{K}}(g)$ and $\mathcal{U}_{\underline{L}}(g)$, are representation of $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$ on $\underline{K}$ and $\underline{L}$ respectively. Finally, in the realization of the theory in a Hilbert space $\underline{\mathfrak{H}}$ one can prove[8] that $\mathcal{U}_{\underline{L}}(g)$ can be extended to $\mathbb{B}(\underline{\mathfrak{H}})$ with the form

$$\mathcal{U}(g)Y = U(g)YU^{*}(g),\quad Y \in \mathbb{B}(\underline{\mathfrak{H}}), \tag{2.7}$$

where $U(g)$ is a unitary up-to-a-factor representation of $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$ on $\underline{\mathfrak{H}}$.

Within such a characterization of the experiments, axiom (2.3) is strongly restrictive. In fact, considering, e.g., the nonrelativistic case, one has couples $(\underline{V},\underline{F})$ such that $\underline{F}$ follows $\underline{V}$ in time; axiom (2.3) implies that for any t_1 and any production process $\underline{V}$ involving times $t \geq t_1$, one can find a process $\underline{V}' \sim \underline{V}$ involving only times $t < t_1$. E.g., if $\underline{V}$ is a preparation of an unstable particle at time $t > t_1$, $\underline{V}'$ must be, loosely speaking, the preparation at time t_1 of particles correlated in such a way to produce with probability 1 the unstable particle at time t. To require that preparations of this type are possible might be a too strong assumption especially for large $t - t_1$ and in the case of a relativistic dynamics in which several channel for the time evolution are open. We feel that assumption (2.3) is connected with the difficulties to obtain a clear description of unstable particles in quantum field theories.

B. Characterization II

Ludwig[9] considers the following *different* characteri-

zation of the experiments in which axiom (2.3) is no longer restrictive. Each preparation part $\underline{\underline{V}}$ is characterized by a space–time frame $R_{\underline{V}}$ (which we shall call preparation frame) and a production process $\alpha_{\underline{V}}$ referred to $R_{\underline{V}}$: $\underline{\underline{V}} =: (R_{\underline{V}}, \alpha_{\underline{V}})$. Each effect part $\underline{\underline{F}}$ is a modification of a given macroscopic process referred to R. The macroscopic physics which is involved into the description of $\underline{\underline{V}}$ and of $\underline{\underline{F}}$ is assumed to be invariant under $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$; then $\underline{\underline{K}}$ and $\underline{\underline{L}}$ are the spaces of two representations $\mathcal{U}_{\underline{\underline{K}}}(g)$, $\mathcal{U}_{\underline{\underline{L}}}(g)$ of $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$. $\mathcal{U}_{\underline{\underline{K}}}(g)$ is given by

$$\mathcal{U}_{\underline{\underline{K}}}(g)\underline{\underline{V}} = (gR_{\underline{V}}, \alpha_{\underline{V}}), \quad \forall\ g \in \mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+}). \tag{2.8}$$

$\mathcal{U}_{\underline{\underline{L}}}(g)$ is defined as in the previous characterization. The experiment $(\underline{\underline{V}}, \underline{\underline{F}})$ consists in the determination of the frequency of occurrence of an effect which is described in $R_{\underline{V}}$ in the same way as $\underline{\underline{F}}$ in R, as a consequence of the production process $\alpha_{\underline{V}}$.

The schematization of an experiment as being composed by a preparation and an effect part is meaningful only if the effect part does not influence the preparation part. In the nonrelativistic case this can be assumed for every pair $(\underline{\underline{V}}, \underline{\underline{F}})$, prescribing that the production process involves times $t \leq 0$ (obviously in $R_{\underline{V}}$) and the effect part involves times $t \geq 0$ (in R). In the relativistic case the space–time points of $\alpha_{\underline{V}}$ must be outside the union of the forward light cones with vertices at space–time points of $\underline{\underline{F}}$; this is obtained most simply, taking $\underline{\underline{F}}$ inside the forward light cone of R and $\alpha_{\underline{V}}$ outside the forward light cone of $R_{\underline{V}}$.

We stress that such prescriptions reduce the symmetry group for the effects to a semigroup: in the nonrelativistic case to the Galilei semigroup $\mathcal{G}^{\uparrow}_{+s_+}$, in the relativistic case, to the Poincaré semigroup $\mathcal{P}^{\uparrow}_{+s_+}$; the positive direction of the time axes is then privileged. The symmetry of the theory under $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$ is expressed by the relation

$$\mu(\mathcal{U}_{\underline{\underline{K}}}(g)\underline{\underline{V}}, \underline{\underline{F}}) = \mu(\underline{\underline{V}}, \underline{\underline{F}}), \quad \forall\ g \in \mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+}), \tag{2.9}$$

and $\forall\ \underline{\underline{F}}$ such that $(\underline{\underline{V}}, \underline{\underline{F}}) \in \underline{\underline{M}}$. Relation (2.9) implies that $\mathcal{U}_{\underline{\underline{K}}}(g)\underline{\underline{V}} \sim \underline{\underline{V}}, \forall\ \underline{\underline{V}} \in \underline{\underline{K}}, \forall g \in \mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$, and therefore one gets only a trivial representation of $\mathcal{P}^{\uparrow}_{+}(\mathcal{G}^{\uparrow}_{+})$ on $\underline{\underline{K}}$.

On the other hand, the symmetry condition does not give any restriction on $\mathcal{U}_{\underline{\underline{L}}}(g)$, $g \in \mathcal{P}^{\uparrow}_{+s_+}(\mathcal{G}^{\uparrow}_{+s_+})$. We see therefore that in the given description of the experiment, in which the effect part is referred to the preparation frame, the symmetry condition has very poor consequences.

However, features which in the characterization I are linked to the symmetry can arise by the very structure of the present one. In fact the experiment $(\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}(g)\underline{\underline{F}})$, $g \in \mathcal{P}^{\uparrow}_{+s_+}$ can be described also as $(\underline{\underline{V}}', \underline{\underline{F}})$ with $\underline{\underline{V}}' = (g^{-1}R_{\underline{V}}, \alpha_{g^{-1}})$, where $\alpha_{g^{-1}}$ is the description given in $g^{-1}R_{\underline{V}}$ of the production process which is described as α in $R_{\underline{V}}$. Therefore, there is an arbitrariness in the specification of $\underline{\underline{K}}$ associated with a set of experiments; "minimal" choices of $\underline{\underline{K}}$ are those in which each concrete preparation part corresponds only to one element of $\underline{\underline{K}}$. With such a choice nothing new about $\mathcal{U}_{\underline{\underline{L}}}(g)$ arises. More fruitful choices are the two following ones:

(a) $\underline{\underline{K}}$ is such that if $(R_{\underline{V}}, \alpha) \in \underline{\underline{K}}$ also $(g^{-1}R_{\underline{V}}, \alpha_{g^{-1}}) \in \underline{\underline{K}}$, $\forall g \in \mathcal{P}^{\uparrow}_{+s_+}(\mathcal{G}^{\uparrow}_{+s_+})$; then on the set of all production processes α a representation of $\mathcal{P}^{\uparrow}_{+s_-}(\mathcal{G}^{\uparrow}_{+s_-})$ is defined.

(b) $\underline{\underline{K}}$ is such that if $(R_{\underline{V}}, \alpha) \in \underline{\underline{K}}$, also $(g^{-1}R_{\underline{V}}, \alpha_{g^{-1}}) \in \underline{\underline{K}}$, $\forall g \in \mathcal{L}^{\uparrow}_{+}(\mathcal{G}_0)$; then on the set of all production processes α a representation of $\mathcal{L}^{\uparrow}_{+}(\mathcal{G}_0)$ is defined.

We stress that the axioms of Ludwig, which require that certain relations hold $\forall\ \underline{\underline{V}} \in \underline{\underline{K}}$, as is the case for axiom (2.2), become the more restrictive the larger $\underline{\underline{K}}$ is. The consistency of the description requires that

$$\underline{\underline{\mu}}(\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}(g)\underline{\underline{F}}) = \mu(\mathcal{V}_{\underline{\underline{K}}}(g^{-1})\underline{\underline{V}}, \underline{\underline{F}}), \quad \forall \underline{\underline{F}} \in \underline{\underline{L}},\ \underline{\underline{V}} = (R_{\underline{V}}, \alpha) \in \underline{\underline{K}}, \tag{2.10}$$

with $\mathcal{V}_{\underline{\underline{K}}}(g^{-1})(R_{\underline{V}}, \alpha) = (g^{-1}R_{\underline{V}}, \alpha_{g^{-1}})$, where $g \in \mathcal{P}^{\uparrow}_{+s_+}(\mathcal{G}^{\uparrow}_{+s_+})$ in the case (a) and $g \in \mathcal{L}^{\uparrow}_{+}(\mathcal{G}_0)$ in the case (b).

In the case (a) it follows immediately that $\mathcal{V}_{\underline{\underline{K}}}(g)$ and $\mathcal{U}_{\underline{\underline{L}}}(g)$ preserve equivalence classes and yield respectively a representation $\mathcal{V}_{\underline{\underline{K}}}(g^{-1})$ of $\mathcal{P}^{\uparrow}_{+s_-}(\mathcal{G}^{\uparrow}_{+s_-})$ on $\underline{\underline{K}}$ and $\mathcal{U}_{\underline{\underline{L}}}(g)$ of $\mathcal{P}^{\uparrow}_{+s_+}(\mathcal{G}^{\uparrow}_{+s_+})$ on $\underline{\underline{L}}$, such that

$$\mu(\mathcal{V}_{\underline{\underline{K}}}(g^{-1})\underline{\underline{V}}, \underline{\underline{F}}) = \mu(\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}(g)\underline{\underline{F}}), \quad \forall \underline{\underline{V}} \in \underline{\underline{K}},\ \underline{\underline{F}} \in \underline{\underline{L}}. \tag{2.11}$$

$\mathcal{V}_{\underline{\underline{K}}}(g^{-1})$, $\mathcal{U}_{\underline{\underline{L}}}(g)$ are affine mappings. In the Hilbert space realization of the theory, $\mathcal{U}_{\underline{\underline{L}}}(g)$ is, by (2.11), continuous on $\underline{\underline{L}}$ in the weak*-topology of $\mathbb{B}(\mathfrak{H})$; therefore, it can be extended as an affine mapping $\mathcal{U}_{\underline{\underline{L}}}(g)$ on L to L. Then one can show[10] that $\mathcal{U}_{\underline{\underline{L}}}(g)$ can be extended to a linear contractive, weak* continuous, order preserving, unity preserving operator $\mathcal{U}(g)$ on $\mathbb{B}(\mathfrak{H})$ to $\mathbb{B}(\mathfrak{H})$. Its adjoint leaves $\tau c(\mathfrak{H})$ invariant and its restriction to $\tau c(\mathfrak{H})$ is a positive linear endomorphism, i.e., it maps K in K; it provides the linear extension $\mathcal{V}(g^{-1})$ of $\mathcal{V}_{\underline{\underline{K}}}(g^{-1})$ to $\tau c(\mathfrak{H})$. The correspondence

$$\mathcal{P}^{\uparrow}_{+s_+}(\mathcal{G}^{\uparrow}_{+s_+}) \ni g \text{-} \mathcal{U}(g)$$

is a representation of $\mathcal{P}^{\uparrow}_{+s_+}(\mathcal{G}^{\uparrow}_{+s_+})$ on $\mathbb{B}(\mathfrak{H})$. The correspondence

$$\mathcal{P}^{\uparrow}_{+s_-}(\mathcal{G}^{\uparrow}_{+s_-}) \ni g \text{-} \mathcal{V}(g)$$

is a representation of $\mathcal{P}^{\uparrow}_{+s_-}(\mathcal{G}^{\uparrow}_{+s_-})$ on $\tau_c(\mathfrak{H})$. For $g \in \mathcal{L}^{\uparrow}_{+}(\mathcal{G}_0)$, $\mathcal{U}_{\underline{\underline{L}}}(g)$ is a bijective application on $\underline{\underline{L}}$. Then $\mathcal{U}(g)$ is an automorphism of the order unit space $\mathbb{B}(\mathfrak{H})$.[11] Such an automorphism has the following structure:

$$\mathcal{U}(g)Y = U(g)YU^{+}(g), \quad \forall Y \in \mathbb{B}(\mathfrak{H}), \tag{2.12}$$

where $U(g)$ is a unitary up to a factor representation of $\mathcal{L}^{\uparrow}_{+}(\mathcal{G}_0)$ on $\mathfrak{H}$.[10]

In the case (b) result (2.12) holds for $g \in \mathcal{L}^{\uparrow}_{+}(\mathcal{G}_0)$, whereas for $g = (a, I)$, $a^2 \geq 0$ $a^0 \geq 0$ $[g = (b, \underline{0}, \underline{0}, I)$, $b \geq 0]$, one cannot even show that $\mathcal{U}_{\underline{\underline{L}}}(g)$ preserves the equivalence classes $\underline{\underline{F}}$.

C. Characterization III

Our aim is to give a description of experiments intermediary between the two previously given, devised in such a way that axiom (2.3) is not too restrictive and on the other hand the space–time symmetry is as fruitful as possible. Let us investigate the reasons why, in characterization II of the experiments, axiom (2.3) is far less restrictive than in characterization I. In the second description, due to the fact that effects are referred in the experiments to the preparation frame, the separation between $\underline{\underline{V}}$ and $\underline{\underline{F}}$ in each experiment is simply obtained, e.g., in the Galilean case, considering preparations involving $t < 0$ and effects involving $t > 0$. However, to meet such a situation, it is sufficient that

only the time specification of the effect part in the experiment is referred to the preparation frame; therefore, in our new description we take preparation frames obtained from R only by time translations, so that $\underline{\underline{V}} =: (b, \alpha)$, where b is a real number and α a production process involving only negative times, referred to the frame R_b obtained from R by the time translation b. The relativistic version of such a characterization consists in taking preparation frames obtained from R only by space–time translations, so that: $\underline{\underline{V}} =: (b_\mu, \alpha)$, where b_μ ($\mu = 0, 1, 2, 3$) is a 4-vector and α a production process, involving only points in the backward light cone, referred to the frame R_{b_μ} obtained from R by the space–time translation b_μ. As in the second description one considers effects involving only space–time points inside the forward light cone of R and in the experiment the effects are referred to R_{b_μ}. Therefore, the set $\underline{\underline{L}}$ as well the representation $\mathcal{U}_{\underline{\underline{L}}}(g)$ of the semigroup $\mathcal{P}^\uparrow_{+s_+}$ ($\mathcal{G}^\uparrow_{+s_+}$) are the same as in characterizations I and II. The definition of $\mathcal{U}_{\underline{\underline{K}}}(g)$ is simpler in the relativistic case, which we consider first. The preparation (b_μ, α) is described in a transformed frame $R' = (a, \Lambda)R$ as $(a_\mu + (\Lambda b)_\mu, \alpha')$, where α' is the description referred to $R'_{a_\mu + (\Lambda b)_\mu}$ of the production process which in R_{b_μ} is described by α. Since $R'_{a_\mu + (\Lambda b)_\mu} = (0, \Lambda)R_{b_\mu}$ one has $\alpha' = u(\Lambda)\alpha$, where $u(\Lambda)$ is a representation of $\mathcal{L}^\uparrow_+$ on the set of all production processes α. In conclusion one has the following representation of $\mathcal{P}^\uparrow_+$ on $\underline{\underline{K}}$:

$$\mathcal{U}_{\underline{\underline{K}}}((a, \Lambda))(b_\mu, \alpha) = (a_\mu + (\Lambda b)_\mu, u(\Lambda)\alpha) \quad \forall (a, \Lambda) \in \mathcal{P}^\uparrow_+, \ (b_\mu, \alpha) \in \underline{\underline{K}}. \tag{2.13}$$

By similar considerations one sees that the symmetry condition is now

$$\mu(\underline{\underline{V}}, \underline{\underline{F}}) = \mu(\mathcal{U}_{\underline{\underline{K}}}(a, \Lambda))\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}((0, \Lambda))\underline{\underline{F}}) \quad \forall (a, \Lambda) \in \mathcal{P}^\uparrow_+, \ \underline{\underline{V}} \in \underline{\underline{K}}, \ \underline{\underline{F}} \in \underline{\underline{L}}. \tag{2.14}$$

By considering the case $\Lambda = I$, Eq. (2.14) implies

$$\mathcal{U}_{\underline{\underline{K}}}((a, I))\underline{\underline{V}} \sim \underline{\underline{V}} \quad \forall a \in R_4, \ \underline{\underline{V}} \in \underline{\underline{K}},$$

and therefore one gets only a trivial representation of translations on $\underline{\underline{K}}$: $\mathcal{U}_{\underline{\underline{K}}}((a, I)) = \mathcal{J}_{\underline{\underline{K}}}$, with $\mathcal{J}_{\underline{\underline{K}}}$ identity operator on $\underline{\underline{K}}$.

On the other hand in the case $a_\mu = 0$, by the same arguments given in connection to Eq. (2.5) one defines $\mathcal{U}_{\underline{\underline{K}}}((0, \Lambda))$ and $\mathcal{U}_{\underline{\underline{L}}}((0, \Lambda))$ and proves that in the Hilbert space realization of the theory $\mathcal{U}_{\underline{\underline{L}}}((0, \Lambda))$ can be extended to $\mathbb{B}(\mathfrak{H})$ with the form

$$\mathcal{U}((0, \Lambda))Y = U(\Lambda)YU^*(\Lambda) \quad \forall Y \in \mathbb{B}(\mathfrak{H}), \tag{2.15}$$

where $U(\Lambda)$ is a unitary up to a factor representation of $\mathcal{L}^\uparrow_+$ on $\mathfrak{H}$. The symmetry condition has no implication on the representation $\mathcal{U}_{\underline{\underline{L}}}((a, I))$ of timelike translations into the future.

In such a way we achieve by space–time symmetry the results obtained in characterization II with the assumption (b). [See (2.12).]

As in the characterization II also in the present one different pairs $(\underline{\underline{V}}, \underline{\underline{F}})$ can exist which are related to the same concrete experiment. In fact $(\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}((a, I))\underline{\underline{F}})$, $a^2 \geq 0$, $a^0 \geq 0$, where $\underline{\underline{V}} = (b_\mu, \alpha)$, can be described also as $(\underline{\underline{V}}', \underline{\underline{F}})$, with $\underline{\underline{V}}' = (b_\mu + a_\mu, \alpha_{(-a, I)})$, $\alpha_{(-a, I)}$ being defined as in characterization II. Then the same set of results which are obtained in the characterization II with the assumption (a), now can be obtained with the following assumption:

(a$'_2$): $\underline{\underline{K}}$ is such that if $(b_\mu, \alpha) \in \underline{\underline{K}}$ also $(b_\mu + a_\mu, \alpha_{(-a, I)}) \in \underline{\underline{K}} \quad \forall a \in R^4, \ a^2 \geq 0, \ a^0 \geq 0.$

Let us consider now the definition of $\mathcal{U}_{\underline{\underline{K}}}(g)$ in the Galilean case. By the same arguments used to obtain Eq. (2.13), one gets the following representation of $\mathcal{G}^\uparrow_+$ on $\underline{\underline{K}}$:

$$\mathcal{U}_{\underline{\underline{K}}}((\tau, \underline{a}, \underline{v}, R))(b, \alpha) = (b + \tau, u(\underline{a} + b\underline{v}, \underline{v}, R)\alpha), \quad (\tau, \underline{a}, \underline{v}, R) \in \mathcal{G}^\uparrow_+, \tag{2.16}$$

where $u(\underline{a}, \underline{v}, R)$ is a representation, on the set of all production processes, of the subgroup $\mathcal{C}$ of $\mathcal{G}^\uparrow_+$ of transformations $(0, \underline{a}, \underline{v}, R)$.

The symmetry condition is

$$\mu(\underline{\underline{V}}, \underline{\underline{F}}) = \mu(\mathcal{U}_{\underline{\underline{K}}}((\tau, \underline{a}, v, R))\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}((0, a + \underline{v}b(\underline{\underline{V}}), \underline{v}, R))\underline{\underline{F}}), \tag{2.17}$$

where $b(\underline{\underline{V}})$ is the specification b in the preparation $\underline{\underline{V}} = (b, \alpha)$. In analogy with the relativistic case one has that

$$\mathcal{U}_{\underline{\underline{K}}}((\tau, \underline{0}, \underline{0}, I)) = \mathcal{J}_{\underline{\underline{K}}}. \tag{2.18}$$

The operators $\mathcal{U}_{\underline{\underline{K}}}((0, \underline{a}, \underline{v}, R))$, which yield a representation of $\mathcal{G}_0$ on $\underline{\underline{K}}$, do not preserve equivalence classes when $\underline{v} \neq 0$, due to the term $\underline{v}b(\underline{\underline{V}})$ in the rhs of Eq. (2.17). Therefore, the representation $\mathcal{U}_{\underline{\underline{K}}}((\tau, \underline{a}, \underline{v}, R))$ of $\mathcal{G}^\uparrow_+$ on $\underline{\underline{K}}$ does not induce in a natural way a representation of $\overline{\mathcal{G}}^\uparrow_+$ on $\underline{\underline{K}}$. On the other hand no nontrivial representation of $\overline{\mathcal{G}}^\uparrow_+$ exists compatible with (2.18). However, writing Eq. (2.17) in the form

$$\mu(\underline{\underline{V}}, \underline{\underline{F}}) = \mu(\mathcal{U}_{\underline{\underline{K}}}((\tau, \underline{a} - \underline{v}b(\underline{\underline{V}}), \underline{v}, R))\underline{\underline{V}}, \mathcal{U}_{\underline{\underline{L}}}((0, \underline{a}, \underline{v}, R))\underline{\underline{F}}), \tag{2.19}$$

one can define a mapping of $\underline{\underline{K}}$ on $\underline{\underline{K}}$ by

$$\mathcal{U}_{\underline{\underline{K}}}(\underline{a}, \underline{v}, R)\underline{\underline{V}} = \underline{\underline{V}}', \tag{2.20}$$

where $\underline{\underline{V}}'$ is the equivalence class containing the elements

$$\mathcal{U}_{\underline{\underline{K}}}((0, \underline{a} - \underline{v}b(\underline{\underline{V}}), \underline{v}, R))\underline{\underline{V}}, \quad \underline{\underline{V}} \in \underline{\underline{V}}.$$

Since

$$\mathcal{U}_{\underline{\underline{K}}}((0, \underline{a} - \underline{v}b(\underline{\underline{V}}), \underline{v}, R))(b, \alpha) = (b, u(\underline{a}, \underline{v}, R)\alpha), \tag{2.21}$$

$\mathcal{U}_{\underline{\underline{K}}}(\underline{a}, \underline{v}, R)$ is a representation of $\mathcal{G}_0$ on $\underline{\underline{K}}$. By Eq. (2.19), $\mathcal{U}_{\underline{\underline{L}}}((0, \underline{a}, \underline{v}, R))$ preserves equivalence classes in $\underline{\underline{L}}$ and yields a representation $\mathcal{U}_{\underline{\underline{L}}}(\underline{a}, \underline{v}, R)$ of $\mathcal{G}_0$ on $\underline{\underline{L}}$. Then the symmetry condition implies that in the Hilbert space realization of the theory $\mathcal{U}_{\underline{\underline{L}}}(\underline{a}, \underline{v}, R)$ can be extended on $\mathbb{B}(\mathfrak{H})$ with the form

$$\mathcal{U}(\underline{a}, \underline{v}, R)Y = U(\underline{a}, \underline{v}, R)YU^*(\underline{a}, \underline{v}, R), \quad \forall Y \in \mathbb{B}(\mathfrak{H}), \tag{2.22}$$

where $U(\underline{a}, \underline{v}, R)$ is a unitary up to a factor representation of $\mathcal{G}_0$ on $\mathfrak{H}$. This is the result (2.12), now obtained

only by symmetry considerations. The results on $\mathcal{U}_{\underline{\underline{L}}}((\tau, \underline{0}, \underline{0}, I))$ obtained in 2B with assumption (a) now follow from assumption:

(a_g) $\underline{\underline{K}}$ is such that if $(b, \alpha) \in \underline{\underline{K}}$, also

$(b + \tau, \alpha_{(-\tau, \underline{0}, \underline{0}, I)}) \in \underline{\underline{K}}$, $\quad \forall b \geq 0$.

From our discussion the following new feature arises for the description of space–time symmetries in quantum mechanics: The usual requirement that space–time translations are represented by unitary operators on the Hilbert space of the system is a not well-motivated restriction; instead one should consider timelike translations into the past of preparations ("states", statistical operators) given by positive linear endomorphisms of $\tau c(\mathfrak{H})$ and timelike translations into the future of the effects given by the adjoints of these mappings. In such a way one has a more fundamental motivation for the use of "dynamical semigroups" considered, e.g., by Kossakowsky.[12] In such a more general context, energy–momentum conservation (energy conservation in the Galilean case) is an additional requirement. We stress, however, that what one calls experimentally energy–momentum conservation in a process concerns only ingoing and outgoing states, so that energy–momentum conservation should become an asymptotic condition in this theory. We observe that axiom (2.3) in the characterization I becomes less and less restrictive for increasing separation between the preparation and the effect parts, so that one can expect that by a more accurate formalization of axiom (2.3) symmetry under space–time translation is again relevant for energy–momentum conservation.

3. IRREDUCIBLE REPRESENTATION OF $\mathcal{P}^{\uparrow}_{+s_+}$ FOR AN UNSTABLE PARTICLE

Let us consider first the case of a stable particle: The space–time symmetry of such a system can be described as in Sec. 2A and, since one expects that symmetry alone determines the description, one requires that the representation (2.7) of $\mathcal{P}^{\uparrow}_{+}$ ($\mathcal{G}_0$) on $\mathfrak{H}$ is irreducible; then one chooses on physical grounds representations characterized by a finite spin j and a nonnegative mass m. If one does not assume *a priori* that the particle is stable, the characterization 2A is too restrictive and 2B or 2C must be used instead. We shall refer to 2C.

One expects that the pure kinematical behavior of one (in general unstable) particle can be still characterized by symmetry consideration alone.

Let $\underline{\underline{M}}^{(1)}$ be the set of experiments concerning the pure kinematics, i.e., no observations on possible decay products are made. For the set $\underline{\underline{M}}^{(1)}$ in the case of an unstable particle the axioms of Ludwig and the condition (a_τ) [(a_g)] are incompatible: e.g., (2.2) cannot be satisfied for $\underline{\underline{V}} = (b_u, \alpha)$ if α is removed to far into the past. One expects, however, that the axioms of Ludwig and symmetry considerations 2C without condition (a_τ) [(a_g)] hold for $\underline{\underline{M}}^{(1)}$ so that one can take the result (2.15) for $\mathcal{U}((0, \Lambda))$ [(2.22) for $\mathcal{U}((0, \underline{a}, \underline{v}, R))$]. Since the theory for an unstable particle should be a possibly straightforward generalization of the theory for a stable particle, one is led to assume that $\mathcal{U}_{\underline{\underline{L}}}((a, I))$ preserves equivalence classes in $\underline{\underline{L}}$, induces an affine mapping $\mathcal{U}_{\underline{L}}((a, I))$ on $\underline{L}$, so that it can be extended by linearity on $\mathbb{B}(\mathfrak{H})$; finally taking into account the Hilbert space structure of the theory, let us assume the following structure in the relativistic case,

$$\mathcal{U}((a, I))Y = U(a) Y U^{+}(a),$$

$$\forall Y \in \mathbb{B}(\mathfrak{H}), \ \forall a^2 \geq 0, \ a^0 \geq 0,$$

and in the Galilean case,

$$\mathcal{U}((b, \underline{0}, \underline{0}, I))Y = U(b) Y U^{+}(b),$$

$$\forall Y \in \mathbb{B}(\mathfrak{H}), \ \forall b \geq 0,$$

where $U(a)$ and $U(b)$ are linear contractive operators on $\mathfrak{H}$.

Defining $U((a, \Lambda)) =: U(a)U(\Lambda)$, $U((b, \underline{a}, \underline{v}, R)) =: U(b)U(\underline{a}, \underline{v}, R)$, one has then a (generally) nonunitary-up-to-a-factor representation of $\mathcal{P}^{\uparrow}_{+s_+}$ ($\mathcal{G}^{\uparrow}_{+s_+}$), which, taking into account that we are describing only the kinematics of the particle, we shall assume to be irreducible.

We consider now only the relativistic case for a particle with positive mass, the Galilean one having been treated in Ref. 5, starting from a less fundamental point of view.

Let us recall that a stable particle corresponds to a unitary representation of $\mathcal{P}^{\uparrow}_{+}$ characterized by a mass m and a spin j. In the nonunitary case a systematic classification of the representations is still lacking.

A representation,[2] which is a straightforward generalization of the forementioned unitary one, is the natural candidate to be associated with an unstable particle of given mass m, spin j, and mean-life time τ_0. The Hilbert space $\mathfrak{H}$ of such a representation is

$$\mathfrak{H} = \sum_{\xi=1}^{2j+1} \oplus \mathfrak{H}^{(\xi)}$$

with $\mathfrak{H}^{(\xi)} = L^2(\mathbb{R}^3, \mathcal{M}, \mu)$, where $\mathcal{M}$ is the Lebesgue σ-algebra of $\mathbb{R}^3$, and

$$\mu(\Omega) = \int_{\Omega} d_3\underline{p} \frac{1}{(\underline{p}^2 + m^2c^2)^{1/2}}, \quad \Omega \in \mathcal{M}.$$

Indicating by $f_\xi(\underline{p})$ an element of $\mathfrak{H}$, the representation of $\mathcal{P}^{\uparrow}_{+s_+}$ is (almost everywhere in $\mathbb{R}^3$)[13]:

$$(U((a, \Lambda))f)_\xi(\underline{p}) = \sum_{\xi'} \exp[i/\hbar)(1 + i\gamma)a \cdot p] Q_{\xi\xi'}(\Lambda, \underline{p}) f_{\xi'}(\underline{p}'), \tag{3.1}$$

with

$$p_0 = +(\underline{p}^2 + m^2c^2)^{1/2}, \quad \gamma = \frac{1}{2}\frac{\lambda}{\tau_0 c}, \quad \lambda = \frac{\hbar}{mc},$$

$$p = (p_0, \underline{p}), \quad p' = \Lambda^{-1}p,$$

$$Q(\Lambda, \underline{p}) = D^{(j)}(B^{-1}(p)\,\Lambda\,B(\Lambda^{-1}p)), \tag{3.2}$$

where $B(p)$ is the boost[14] transforming the 4-vector $(m, 0, 0, 0)$ into p and $D^{(j)}$ is the $(2j+1)$-dimensional representation of $SU(2)$. To simplify the notation, we have always indicated the elements Λ of the homogeneous Lorentz group instead of the corresponding element of $SL(2, \mathbb{C})$. We shall see that in this frame-

work a completely satisfactory description of a single particle system can be given.

For stable particle one associates also a linear "wave equation" to the particle (e. g., Klein—Gordon, Dirac equation). Such equations do not add anything to the description of the particle, but become relevant if considered as classical field equations. In fact the quantization of such fields provides the theory for systems of many particles and antiparticles. The correspondence between the quantum mechanical description of the particle and the classical field description is the following: There is a mapping $\mathfrak{M}$ of the Hilbert space $\mathfrak{H}$ onto a suitable set of solutions of the wave equation such that the wavefunction transforms as follows:

$$(\tilde{U}((a,\Lambda))\varphi)_\xi(x) = \sum_{\xi'} D_{\xi\xi'}(\Lambda)\varphi_{\xi'}(\Lambda^{-1}(x-a)), \tag{3.3}$$

where

$$\tilde{U}((a,\Lambda))\mathfrak{M} = \mathfrak{M}U((a,\Lambda)) \tag{3.4}$$

and $D(\Lambda)$ is a representation of the homogeneous Lorentz group. [14]

In the case of unstable particle one can find an analogous mapping $\mathfrak{M}$ and write Eqs. (3.3), (3.4) with the only difference being that the wavefunction is defined only in the forward light cone and that in (3.3) $a^2 \geq 0$, $a_0 \leq 0$ and that $U((a,\Lambda))$ on the rhs of Eq. (3.4) must be replaced by $U^+((-\Lambda^{-1}a, \Lambda^{-1}))$ with $a^2 \geq 0$, $a_0 \leq 0$. In fact one looks for the correspondence in the Schrödinger picture; in such a picture one has, with our characterization of space—time symmetries, only timelike translations into the past. We give explicitly the mapping $\mathfrak{M}$ in the case of a spinless particle:

$$\varphi(x) = \mathfrak{M}\psi =: \int d_3\underline{p} \frac{1}{(\underline{p}^2 + m^2c^2)^{1/2}} \exp[-(i/\hbar)(1 - i\gamma)p \cdot x]\psi(\underline{p}),$$
$$\psi \in \mathfrak{H}, \quad x^2 \geq 0, \quad x_0 \geq 0 \tag{3.5}$$

$\varphi(x)$ is a "positive frequency" solution of the Klein—Gordon equation with "complex mass."

4. PHYSICAL INTERPRETATION OF THE SINGLE PARTICLE THEORY

The key point of the physical interpretation of the theory of a single particle is the definition of the observables momentum and position. Usually an observable is associated with a self-adjoint operator. However, such an association is rather a consequence of a more fundamental mathematical characterization of an observable, as it has been stressed particularly by Ludwig. [4] An observable is a field of "coexistent" effects; such a field yields in the Hilbert space realization a measure with values in the $[0, \mathbb{1}]$ interval of $\mathbb{B}(\mathfrak{H})$. In particular, if the measure is projection-valued, it generates an Abelian algebra of self-adjoint operators. Such operators are then called observables.

Let us consider first the case of a stable particle. To define a position observable at time t, one looks for a projection-valued measure $E_{x_0}(\Omega)$ on the Borel σ-algebra of $\mathbb{R}_3$. The effect $E_{x_0}(\Omega)$ corresponds to the following property: The particle is at time $t = x_0/c$ inside the region Ω. Since in our scheme the effects are inside the future light cone, one considers only regions Ω such that, for $\underline{x} \in \Omega$, $|\underline{x}| \leq ct$. By its physical interpretation $E_{x_0}(\Omega)$ must transform in the following obvious way under rotations and space—time translations:

$$U((a,R))E_{x_0}(\Omega)U^+((a,R)) = E_{x_0+a_0}(\Omega'), \tag{4.1}$$

where $\Omega' =: \{\underline{x}' \mid \underline{x}' = R\underline{x} + \underline{a}, \underline{x} \in \Omega\}$.

The family $E_{x_0}(\Omega)$, which satisfies Eq. (4.1), is given explicitly by

$$E_{x_0}(\Omega) =: U((x_0, \underline{0}; I))E(\Omega)U^+((x_0, \underline{0}; I)) \tag{4.2}$$

with

$$E(\Omega) =: P_0^{1/2}\mathcal{J}^{-1}\tilde{E}(\Omega)\mathcal{J}P_0^{-1/2},$$

where

$$\begin{aligned}
&(\tilde{E}(\Omega)f)_\xi(\underline{p}) =: X_\Omega(\underline{p})f_\xi(\underline{p}),\\
&(\mathcal{J}f)_\xi(\underline{x}) =: \frac{1}{(2\pi\hbar)^{3/2}} \int d_3\underline{p} \exp[(i/\hbar)\underline{p} \cdot \underline{x}]f_\xi(\underline{p}),\\
&(\mathcal{J}^{-1}f)_\xi(\underline{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d_3\underline{x} \exp[-(i/\hbar)\underline{p} \cdot \underline{x}]f_\xi(\underline{x}),\\
&(P_0 f)_\xi(\underline{p}) =: p_0 f_\xi(\underline{p}).
\end{aligned} \tag{4.3}$$

In the theory of a stable particle according to description I, in which effects are not restricted to the future light cone, $E(\Omega)$ can be interpreted as the measure associated with the position operator $\hat{\underline{x}}$ at time $t = 0$:

$$(\hat{\underline{x}}f)_\xi(\underline{p}) =: i\hbar\left(\frac{\partial}{\partial_f} - \frac{f}{2(\underline{p}^2 + m^2c^2)}\right) f_\xi(\underline{p}). \tag{4.4}$$

Such position operator does not transform in a covariant way under velocity transformations. This is in no way a difficulty since the physical interpretation of the spectral measure of $\hat{\underline{x}}$ requires only the transformation property (4.1).

A momentum observable at time $t = x_0/c$ is a projection valued measure $\tilde{E}_{x_0}(\Omega)$ on the Borel σ-algebra of $\mathbb{R}_3$ with the following physical interpretation of $\tilde{E}_{x_0}(\Omega)$: the particle has at time t momentum $\underline{p} \in \Omega$. Then $\tilde{E}_{x_0}(\Omega)$ must transform in the following way:

$$U((a,\Lambda))\tilde{E}_{x_0}(\Omega)U^+((a,\Lambda)) = \tilde{E}_{x_0}(\Omega'), \tag{4.5}$$

where

$$\Omega' =: \left\{\underline{p}' \,\middle|\, \underline{p}'_k = \sum_1^3 \Lambda_k^l p_l + \Lambda_k{}^0(\underline{p}^2 + m^2c^2)^{1/2}, \; K = 1,2,3, \; \underline{p} \in \Omega\right\}.$$

$\tilde{E}_{x_0}(\Omega)$ is given explicitly by

$$\tilde{E}_{x_0}(\Omega) = \tilde{E}(\Omega), \tag{4.6}$$

where $\tilde{E}(\Omega)$ is given by (4.3).

Obviously the selfadjoint operators $\hat{\underline{p}}$ related to $\tilde{E}(\Omega)$ are

$$(\hat{\underline{p}}f)_\xi(\underline{p}) = \underline{p}f_\xi(\underline{p}). \tag{4.7}$$

The operators $\hat{\underline{x}}$ and $\hat{\underline{p}}$ obey the canonical commutation relations. It is useful to introduce a coarse grained position-momentum observable, which is more adherent to the actual measurements of position and momentum of a particle: It is given by the field of coexistent effects generated by the following projections:

$$E_{x_0}(\underline{n}, \underline{r}) =: U(\underline{x}_0, \underline{0}; I)E(\underline{n}, \underline{r})U^+(x_0, \underline{0}; I),$$

$$(E(\underline{n},\underline{r})f)_{\underline{\varepsilon}}(\underline{p}) =: u^{(\underline{n},\underline{r})}(p)\int d_3\underline{p}'\frac{1}{(\underline{p}'^2+m^2c^2)^{1/2}} \times u^{(\underline{n},\underline{r})}(\underline{p}')f_{\underline{\varepsilon}}(\underline{p}'), \tag{4.8}$$

$$u^{(\underline{n},\underline{r})}(\underline{p}) =: \exp[-(i/\hbar)\underline{p}\cdot\underline{x}_{\underline{n}}]\frac{1}{(\Delta p)^{3/2}}\chi_{\underline{r}}(\underline{p})(\underline{p}^2+m^2c^2)^{1/4},$$

where $\chi_{\underline{r}}(\underline{p})$ is the characteristic function of the cube $\Omega_{\underline{r}}$ of volume $(\Delta p)^3$ centered in $\underline{p}_{\underline{r}}=\underline{r}\Delta p$ $(r_i=0,\pm1, \pm2,\cdots,\ i=1,2,3)$ and $\underline{x}_{\underline{n}}=(2\pi/\Delta p)\hbar\underline{n}$ $(n_i=0,\pm1,\pm2,\cdots, i=1,2,3)$.

The effect $E_{x_0}(\underline{n},\underline{r})$ corresponds to the following property: The particle at time $t=x_0/c$ has momentum $\underline{p}\in\Omega_{\underline{r}}$ and is somewhere in a region around $\underline{x}_{\underline{n}}$ with volume $\sim\hbar^3/(\Delta p)^3$. Such an interpretation is possible since

$$\sum_{\underline{n},\underline{r}} E_{x_0}(\underline{n},\underline{r}) = \mathbb{1}. \tag{4.9}$$

Obviously $E_{x_0}(\underline{n},\underline{r})$ is a meaningful effect if $|\underline{x}_{\underline{n}}|<x_0$. In the case of an unstable particle, due to the way in which $U((a,\Lambda))$ depends on γ, one is led to consider the following sets of operators:

$$F_{x_0}(\Omega) =: \exp[(i/\hbar)x_0(1+i\gamma)P_0]P_0^{1/2}\mathcal{J}_\gamma^+\tilde{E}(\Omega) \times\mathcal{J}_\gamma P_0^{-1/2}\exp[-(i/\hbar)x_0(1-i\gamma)P_0] \tag{4.10}$$

with

$$(\mathcal{J}_\gamma f)_{\underline{\varepsilon}}(\underline{x}) =: \frac{1}{(2\pi\hbar)^{3/2}}\int d_3\underline{p}\exp[(i/\hbar)(1-i\gamma)\underline{p}\cdot\underline{x}]f(\underline{p}),$$

$$(\mathcal{J}_\gamma^+ f)_{\underline{\varepsilon}}(\underline{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d_3\underline{x}\exp[-(i/\hbar)(1+i\gamma)\underline{p}\cdot\underline{x}]f(\underline{x}),$$

Ω such that $\underline{x}\in\Omega\Rightarrow|\underline{x}|<x_0$;

$$\tilde{F}_{x_0}(\Omega) =: \exp[-(2/\hbar)\gamma x_0 P_0]\tilde{E}(\Omega), \tag{4.11}$$

$$(F_{x_0}(\underline{n},\underline{r})f)_{\underline{\varepsilon}}(\underline{p}) =: u_{x_0,\gamma}^{(\underline{n},\underline{r})}(\underline{p})\int d_3\underline{p}'\frac{1}{(\underline{p}'^2+m^2c^2)^{1/2}} \times\overline{u_{x_0,\gamma}^{(\underline{n},\underline{r})}(\underline{p}')}f_{\underline{\varepsilon}}(\underline{p}'), \tag{4.12}$$

$$u_{x_0,\gamma}^{(\underline{n},\underline{r})}(\underline{p}) =: \exp[-(i/\hbar)(1+i\gamma)(\underline{p}\cdot\underline{x}_{\underline{n}}-p_0x_0)]\frac{1}{(\Delta p)^{3/2}} \times\chi_{\underline{r}}(\underline{p})(\underline{p}^2+m^2c^2)^{1/4}.$$

However, there is no evidence that Eq. (4.10) defines an operator $<\mathbb{1}$. On the other hand, one expects that a localization in arbitrarily small regions is not possible for an unstable particle which one describes in a modelistic way as a "resonance" of stable particles.

There is no problem in connection to (4.11): It defines the field of coexistent effects of the observable "momentum." The effects $\tilde{F}_{x_0}(\Omega)$ are not projections.

The operators $F_{x_0}(\underline{n},\underline{r})$ are effects; in fact:

$$(f,F_{x_0}(\underline{n},\underline{r})f) = \sum_{\xi=1}^{2j+1}\left|\int d_3\underline{p}\frac{1}{(\underline{p}^2+m^2c^2)^{1/2}} \times\overline{u_{x_0,\gamma}^{(\underline{n},\underline{r})}(\underline{p})}f_{\underline{\varepsilon}}(\underline{p})\right|^2$$
$$= \sum_{\xi=1}^{2j+1}\int d_3\underline{p}\frac{1}{(\underline{p}^2+m^2c^2)^{1/2}} \times\exp[(2/\hbar)(\underline{p}\cdot\underline{x}_{\underline{n}}-p_0x_0)\gamma]\,|f_{\underline{\varepsilon}}(\underline{p})|^2$$
$$\times\int d_3\underline{p}\frac{1}{(\Delta p)^3}\chi_{\underline{r}}(\underline{p})$$
$$\leq\|f\|^2,\quad\forall f\in\ . \tag{4.13}$$

They provide the expected kinematical description for the unstable particle. In fact let us evaluate the expression $(f,F_{x_0}(\underline{n},\underline{r})f)$ given by Eq. (4.13), using the method of the stationary phase. Let us choose $f_{\underline{\varepsilon}}(\underline{p})$ peaked in $\underline{p}=\underline{p}_{\underline{r}_0}$, such that its phase is practically constant; then the condition of stationary phase, which selects the effects which have the highest frequency, is

$$\underline{x}_{\underline{n}}-\underline{p}_{\underline{r}}x_0/(\underline{p}_{\underline{r}}^2+m^2c^2)^{1/2}=0. \tag{4.14}$$

For the effect $F_{x_0}(\underline{n},\underline{r}_0)$, with $x_0,\underline{n},\underline{r}_0$ satisfying Eq. (4.14), one has

$$(f,F_{x_0}(\underline{n},\underline{r})f) = \sum_{\xi=1}^{2j+1}\left|\int d_3\underline{p}\exp[(\gamma/\hbar)(\underline{p}\underline{x}_{\underline{n}}-p_0x_0)\frac{\chi_{\underline{r}}(\underline{p})}{(\Delta p)^3} \times\frac{\exp[(i/\hbar)(\underline{p}\underline{x}_{\underline{n}}-p_0x_0)]f_{\underline{\varepsilon}}(\underline{p})}{(\underline{p}^2+m^2c^2)^{1/4}}\right|^2$$
$$\approx\exp[(2\gamma/\hbar)(\underline{p}_{\underline{r}_0}\cdot\underline{x}_{\underline{n}}-(\underline{p}_{\underline{r}_0}^2+m^2c^2)^{1/2}x_0)] \times\sum_{\xi=1}^{2j+1}\left|\int d_3\underline{p}\frac{\chi_{\underline{r}}(\underline{p})}{(\Delta p)^3}\frac{\exp[(i/\hbar)(\underline{p}\underline{x}_{\underline{n}}-p_0x_0)f_{\underline{\varepsilon}}(\underline{p})}{(\underline{p}^2+m^2c^2)^{1/4}}\right|^2. \tag{4.15}$$

Equations (4.14) and (4.15) give the expected kinematical description of an unstable particle with mass m and mean-life time $\tau_0=1/2\gamma m$. The effects $F_{x_0}(\underline{n},\underline{r})$ generate a field of coexistent effects if for any subset I of vectors $(\underline{n},\underline{r})$ such that $|\underline{x}_{\underline{n}}|<x_0$, one has

$$\sum_{(\underline{n},\underline{r})\in I}F_{x_0}(\underline{n},\underline{r})\leq\mathbb{1}. \tag{4.16}$$

Such field defines a coarse-grained position-momentum observable. Condition (4.16) is immediately verified if the effect $F_{x_0}(\underline{n},\underline{r})$ is replaced by $F'_{x_0}(\underline{n},\underline{r})$ defined as follows:

$$(F'_{x_0}(\underline{n},\underline{r})f)_{\underline{\varepsilon}}(\underline{p}) =: u_{x_0}^{(\underline{n},\underline{r})}(\underline{p})\exp\{(2\gamma/\hbar)[\underline{p}_{\underline{r}}\cdot\underline{x}_{\underline{n}}-(\underline{p}_{\underline{r}}^2+m^2c^2)^{1/2}x_0]\} \times\int d_3f'\overline{\mu_{x_0}^{(\underline{n},\underline{r})}}(f')\frac{f_{\underline{\varepsilon}}(f')}{(f'^2+m^2c^2)^{1/2}} \tag{4.17}$$
$$u_{x_0}^{(\underline{n},\underline{r})}(\underline{p}) =: \exp(ip_0x_0)u^{(\underline{n},\underline{r})}(\underline{p}).$$

On the other hand one can see that expression $\sum_{\underline{n},\underline{r}}|(f,[F_{x_0}(\underline{n},\underline{r})-F'_{x_0}(\underline{n},\underline{r})]f)|$ becomes arbitrarily small, uniformly with respect to f, by choosing Δp small enough.

One can give a connection between the effects (4.12) and the operators (4.10), by which the practical use of the latter can be justified under suitable conditions. In fact let us take a state f, where $f_{\underline{\varepsilon}}(\underline{p})=\chi_{\underline{r}}(\underline{p})f_{\underline{\varepsilon}}(p)$ and let us consider the effect $F'_{x_0}(\Omega) =: \sum_{\underline{n},\underline{r},\underline{x}_{\underline{n}}\in\Omega}F_{x_0}(\underline{n},\underline{r})$, where Ω is a region such that $\underline{x}\in\Omega\Rightarrow|\underline{x}|\leq x_0$. One has

$$(f,F'_{x_0}(\Omega)f) = \sum_{\underline{n},\underline{r},\underline{x}_{\underline{n}}\in\Omega}\frac{1}{(\Delta p)^3}\sum_{\xi=1}^{2j+1}\left|\int_\Omega d_3\underline{p}\exp[(i/\hbar)(1+i\gamma)(\underline{p}\underline{x}_{\underline{n}}-p_0x_0)] \times\frac{1}{(\underline{p}^2+m^2c^2)^{1/4}}f_{\underline{\varepsilon}}(\underline{p})\right|^2 \tag{4.18}$$
$$\approx\sum_{\xi=1}^{2j+1}\int d_3\underline{x}\left|\frac{1}{(2\pi\hbar)^{3/2}}\int d_3\underline{p}\exp[(i/\hbar)(1+i\gamma)(\underline{p}\cdot\underline{x}-p_0x_0)]\right.$$

$$\times \frac{1}{(\underline{p}^2 + m^2c^2)^{1/4}} f_\xi(\underline{p}) \Big|^2 = (f, F_{x_0}(\Omega) f),$$

where $F_{x_0}(\Omega)$ is defined in (4.10); Δp must be chosen in such a way that $F'_{x_0}(\Omega) \leq \mathbb{1}$ and the continuous approximation in (4.18) hold together. Then Eq. (4.18) defines in a natural way a position probability amplitude which coincides with the wavefunction (1.1) introduced, e.g., by Zwanziger and Schulman.

The observable related to momentum and to position which we have introduced are coexistent with the spin observables, e.g., S_z defined by the field, generated by the following effects,

$$(F_{x_0}(\xi) f)_\xi(\underline{p}) = \exp[-(2\gamma/\hbar) p_0 x_0] \delta_{\xi\xi} f_\xi(\underline{p}), \quad \xi = 1, 2, \ldots, 2j+1, \tag{4.19}$$

so that, e.g., the observable "coarse grained position-momentum and S_z" is associated with the effects

$$F_{x_0}(\underline{n}, \underline{r}; \xi) = : U(x_0, \underline{0}; I) F(\underline{n}, \underline{r}; \xi) U^+(x_0, \underline{0}; I),$$

$$F(\underline{n}, \underline{r}; \xi) = F_0(\underline{n}, \underline{r}) \cdot F_0(\xi).$$

[1] D. Zwanziger, Phys. Rev. 131, 2818 (1963).
[2] L.S. Schulman, Ann. Phys. 59, 201 (1970).
[3] M. Simonius, Helv. Phys. Acta 43, 223 (1970).
[4] G. Ludwig, *Lecture Notes in Physics n.*4 (Springer-Verlag, Berlin, 1970).
[5] L. Lanz, L.A. Lugiato, and G. Ramella, Int. Theor. Phys. 8, (5), 341 (1973).
[6] H.H. Schaefer, *Topological Vector Spaces* (Springer-Verlag, Berlin, 1970).
[7] K. Yosida, *Functional Analysis* (Springer-Verlag, Berlin 1971).
[8] We refer to 2B, where (2.7) is discussed in a more general context.
[9] Such a characterization is given by Ludwig in Ref. 4, p. 186—87; see also A. Hartkämper, in *Lecture Notes in Physics* 29 (Springer-Verlag, Berlin, 1974).
[10] G. Ludwig, "Notes in Mathematical Physics (1971)," NMP4 Marburg.
[11] Such results about $J(g)$ and $J(g^{-1})$ refer essentially to the following structure of the spaces $\tau c(\mathfrak{H})$ and $\mathbb{B}(\mathfrak{H})$: they are a dual pair of Banach spaces B, B', $\tau c(\mathfrak{H})$ being a base norm space, $\mathbb{B}(\mathfrak{H})$ its dual order unit space; $\underline{K}$ is norm dense in the base K of B and L is $\sigma(B', B)$ dense in the $[0, 1]$ order interval of B'. Such structure does not require the underlying Hilbert space .
[12] A. Kossakowsky, Rep. Math. Phys. 3, 247 (1972); Bull. Acad. Polon des Sciences 20, 1021 (1972).
[13] $U((a, \Lambda))$ is a representation of $\mathcal{P}^\uparrow_{+4}$ on $\mathfrak{H}$: the set of operators $U((a, \Lambda))$ can be "extrapolated" on the group $\mathcal{P}^\uparrow_+$ by the rhs of Eq. (3.1) in which a_μ is an arbitrary 4-vector; however, such extrapolated operators are unbounded and give a representation of $\mathcal{P}^\uparrow_+$, e.g., on the linear manifold of elements f with bounded support.
[14] G. Parravicini and A. Sparzani, Nuovo Cimento A 66, 579 (1970).

Correction terms for Padé approximants

M. F. Barnsley

School of Mathematics, Bradford University, England
(Received 7 May 1974)

Let $f(x)$ be a function of the form $f(x) = \int_0^\infty d\varphi(u)/(1+ux)$, $x \geq 0$, where $\varphi(u)$ is of bounded variation and piecewise differentiable on $0 \leq u < \infty$; and suppose that the $[N-1/N]$ and $[N/N]$ Padé approximants (PA's) to $f(x)$ can be constructed. Then correction terms $b_N(x)$ and $c_N(x)$ such that $[N-1/N]-b_N(x) \leq f(x) \leq [N/N]+c_N(x)$, $x \geq 0$, are considered. Suitable corrections are shown to have the structure $x^{2N}\{\text{positive constant}\}/\{\text{denominator of corresponding PA}\}^2$. The nature of the constants is examined: They vanish when $f(x)$ is a series of Stieltjes, and given appropriate information about $f(x)$ they can be calculated. Applications are considered.

I. INTRODUCTION

In this paper we consider the following problem: Suppose $f(x)$ is a function of the form

$$f(x)=\int_0^\infty \frac{d\varphi(u)}{(1+ux)}, \quad x \geq 0, \tag{1.1}$$

where $\varphi(u)$ is of bounded variation and piecewise differentiable on $0 \leq u < \infty$; and suppose that the $[N\text{-}1/N]$ and $[N/N]$ Padé approximants (PA's) to $f(x)$ can be constructed. Then we ask if it is possible to evaluate *correction terms* $b_N(x)$ and $c_N(x)$ such that

$$[N-1/N]-b_N(x) \leq f(x) \leq [N/N]+c_N(x), \quad x \geq 0. \tag{1.2}$$

We will establish explicit formulas for such corrections. Except for a constant multiplier, at fixed N, these use the same information as is used to construct the PA's themselves. Given certain additional information about $f(x)$, the requisite constants can be evaluated.

The motivation for this investigation is that in the case $f(x)$ is a series of Stieltjes, which corresponds to $\varphi(u)$ being a bounded monotone *nondecreasing* function in (1.1), we have the inequalities[1]

$$[N-1/N] \leq f(x) \leq [N/N], \quad x \geq 0. \tag{1.3}$$

These bounds have many applications[2] both because they are in practice usually found to be tight and because they require a relatively small amount of information about $f(x)$, namely the first $2N+1$ terms in the asymptotic expansion of $f(x)$ at $x=0$. One is led to expect that the PA's themselves in (1.2) will be good approximations to $f(x)$ and to hope that relatively small corrections can be found. Since functions of the form (1.1) occur even more often than series of Stieltjes, the nature of simple correction terms such that (1.2) is true is interesting, and explicit formulas for them should find many uses.

Our approach involves a bivariational bounding technique described recently by Barnsley and Robinson.[3] In Sec. 2 we construct a real Hilbert space $\mathfrak{H}$ with symmetric inner product $\langle\ ,\ \rangle$, a pair of vectors ξ and η in $\mathfrak{H}$, and a positive, self-adjoint linear operator L in $\mathfrak{H}$, such that

$$f(x)=\langle \xi, (1+xL)^{-1}\eta\rangle, \quad x \geq 0. \tag{1.4}$$

This latter quantity is in a suitable form for bounding by means of bivariational functionals. In Sec. 3 we show how formulas of the form (1.2) are obtained by choosing appropriate trial vectors in the functionals. We obtain the central result that *the correction terms each have the structure*

$$\frac{x^{2N}\{\text{positive constant}\}}{\{\text{denominator of corresponding PA}\}^2}. \tag{1.5}$$

We show that the constants vanish when $f(x)$ is a series of Stieltjes, thus reducing the bounds (1.2) to the usual PA ones in this case.

In Sec. 4 we consider the evaluation of the constants in the correction terms. We find that the necessary constants may be calculated explicitly provided we know two sets of numbers, $\{f_n\}_{n=0}^{2N}$ and $\{F_n\}_{n=0}^{2N}$. The former are simply coefficients from the formal expansion of $f(x)$ about $x=0$, written

$$f(x)=\sum_{n=0}^{\infty}(-x)^n f_n, \tag{1.6}$$

so that

$$f_n=\int_0^\infty u^n d\varphi(u), \quad n=0,1,\cdots. \tag{1.7}$$

These numbers are precisely the ones used to construct the $[N-1/N]$ and $[N/N]$ PA's to $f(x)$ (see below). The second set of numbers, $\{F_n\}_{n=0}^{2N}$, are coefficients from the formal expansion of the function

$$F(x)=\int_0^\infty \frac{|d\varphi(u)|}{(1+ux)}=\sum_{n=0}^{\infty}(-x)^n F_n, \tag{1.8}$$

so that

$$F_n=\int_0^\infty u^n |d\varphi(u)|, \quad n=0,1,\cdots, \tag{1.9}$$

where $|d\varphi(u)|$ denotes the absolute value of the increment $d\varphi(u)$.

Requiring the latter numbers is clearly too stringent a condition to be useful in most cases. However, in Sec. 4B we show that the set $\{F_n\}_{n=0}^{2N}$ may often be replaced by a new set of numbers $\{\tilde{F}_n\}_{n=0}^{2N}$, obtained as follows. Let $\theta(u)$ be any function such that

$$d\theta(u) \geq |d\varphi(u)|, \quad \text{for all } 0 \leq u < \infty. \tag{1.10}$$

By this notation we mean that $\theta'(u) \geq |\varphi'(u)|$ on all intervals where the derivative $\varphi'(u)$ exists and that $\theta(u)$ has a larger positive "jump" than the magnitude of the jump in $\varphi(u)$ at each point of discontinuity of $\varphi(u)$. Then the $\tilde{F}_n$'s are given by

$$\tilde{F}_n=\int_0^\infty u^n d\theta(u), \quad n=0,1,\cdots, \tag{1.11}$$

which should be compared with (1.9). We assume that the requisite $\tilde{F}_n$'s are finite.

When all is established, we see that *one is often able to use PA's plus correction terms to derive bounds on functions of the form* (1.1) *in much the same way as*

PA's are usually used to bound series of Stieltjes: The point is that the additional information needed, the $\tilde{F}_n$'s, is usually accessible. In Sec. 5 we test the method with an example, and briefly consider applications and extensions.

For reference later on we give the definition and formula for the $[M/N]$ PA to $f(x)$. The approximant take the form of a polynomial of degree M divided by one of degree N. The coefficients, not all zero, are obtained by equating powers of x in the equation

$$\left(\sum_{n=0}^{M+N}(-x)^n f_n\right) Q(x) - P(x) = O(x^{M+N+1}), \tag{1.12}$$

where $P(x)/Q(x)$ is the $[M/N]$ PA to $f(x)$. Provided that $D(M-N+1, N-1) \neq 0$ we have[4]

$$[M/N] = \sum_{j=0}^{M-N}(-x)^j f_j - (-x)^{M-N+1} \times \frac{\begin{vmatrix} 0 & f_{M-N+1} & \cdots & f_M \\ f_{M-N+1} & (f_{M-N+1}+xf_{M-N+2}) & \cdots & (f_M+xf_{M+1}) \\ \vdots & & & \\ f_M & (f_M+xf_{M+1}) & \cdots & (f_{M+N-1}+xf_{M+N}) \end{vmatrix}}{\begin{vmatrix} (f_{M-N+1}+xf_{M-N+2}) & \cdots & (f_M+xf_{M+1}) \\ \vdots & & \\ (f_M+xf_{M+1}) & \cdots & (f_{M+N-1}+xf_{M+N}) \end{vmatrix}} \tag{1.13}$$

and the approximant displays the familiar property

$$f(x) - [M/N] = O(x^{M+N+1}). \tag{1.14}$$

In the above we have the persymmetric determinants[5]

$$D(m,n) = \begin{vmatrix} f_m & f_{m+1} & \cdots & f_{m+n} \\ f_{m+1} & f_{m+2} & \cdots & f_{m+n+1} \\ \vdots & \vdots & & \\ f_{m+n} & f_{m+n+1} & \cdots & f_{m+2n} \end{vmatrix}, \tag{1.15}$$

and we adopt the convention $f_j = 0$ for $j < 0$. For simplicity we assume throughout that

$$D(0, N-1) \neq 0 \quad \text{and} \quad D(1, N-1) \neq 0, \tag{1.16}$$

thereby ensuring the validity of (1.13) in the case of $[N-1/N]$ and $[N/N]$ PA's. We will use the notation

$$Q_{[M/N]}(x) = \begin{vmatrix} (f_{M-N+1}+xf_{M-N+2}) & \cdots & (f_M+xf_{M+1}) \\ \vdots & & \vdots \\ (f_M+xf_{M+1}) & \cdots & (f_{M+N-1}+xf_{M+N}) \end{vmatrix} \tag{1.17}$$

for the polynomial in the denominator of the $[M/N]$ PA.

2. BIVARIATIONAL BOUNDS FOR $f(x)$

A. Construction of a representation $f(x) = \langle \xi, (1+xL)^{-1}\, \eta \rangle$

Here we construct[6] a real Hilbert space $\mathfrak{H}$ with symmetric inner product $\langle\ ,\ \rangle$, a pair of vectors ξ and η in $\mathfrak{H}$, and a positive self-adjoint operator L in $\mathfrak{H}$, such that $f(x)$ can be written in the form (1.4).

Let $\mathfrak{H}$ be the Hilbert space $L^2[0,\infty)$ of real square integrable functions on $[0,\infty)$, with the symmetric inner product

$$\langle \zeta_1, \zeta_2 \rangle = \int_0^\infty \zeta_1(u)\,\zeta_2(u)\,du, \qquad \zeta_1 \text{ and } \zeta_2 \text{ in } \mathfrak{H}. \tag{2.1}$$

Now let L be the linear operator in $\mathfrak{H}$ defined by[7]

$$L\zeta(u) = u\zeta(u), \quad \zeta \in \mathcal{D}(L). \tag{2.2}$$

Here $\mathcal{D}(L)$ is the domain of L, and consists of all ζ in $\mathfrak{H}$ such that

$$\|L\zeta\|^2 = \langle L\zeta, L\zeta \rangle = \int_0^\infty \{u\zeta(u)\}^2\, du < \infty; \tag{2.3}$$

$\mathcal{D}(L)$ can be shown to be dense in $\mathfrak{H}$. It is then readily established that L is both positive and self-adjoint. We have, for example,

$$\langle \zeta, L\zeta \rangle = \int_0^\infty u\{\zeta(u)\}^2\, du > 0 \quad \text{for } \zeta \neq 0,\ \zeta \in \mathcal{D}(L), \tag{2.4}$$

and

$$\langle \zeta_1, L\zeta_2 \rangle = \int_0^\infty \zeta_1(u)\, u\zeta_2(u)du = \langle L\zeta_1, \zeta_2 \rangle,$$
$$\zeta_1 \text{ and } \zeta_2 \text{ in } \mathcal{D}(L). \tag{2.5}$$

In particular, the operator $(1+xL)^{-1}$, $x \geq 0$, is a bounded, linear, self-adjoint operator whose domain is the whole of $\mathfrak{H}$.[8] Its operation is simply

$$(1+xL)^{-1}\ \zeta(u) = (1+xu)^{-1}\,\zeta(u), \quad \zeta(u) \in \mathfrak{H}. \tag{2.6}$$

The final step is to select any pair ξ and η of vectors in $\mathfrak{H}$ such that

$$\int_0^u \xi(\nu)\eta(\nu)d\nu = \int_0^u d\varphi(\nu), \quad \text{for all } 0 \leq u < \infty. \tag{2.7}$$

Suppose for the moment that this has been done. Then

$$\begin{aligned} \langle \xi, (1+xL)^{-1}\eta \rangle &= \int_0^\infty \xi(u)(1+xu)^{-1}\eta(u)du \\ &= \int_0^\infty (1+xu)^{-1}\, d\left(\int_0^u \xi(\nu)\eta(\nu)d\nu\right) \\ &= \int_0^\infty (1+xu)^{-1}\, d\left(\int_0^u d\varphi(\nu)\right) \\ &= \int_0^\infty \frac{d\varphi(u)}{(1+xu)}, \quad x \geq 0, \end{aligned} \tag{2.8}$$

which is just what we want.

The existence of vectors ξ and η in $\mathfrak{H}$ such that (2.7) is true is easily established if we assume $\varphi(u)$ is differentiable on $0 \leq u < \infty$. In this case we can choose for example

$$\eta(u) = |\varphi'(u)|^{1/2} \quad \text{and} \quad \xi(u) = \operatorname{sgn}\{\varphi'(u)\}\ |\varphi'(u)|^{1/2}, \tag{2.9}$$

where $\operatorname{sgn}\{\Gamma\}$ takes the values $+1$ and -1 according as the real number Γ is nonnegative or negative, respectively. Then these functions belong to $\mathfrak{H}$ because

$$\int_0^\infty [\eta(u)]^2\, du = \int_0^\infty [\xi(u)]^2\, du$$

$$= \int_0^\infty |\varphi'(u)|\,du = \int_0^\infty |d\varphi(u)| < \infty, \quad (2.10)$$

where we have used the property that $\varphi(u)$ is of bounded variation for $0 \leq u < \infty$. With this choice we have

$$\int_0^u \eta(\nu)\,\xi(\nu)d\nu = \int_0^u \operatorname{sgn}\{\varphi'(u)\}\,|\varphi'(u)|\,du$$

$$= \int_0^u \varphi'(u)du = \int_0^u d\varphi(u). \quad (2.11)$$

If $\varphi(u)$ has discontinuities ν_i at points $\omega_i \in [0, \infty)$, say

$$\varphi(\omega_i +) - \varphi(\omega_i) = \nu_i \neq 0 \quad (i = 0, 1, \cdots), \quad (2.12)$$

then we may adjoin the contributions

$$\sum_{i=0}^{\infty} |v_i|^{1/2}\,[\delta(u - w_i)]^{1/2},$$

$$\sum_{i=0}^{\infty} \operatorname{sgn}\{v_i\}\,|v_i|^{1/2}\,[\delta(u - w_i)]^{1/2}, \quad (2.13)$$

to $\eta(u)$ and $\xi(u)$, respectively. The inclusion of such functions in $\mathfrak{H}$, along with the use of the usual rules for evaluating integrals involving delta functions, can be rigorously justified.[9] With these additions it is readily verified that $\eta(u)$ and $\xi(u)$ satisfy (2.7) in the case where $\varphi(u)$ is piecewise differentiable.

We observe that $f(x)$ being a series of Stieltjes corresponds to the case $\xi = \eta$. Similarly, $f(x)$ is the negative of a series of Stieltjes when $\xi = -\eta$. We also note that the coefficients in the expansion of $f(x)$, as in (1.6), are related to inner products in involving powers of L and the two vectors η and ξ, by

$$\langle L^m\xi, L^n\eta\rangle = \int_0^\infty u^{m+n}\,d\varphi(u) = f_{m+n}, \quad m, n \geq 0. \quad (2.14)$$

B. Bivariational bounds

Let A be any linear self-adjoint operator in a Hilbert space $\mathfrak{H}$, such that

$$\langle \zeta, A\zeta\rangle \geq \langle \zeta, \zeta\rangle, \quad \zeta \in \mathcal{D}(A). \quad (2.15)$$

Suppose ξ and η are vectors in $\mathfrak{H}$. Then if ϕ satisfies the linear equation

$$A\phi = \xi, \quad (2.16)$$

bivariational upper and lower bounds can be imposed on the inner product $\langle \phi, \eta\rangle = \langle \xi, A^{-1}\eta\rangle$. There are *two pairs* of bounding functionals[3]:

$$\mathcal{J} + \mathcal{S} - \{S_\xi S_\eta\}^{1/2} \leq \langle \xi, A^{-1}\eta\rangle \leq \mathcal{J} + \{S_\xi S_\eta\}^{1/2} \quad (2.17a)$$

and

$$\mathcal{J} - \{S_\xi S_\eta\}^{1/2} \leq \langle \xi, A^{-1}\eta\rangle \leq \mathcal{J} + \mathcal{S} + \{S_\xi S_\eta\}^{1/2}, \quad (2.17b)$$

where

$$\mathcal{J} = \mathcal{J}(\Phi, \Psi) = -\langle \Phi, A\Psi\rangle + \langle \Phi, \eta\rangle + \langle \Psi, \xi\rangle, \quad (2.18)$$

$$S_\xi = S_\xi(\Phi) = \langle A\Phi - \xi, A\Phi - \xi\rangle,$$
$$S_\eta = S_\eta(\Psi) = \langle A\Psi - \eta, A\Psi - \eta\rangle, \quad (2.19)$$

and

$$\mathcal{S} = \mathcal{S}(\Phi, \Psi) = \langle A\Phi - \xi, A\Psi - \eta\rangle. \quad (2.20)$$

The trial vectors Φ and Ψ must belong to $\mathcal{D}(A)$, and are approximations respectively to the solutions of (2.16) and the auxiliary equation

$$A\psi = \eta. \quad (2.21)$$

We observe that the second pair of bounds may be derived from the first by using $-\xi$ in place of ξ, and then using the trial vector $-\Phi$ in place of Φ. (The need for two pairs of functionals will become clear in the next section.) By writing $\Phi = \phi + \delta\phi$ and $\Psi = \psi + \delta\psi$, the bounding properties of the functionals may be verified directly.

If we set

$$A = (1 + xL), \quad x \geq 0, \quad (2.22)$$

L being the operator discussed in Sec. 2A, then A is linear, self-adjoint, and satisfies (2.15). The functionals in (2.17) now impose upper and lower bounds on

$$\langle \xi, A^{-1}\eta\rangle = \langle \xi, (1 + xL)^{-1}\eta\rangle = f(x), \quad x \geq 0, \quad (2.23)$$

which is just what we want.

3. PADÉ APPROXIMANTS AND CORRECTION TERMS

To obtain formulas like (1.2) we will use trial vectors

$$\Phi = \Phi^N = \sum_{n=0}^{N-1} a_n L^n\xi \quad \text{and} \quad \Psi = \Psi^N = \sum_{n=0}^{N-1} b_n L^n\eta, \quad (3.1)$$

in the functionals (2.17), where the parameters a_n and b_n $(n = 0, 1, \ldots, N-1)$ have yet to be chosen. Here we assume that both ξ and η belong to $\mathcal{D}(L^n)$ for $n = 1, 2, \ldots, N$, and at the end of Sec. 4A we will show that this is assured by the assumption that F_n, defined in (1.9), is finite $(n = 1, 2, \ldots, 2N)$. Rather than choosing the parameters in the trial vectors so as to optimize the functionals in each case, we will instead choose them so as to make either

$$\mathcal{J}(\Phi^N, \Psi^N) = \mathcal{J}(a, b), \quad (3.2)$$

or else

$$\mathcal{G}(\Phi^N, \Psi^N) = \mathcal{G}(a, b) = \mathcal{J}(\Phi^N, \Psi^N) + \mathcal{S}(\Phi^N, \Psi^N), \quad (3.3)$$

stationary. The reason for this is that when $\mathcal{J}(a, b)$ is made stationary with respect to variations of the a_n's and b_n's, the value about which it becomes stationary is precisely the $[N - 1/N]PA$ to $f(x)$. Similarly, making $\mathcal{G}(a, b)$ stationary yields the $[N/N]$ PA to $f(x)$.

The above results are well known in the context of the Schwinger and Kohn variational principles, as described by Nuttall,[10] and their derivation follows familiar lines. As an example we will show how $\mathcal{J}(a, b)$ yields the $[N - 1/N]$ PA. We have

$$\mathcal{J}(a, b) = -a^+Ab + (a^+ + b^+)c. \quad (3.4)$$

Here A is the $N \times N$ matrix with elements $A_{ij} = \langle L^i\xi, (1 + xL)L^j\eta\rangle = f_{i+j} + xf_{i+j+1}$ $(i, j = 0, 1, \ldots, N-1)$, c is the column vector with elements $c_i = \langle L^i\xi, \eta\rangle = \langle L^i\eta, \xi\rangle = f_i$ $(i = 0, 1, \ldots, N-1)$, where in both of the latter we have used (2.14), and a, b are the column vectors with elements a_i, b_i $(i = 0, 1, \ldots, N-1)$, respectively. We now find that $\mathcal{J}(a, b)$ becomes stationary when

$$\frac{\partial \mathcal{J}(a, b)}{\partial a} = \frac{\partial \mathcal{J}(a, b)}{\partial b} = 0, \quad \text{so that } a = b = A^{-1}c, \quad (3.5)$$

and correspondingly

$$\mathcal{J}(a_{\text{opt}}, b_{\text{opt}}) = c^+A^{-1}c \quad (3.6)$$

$$= -\begin{vmatrix} 0 & f_0 & \cdots & f_{N-1} \\ f_0 & (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & \vdots & & \vdots \\ f_{N-1} & (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix}$$

$$\begin{vmatrix} (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & & \vdots \\ (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix}$$

We see by comparison with (1.13) that this is indeed the $[N-1/N]$ PA to $f(x)$. The $[N/N]$ PA is obtained in a similar way from $\mathcal{G}(a,b)$.

Let us introduce the notation $\Phi^N_{\mathcal{J}}$, $\Psi^N_{\mathcal{J}}$, and $\Phi^N_{\mathcal{G}}$, $\Psi^N_{\mathcal{G}}$, for the optimized pairs Φ^N, Ψ^N, which yield the $[N-1/N]$ and $[N/N]$ PA's on use in $\mathcal{J}$ and $\mathcal{G}$, respectively. Then we will shortly require the formulas[11]

$$\Phi^N_{\mathcal{J}} = -\begin{vmatrix} 0 & f_0 & \cdots & f_{N-1} \\ \xi & (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & \vdots & & \\ L^{N-1}\xi & (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix} \div Q_{[N-1/N]}(x) \tag{3.7}$$

and

$$\Phi^N_{\mathcal{G}} = -\begin{vmatrix} 0 & f_1 & \cdots & f_N \\ \xi & (f_1 + xf_2) & \cdots & (f_N + xf_{N+1}) \\ \vdots & \vdots & & \vdots \\ L^{N-1}\xi & (f_N + xf_{N+1}) & \cdots & (f_{2N-1} + xf_{2N}) \end{vmatrix} \div Q_{[N/N]}(x), \tag{3.8}$$

together with similar expressions for $\Psi^N_{\mathcal{J}}$ and $\Psi^N_{\mathcal{G}}$, wherein ξ is replaced by η. Here we have used the notation (1.17).

We are now in a position to obtain bounds on $f(x)$ of the form (1.2). We begin by rewriting our variational bounds (2.17) as

$$\mathcal{J} - [\{S_\xi S_\eta\}^{1/2} - \mathcal{S}] \le f(x) \le \mathcal{G} + [\{S_\xi S_\eta\}^{1/2} - \mathcal{S}] \tag{3.9a}$$

and

$$\mathcal{G} - [\{S_\xi S_\eta\}^{1/2} + \mathcal{S}] \le f(x) \le \mathcal{J} + [\{S_\xi S_\eta\}^{1/2} + \mathcal{S}], \tag{3.9b}$$

for $x \ge 0$. Now consider for example the lower bound in (3.9a). If we insert the pair of trial vectors $\Phi^N_{\mathcal{J}}$, $\Psi^N_{\mathcal{J}}$, we obtain

$$[N-1/N] - b_N(x) \le f(x), \quad x \ge 0, \tag{3.10}$$

where

$$b_N(x) = \left\{S_\xi\left(\Phi^N_{\mathcal{J}}\right) S_\eta\left(\Psi^N_{\mathcal{J}}\right)\right\}^{1/2} - \mathcal{S}\left(\Phi^N_{\mathcal{J}}, \Psi^N_{\mathcal{J}}\right). \tag{3.11}$$

Similarly, using the pair $\Phi^N_{\mathcal{G}}$, $\Psi^N_{\mathcal{G}}$ in the right-hand side of (3.9a), we obtain

$$f(x) \le [N/N] + c_N(x), \quad x \ge 0, \tag{3.12}$$

where

$$c_N(x) = \left\{S_\xi\left(\Phi^N_{\mathcal{G}}\right) S_\eta\left(\Psi^N_{\mathcal{G}}\right)\right\}^{1/2} - \mathcal{S}\left(\Phi^N_{\mathcal{G}}, \Psi^N_{\mathcal{G}}\right). \tag{3.13}$$

A different pair of bounds on $f(x)$ can be obtained from (3.9b). Using $\Phi^N_{\mathcal{G}}, \Psi^N_{\mathcal{G}}$ in the left-hand side of (3.9b), and $\Phi^N_{\mathcal{J}}, \Psi^N_{\mathcal{J}}$ in the right-hand side, yields

$$[N/N] - B_N(x) \le f(x) \le [N-1/N] + C_N(x), \quad x \ge 0, \tag{3.14}$$

where

$$B_N(x) = \left\{S_\xi\left(\Phi^N_{\mathcal{G}}\right) S_\eta\left(\Psi^N_{\mathcal{G}}\right)\right\}^{1/2} + \mathcal{S}\left(\Phi^N_{\mathcal{G}}, \Psi^N_{\mathcal{G}}\right) \tag{3.15}$$

and

$$C_N(x) = \left\{S_\xi\left(\Phi^N_{\mathcal{J}}\right) S_\eta\left(\Psi^N_{\mathcal{J}}\right)\right\}^{1/2} + \mathcal{S}\left(\Phi^N_{\mathcal{J}}, \Psi^N_{\mathcal{J}}\right) \tag{3.16}$$

We now simplify the above expressions for the correction terms $b_N(x)$, $c_N(x)$, $B_N(x)$ and $C_N(x)$, by showing that each one can be written in the form (1.5); that is,

$$\frac{x^{2N}\{\text{positive constant}\}}{\{\text{denominator of corresponding PA}\}^2}.$$

We will then explain the need for having the second pair of bounds (3.14).

Consider first $b_N(x)$, (3.11). In the evaluation of this term we use

$$A\,\Phi^N_{\mathcal{J}} - \xi = (1+xL)\Phi^N_{\mathcal{J}} - \xi = \frac{-\begin{vmatrix} 0 & f_0 & \cdots & f_{N-1} \\ (\xi + xL\xi) & (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & \vdots & & \vdots \\ (L^{N-1}\xi + xL^N\xi) & (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix} - \begin{vmatrix} \xi & 0 & \cdots & 0 \\ 0 & (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & \vdots & & \vdots \\ 0 & (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix}}{\begin{vmatrix} (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & & \vdots \\ (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix}}$$

$$= -\begin{vmatrix} \xi & f_0 & \cdots & f_{N-1} \\ (\xi + xL\xi) & (f_0 + xf_1) & \cdots & (f_{N-1} + xf_N) \\ \vdots & \vdots & & \\ (L^{N-1}\xi + xL^N\xi) & (f_{N-1} + xf_N) & \cdots & (f_{2N-2} + xf_{2N-1}) \end{vmatrix} \div Q_{[N-1/N]}(x) = -x^N \begin{vmatrix} \xi & f_0 & \cdots & f_{N-1} \\ L\xi & f_1 & \cdots & f_N \\ \vdots & \vdots & & \vdots \\ L^N\xi & f_N & \cdots & f_{2N-1} \end{vmatrix} \div Q_{[N-1/N]}(x), \tag{3.17}$$

where in the last step we have subtracted the first row from the second, taken out a factor x, subtracted the resulting second row from the third, and so on. Introducing the notation

$$D_\xi(m,n) = \begin{vmatrix} \xi & f_m & \cdots & f_{m+n-1} \\ L\xi & f_{m+1} & \cdots & f_{m+n} \\ \vdots & \vdots & & \vdots \\ L^n\xi & f_{m+n} & \cdots & f_{m+2n-1} \end{vmatrix},$$

$$\xi \in \mathfrak{H} \cap \mathcal{D}(L) \cap \cdots \cap \mathcal{D}(L^n), \tag{3.18}$$

we express (3.17) by

$$A\Phi_{\mathcal{J}}^N - \xi = -x^N D_\xi(0,N)/Q_{[N-1/N]}(x). \tag{3.19}$$

In a similar way we obtain

$$A\Psi_{\mathcal{J}}^N - \eta = -x^N D_\eta(0,N)/Q_{[N-1/N]}(x), \tag{3.20}$$

the only difference being that ξ is replaced by η. In particular, we now have

$$S\left(\Phi_{\mathcal{J}}^N, \Psi_{\mathcal{J}}^N\right) = \langle A\Phi_{\mathcal{J}}^N - \xi, A\Psi_{\mathcal{J}}^N - \eta \rangle$$

$$= \frac{x^{2N}}{[Q_{[N-1/N]}(x)]^2} \langle D_\xi(0,N), D_\eta(0,N) \rangle, \tag{3.21}$$

$$S_\xi\left(\Phi_{\mathcal{J}}^N\right) = \langle A\Phi_{\mathcal{J}}^N - \xi, A\Phi_{\mathcal{J}}^N - \xi \rangle$$

$$= \frac{x^{2N}}{[Q_{[N-1/N]}(x)]^2} \langle D_\xi(0,N), D_\xi(0,N) \rangle \tag{3.22}$$

$$= \frac{x^{2N}}{[Q_{[N-1/N]}(x)]^2} \cdot \|D_\xi(0,N)\|^2,$$

and similarly

$$S_\eta\left(\Psi_{\mathcal{J}}^N\right) = \frac{x^{2N}}{[Q_{[N-1/N]}(x)]^2} \cdot \|D_\eta(0,N)\|^2. \tag{3.23}$$

Now substituting into (3.11), we have

$$b_N(x) = x^{2N} b_N / [Q_{[N-1/N]}(x)]^2, \tag{3.24}$$

where

$$b_N = \|D_\xi(0,N)\| \cdot \|D_\eta(0,N)\| - \langle D_\xi(0,N), D_\eta(0,N) \rangle. \tag{3.25}$$

In like manner we derive

$$\begin{aligned} c_N(x) &= x^{2N} c_N / [Q_{[N/N]}(x)]^2, \\ B_N(x) &= x^{2N} B_N / [Q_{[N/N]}(x)]^2, \\ C_N(x) &= x^{2N} c_N / [Q_{[N-1/N]}(x)]^2, \end{aligned} \tag{3.26}$$

where

$$c_N = \|D_\xi(1,N)\| \cdot \|D_\eta(1,N)\| - \langle D_\xi(1,N), D_\eta(1,N) \rangle, \tag{3.27}$$

$$B_N = \|D_\xi(1,N)\| \cdot \|D_\eta(1,N)\| + \langle D_\xi(1,N), D_\eta(1,N) \rangle, \tag{3.28}$$

$$C_N = \|D_\xi(0,N)\| \cdot \|D_\eta(0,N)\| + \langle D_\xi(0,N), D_\eta(0,N) \rangle. \tag{3.29}$$

Thus, in each case, the correction term takes the form (1.5): The numbers b_N, c_N, B_N, and C_N are independent of x and nonnegative by Schwartz's inequality.

We now show how our bounds reduce to the usual PA bounds, see (1.3), when $f(x)$ is a series of Stieltjes. In so doing we uncover the reason for having two pairs of bounding formulas.

From Sec. 2A, the case $f(x)$ is a series of Stieltjes corresponds to $\xi = \eta$. On making this substitution in (3.25) and (3.27) we obtain $b_N = c_N = 0$, and (1.2) becomes the usual PA bounds. Making the same substitution in (3.28) and (3.29) yields

$$B_N = 2\|D_\xi(1,N)\|^2, \quad C_N = 2\|D_\xi(0,N)\|^2, \tag{3.30}$$

and the resulting bounds on $f(x)$ are certainly not the PA ones; indeed, these bounds can be shown to be broader than the PA bounds. However, if $\xi = -\eta$, which is the case where $f(x)$ is the negative of a series of Stieltjes, then just the opposite of the above happens; (3.14) gives

$$\begin{aligned} &[N/N] \le f(x) \le [N-1/N], && x \ge 0, \\ \text{i.e.,}\quad &-[N-1/N] \le -f(x) \le -[N/N], && x \ge 0, \end{aligned} \tag{3.31}$$

while (1.2) yields a pair of bounds which are distinct from the PA ones. Thus, our bounds reduce to the usual PA bounds in both the cases $f(x) = \pm$ a series of Stieltjes. This is the feature which one would naturally expect of "PA's + correction terms"; we see how, for this to occur, two pairs of formulas are needed.

4. EVALUATION OF THE CONSTANTS IN THE CORRECTION TERMS

In this section we will be concerned with the evaluation of the constants b_N, c_N, B_N, and C_N, which occur in the correction terms. The ultimate objective is to show how suitable values for the constants can be calculated while assuming only a set of information about $f(x)$ which is likely to be easily obtained, over and above the coefficients $\{f_n\}_{n=0}^{2n}$ which are already needed to construct the PA's themselves. We begin by discovering that we need to know the coefficients $\{F_n\}_{n=0}^{2n}$, described circa (1.9). It is then shown that in many cases F_n may be replaced by $\tilde{F}_n$, $n = 0, 1, \ldots, 2N$, see (1.11), while preserving the bounding properties of the corrected PA's.

A. Evaluation of constants using $\{F_n\}_{n=0}^{2n}$

The terms $\langle D_\xi(0,N), D_\eta(0,N)\rangle$ and $\langle D_\xi(1,N), D_\eta(1,N)\rangle$ can always be evaluated using only $\{f_n\}_{n=0}^{2n}$. We have for example

$$\langle D_\xi(0,N), D_\eta(0,N)\rangle = \left\langle \begin{vmatrix} \xi & f_0 & \cdots & f_{N-1} \\ L\xi & f_1 & \cdots & f_N \\ \vdots & \vdots & & \vdots \\ L^N\xi & f_N & \cdots & f_{2N-1} \end{vmatrix}, \begin{vmatrix} \eta & f_0 & \cdots & f_{N-1} \\ L\eta & f_1 & \cdots & f_N \\ \vdots & \vdots & & \vdots \\ L^N\eta & f_N & \cdots & f_{2N-1} \end{vmatrix} \right\rangle, \tag{4.1}$$

and, observing that

$$\left\langle L^n\xi, \begin{vmatrix} \eta & f_0 & \cdots & f_{N-1} \\ L\eta & f_1 & \cdots & f_N \\ \vdots & \vdots & & \vdots \\ L^N\eta & f_N & \cdots & f_{2N-1} \end{vmatrix} \right\rangle \equiv \begin{vmatrix} f_n & f_0 & \cdots & f_{N-1} \\ f_{n+1} & f_1 & & f_N \\ \vdots & \vdots & & \vdots \\ f_{n+N} & f_N & \cdots & f_{2N-1} \end{vmatrix} = 0$$

$$\text{for } n = 0, 1, \ldots, N-1, \tag{4.2}$$

where we have made use of (2.17), we find that

$$\langle D_\xi(0,N), D_\eta(0,N)\rangle = D(0,N-1)D(0,N). \tag{4.3}$$

In the same way we derive

$$\langle D_\xi(1,N), D_\eta(1,N)\rangle = D(2,N-1)D(0,N) \tag{4.4}$$

and in each case only the coefficients $\{f_n\}_{n=0}^{2n}$ are used.

However, the constants also involve the quantities $\|D_\xi(0,N)\|$, $\|D_\eta(0,N)\|$, $\|D_\xi(1,N)\|$, and $\|D_\eta(1,N)\|$, where for example

$$\|D_\xi(0,N)\|^2 = \langle D_\xi(0,N), D_\xi(0,N)\rangle$$

$$= \left\langle \begin{vmatrix} \xi & f_0 & \cdots & f_{N-1} \\ L\xi & f_1 & \cdots & f_N \\ \vdots & \vdots & & \vdots \\ L^N\xi & f_N & \cdots & f_{2N-1} \end{vmatrix}, \begin{vmatrix} \xi & f_0 & \cdots & f_{N-1} \\ L\xi & f_1 & \cdots & f_N \\ \vdots & \vdots & & \vdots \\ L^N\xi & f_N & \cdots & f_{2N-1} \end{vmatrix} \right\rangle \tag{4.5}$$

In order to evaluate these, we clearly need to know

$$\langle \xi, L^n\xi\rangle \text{ and } \langle \eta, L^n\eta\rangle \text{ for } n = 0, 1, \ldots, 2N. \tag{4.6}$$

Choosing ξ and η as in (2.9) and using (1.9), we have

$$\langle \xi, L^n\xi\rangle = \langle \eta, L^n\eta\rangle = \int_0^\infty u^n |d\varphi(u)| = F_n, \tag{4.7}$$

and in this case

$$\|D_\eta(0,N)\| = \|D_\xi(0,N)\| \text{ and } \|D_\eta(1,N)\| = \|D_\xi(1,N)\|. \tag{4.8}$$

Given that we know $\{F_n\}_{n=0}^{2N}$, it is now a straightforward matter to evaluate the constants b_N, c_N, B_N, and C_N. For example, when $N=1$, we have from (3.25)

$$b_1 = \|D_\xi(0,1)\| \cdot \|D_\eta(0,1)\| - \langle D_\xi(0,1), D_\eta(0,1)\rangle$$

$$= \langle D_\xi(0,1), D_\xi(0,1)\rangle - D(0,0)D(0,1),$$

by (4.3) and (4.8),

$$= \left\langle \begin{vmatrix} \xi & f_0 \\ L\xi & f_1 \end{vmatrix}, \begin{vmatrix} \xi & f_0 \\ L\xi & f_1 \end{vmatrix} \right\rangle - f_0 \begin{vmatrix} f_0 & f_1 \\ f_1 & f_2 \end{vmatrix}$$

$$= \langle f_1\xi - f_0 L\xi,\ f_1\xi - f_0 L\xi\rangle - f_0(f_0 f_2 - f_1^2)$$

$$= (f_1^2 F_0 - 2f_0 f_1 F_1 + f_0^2 F_2) - f_0(f_0 f_2 - f_1^2), \text{ using (4.7);} \tag{4.9}$$

and correspondingly

$$b_1(x) = \frac{x^2[(f_1^2 F_0 - 2f_0 f_1 F_1 + f_0^2 F_2) - f_0(f_0 f_2 - f_1^2)]}{(f_0 + x f_1)^2}. \tag{4.10}$$

Similarly we find

$$c_1(x) = \frac{x^2[(f_2^2 F_0 - 2f_1 f_2 F_1 + f_1^2 F_2) - f_2(f_0 f_2 - f_1^2)]}{(f_1 + x f_2)^2}. \tag{4.11}$$

In general, there does not seem to be any succinct method for evaluating the inner products $\langle D_\xi(0,N), D_\xi(0,N)\rangle$ and $\langle D_\xi(1,N), D_\xi(1,N)\rangle$; for each N one has to proceed straightforwardly via expansion of the corresponding determinants, $D_\xi(0,N)$ and $D_\xi(1,N)$, as illustrated above.

We recall here the remark made at the beginning of Sec. 3. The assumption that F_n is finite ($n = 1, 2, \ldots 2N$) means in particular that $\langle L^m\xi, L^m\xi\rangle = \langle \xi, L^{2m}\xi\rangle = F_{2m}$ ($m = 1, 2, \ldots, N$) is finite, using (4.7). Hence ξ, and similarly η, belong to $\mathcal{D}(L^m)$ ($m = 1, 2, \ldots N$), as was claimed.

B. Evaluation of constants using $\{\tilde{F}_n\}_{n=0}^{2N}$

The requirement that in addition to $\{f_n\}_{n=0}^{2N}$, we also need to know $\{F_n\}_{n=0}^{2N}$ is a very stringent one. However, provided we know a function $\theta(u)$ such that $d\theta(u) \geq |d\varphi(u)|$ for $0 \leq u < \infty$, we can often still obtain suitable values for the constants b_N, c_N, B_N, and C_N.

Let us suppose for simplicity that $\varphi(u)$ is constant outside $0 \leq u \leq 1/R$, for some $0 < R < \infty$, and that $\varphi(u)$ possesses a continuous derivative $\varphi'(u)$ over this interval. Then

$$f(x) = \int_0^{1/R} \frac{\varphi'(u)du}{(1+ux)} \tag{4.12}$$

is the analog of a series of Stieltjes with radius of convergence R. Let $\theta(u)$ be any monotone nondecreasing function with a continuous derivative $\theta'(u)$ such that

$$\theta'(u) \geq |\varphi'(u)| \quad \text{for} \quad 0 \leq u \leq 1/R. \tag{4.13}$$

It seems generally likely that, while not knowing $|\varphi'(u)|$ and hence not knowing the F_n's, one would still have available a bound $\theta'(u)$, such as a constant $M \geq |\varphi'(u)|$ for $0 \leq u \leq 1/R$.

We now claim that, on defining

$$\tilde{F}_n = \int_0^{1/R} u^n d\theta(u), \quad n = 0, 1, \ldots, 2N, \tag{4.14}$$

and putting

$$\langle \xi, L^n\xi\rangle = \langle \eta, L^n\eta\rangle = \tilde{F}_n, \quad n = 0, 1, \ldots, 2N, \tag{4.15}$$

in place of the F_n's used in Sec. 4A to evaluate b_N, c_N, B_N, and C_N, the resulting constants will be such that the bounding formulas (1.2) and (3.14) remain valid.

In the proof of this result the central idea is the

following. We consider replacing the distribution $d\varphi(u)$ in the definition of $f(x)$ by a distribution whose value at each point $u \in [0, 1/R]$ is either $+d\theta(u)$ or $-d\theta(u)$: $f(x)$ may be approximated arbitrarily closely in this way for $x \geq 0$. The result is then obtained by observing that the "F_n's" associated with the $\pm d\theta(u)$ distribution are exactly the $\tilde{F}_n$'s.

More precisely, given $\theta(u)$ and $\varphi(u)$ as in (4.13), there exists a sequence of piecewise continuous functions $\{\chi_M(u)\}_{M=1}^{\infty}$ with the property that for each M

$$\chi_M(u) = \text{either } +1 \text{ or } -1, \quad \text{each } u \in [0, 1/R]. \tag{4.16}$$

We define

$$\rho_M(u) = \int_0^u \chi_M(u)\, d\theta(u), \tag{4.17}$$

and an associated sequence of functions $\{f_M(x)\}_{M=1}^{\infty}$ by

$$f_M(x) = \int_0^{1/R} \frac{d\rho_M(u)}{(1+ux)}, \qquad M = 1, 2, \cdots. \tag{4.18}$$

Then the sequence $\{\chi_M(u)\}_{M=1}^{\infty}$ is such that

$$f_M(x) \xrightarrow{u} f(x), \quad 0 \leq x \leq X, \tag{4.19}$$

for any $0 < X < \infty$. We use "$\xrightarrow{u}$" to mean uniform convergence with increasing M, over the stated interval. Moreover, if

$$f_{nM} = \int_0^{1/R} u^n d\rho_M(u), \quad M = 1, 2, \cdots, \tag{4.20}$$

then

$$\lim_{M\to\infty} f_{nM} = f_n, \quad n = 0, 1, 2, \cdots. \tag{4.21}$$

These results having been established, the rest is easy. For large enough M the PA's plus correction terms *to* $f_M(x)$ certainly exist [i.e., the associated determinants like (1.16) do not vanish because of (4.21)]. Moreover, the requisite "F_n's" needed to evaluate the constants in the correction terms are

$$\begin{aligned}\int_0^{1/R} u^n |d\rho_M(u)| &= \int_0^{1/R} u^n |\chi_M(u)|\, |d\theta(u)| \\ &= \int_0^{1/R} u^n d\theta(u) = \tilde{F}_n, \quad n = 0, 1, \ldots, 2N,\end{aligned} \tag{4.22}$$

independently of M. Hence we have

$$[N - 1/N]^M - b_N^M(x) \leq f_M(x) \leq [N/N]^M + c_N^M(x), \quad x \geq 0, \tag{4.23}$$

where the M superscript indicates approximants to $f_M(x)$; and on taking the limit as $M \to \infty$ we obtain

$$[N - 1/N] - \tilde{b}_N(x) \leq f(x) \leq [N/N] + \tilde{c}_N(x), \quad x \geq 0, \tag{4.24}$$

where the tildes mean that $\tilde{F}_n$'s are used in place of the F_n's in evaluating the correction terms. A parallel derivation applies to the other pair of bounds (3.14) and yields

$$[N/N] - \tilde{B}_N(x) \leq f(x) \leq [N - 1/N] + \tilde{C}_N(x), \quad x \geq 0, \tag{4.25}$$

in the obvious notation.

To prove these results, we must establish the existence of a sequence of functions $\{\chi(u)\}_{M=1}^{\infty}$ such that the requirements (4.16), (4.19), and (4.21) are fulfilled.

We assume, without any loss of generality, that $R = 1$. Then we begin by defining a set of partitions $\{\Delta_M\}_{M=1}^{\infty}$ of the interval $0 \leq u \leq 1$. We take Δ_M to be the set of points

$$0 = u_0^M < u_1^M < \cdots < u_M^M = 1, \tag{4.26}$$

where

$$u_m^M - u_{m-1}^M = 1/M, \quad m = 1, 2, \ldots, M, \tag{4.27}$$

so that

$$u_m^M = m/M. \tag{4.28}$$

Each Δ_M is now subdivided to form a new partition $\tilde{\Delta}_M$ in the following way: Let v_m^M, w_m^M be such that

$$u_{m-1}^M \leq v_{m-1}^M \leq w_{m-1}^M \leq u_m^M, \quad m = 1, 2, \ldots, M, \tag{4.29}$$

where

$$u_m^M - w_{m-1}^M = \delta_m^M = \begin{cases} (1/M)\,|\varphi'(u_m^M)|\,/\theta'(u_m^M) & \text{if } \theta'(u_m^M) \neq 0 \\ 0 & \text{if } \theta'(u_m^M) = 0 \end{cases} \tag{4.30}$$

and

$$w_{m-1}^M - v_{m-1}^M = v_{m-1}^M - u_{m-1}^M = \gamma_m^M \tag{4.31}$$

with

$$\gamma_m^M = \tfrac{1}{2}[(u_m^M - u_{m-1}^M) - \delta_m^M] = \tfrac{1}{2}[1/M - \delta_m^M]; \tag{4.32}$$

then $\tilde{\Delta}_M$ is the set of points

$$\begin{aligned}0 = u_0^M \leq v_0^M \leq w_0^M \leq u_1^M \leq \cdots \leq v_{m-1}^M \\ \leq w_{m-1}^M \leq u_m^M \leq \cdots \leq u_M^M = 1.\end{aligned} \tag{4.33}$$

We observe that the relationships (4.30) and (4.31) are in harmony with (4.29) because by assumption

$$0 \leq |\varphi'(u)| \leq |\theta'(u)|, \quad 0 \leq u \leq 1, \tag{4.34}$$

so that

$$0 \leq \delta_m^M \leq 1/M, \quad m = 1, 2, \ldots, M. \tag{4.35}$$

The piecewise continuous function $\chi_M(u)$ on $0 \leq u \leq 1$ is now associated with $\tilde{\Delta}_M$ as follows. We define

$$\chi_M(u) = \begin{cases} -1, & u_{m-1}^M < u \leq v_{m-1}^M \\ +1, & v_{m-1}^M < u \leq w_{m-1}^M, \\ \operatorname{sgn}\{\varphi'(u_m^M)\}, & w_{m-1}^M < u \leq u_m^M, \end{cases}$$

$$m = 1, 2, \ldots, M, \tag{4.36}$$

together with, say, $\chi_M(0) = -1$. Then it is clear that each $\chi_M(u)$ is piecewise continuous and satisfies (4.16). We must show that the sequence has the properties (4.19) and (4.21).

We will first establish (4.19). From (4.18) and (4.36) we have

$$\begin{aligned}f_M(x) &= \int_0^1 \frac{d\rho_M(x)}{(1+ux)} = \int_0^1 \frac{\chi_M(u)\theta'(u)du}{(1+ux)} \\ &= \sum_{m=1}^{M} \left(-\int_{u_{m-1}^M}^{v_{m-1}^M} \frac{\theta'(u)du}{(1+ux)} + \int_{v_{m-1}^M}^{w_{m-1}^M} \frac{\theta'(u)du}{(1+ux)} \right) \\ &\quad + \sum_{m=1}^{M} \int_{w_{m-1}^M}^{u_m^M} \frac{\operatorname{sgn}\{\varphi'(u_m^M)\}\,\theta'(u)du}{(1+ux)}\end{aligned} \tag{4.37}$$

$$= g_M(x) + h_M(x),$$

where $g_M(x)$ and $h_M(x)$ denote the first and second sums in the previous line, respectively. We claim that

$$g_M(x) \xrightarrow{u} 0, \qquad 0 \le x \le X, \tag{4.38}$$

while

$$h_M(x) \xrightarrow{u} f(x), \quad 0 \le x \le X. \tag{4.39}$$

Consider $h_M(x)$. Defining

$$s_M(x) = \frac{1}{M} \sum_{m=1}^{M} \frac{\varphi'(u_m^M)}{(1+u_m^M x)}, \tag{4.40}$$

we will prove first that

$$h_M(x) \xrightarrow{u} s_M(x), \quad 0 \le x \le X, \tag{4.41}$$

and then that

$$s_M(x) \xrightarrow{u} f(x), \qquad 0 \le x \le X, \tag{4.42}$$

thereby proving (4.39).

We have

$$\begin{aligned}
&|h_M(x) - s_M(x)| \\
&= \left| \sum_{m=1}^{M} \left(\int_{w_{m-1}^M}^{u_m^M} \frac{\operatorname{sgn}\{\varphi'(u_m^M)\}\theta'(u)du}{(1+ux)} - \frac{1}{M}\frac{\varphi'(u_m^M)}{(1+u_m^M x)} \right) \right| \\
&= \left| \sum_{m=1}^{M} \int_{w_{m-1}^M}^{u_m^M} \left(\frac{\operatorname{sgn}\{\varphi'(u_m^M)\}\theta'(u)}{(1+ux)} - \frac{\operatorname{sgn}\{\varphi'(u_m^M)\}\theta'(u_m^M)}{(1+u_m^M x)} \right) du \right| \\
&\le \sum_{m=1}^{M} \int_{w_{m-1}^M}^{u_m^M} \left| \frac{\theta'(u)}{(1+ux)} - \frac{\theta'(u_m^M)}{(1+u_m^M x)} \right| du, \quad 0 \le x \le X.
\end{aligned} \tag{4.43}$$

If we set

$$\begin{aligned}
\measuredangle_m^M &= \min\{\theta'(u) \,|\, u_{m-1}^M \le u \le u_m^M\}, \\
/\!\!\eta_m^M &= \max\{\theta'(u) \,|\, u_{m-1}^M \le u \le u_m^M\},
\end{aligned} \tag{4.44}$$

then we observe that the assumed continuity of $\theta'(u)$ on $0 \le u \le 1$ implies it is uniformly continuous over this interval, and hence there exists an integer $M(\epsilon)$ such that

$$/\!\!\eta_m^M - \measuredangle_m^M < \epsilon, \quad m = 1, 2, \ldots M, \text{ for all } M > M(\epsilon) \tag{4.45}$$

for any $\epsilon > 0$, prescribed arbitrarily small. Further, let

$$/\!\!\eta = \max\{\theta'(u) \,|\, 0 \le u \le 1\}. \tag{4.46}$$

From (4.43) we now have

$$\begin{aligned}
&|h_M(x) - s_M(x)| \\
&\le \sum_{m=1}^{M} \int_{w_{m-1}^M}^{u_m^M} \left| \frac{(\theta'(u) - \theta'(u_m^M))(1+u_m^M x) + (u_m^M - u)x\theta'(u_m^M)}{(1+ux)(1+u_m^M x)} \right| du \\
&\le \sum_{m=1}^{M} \int_{w_{m-1}^M}^{u_m^M} [(/\!\!\eta_m^M - \measuredangle_m^M) + (u_m^M - u)X/\!\!\eta]\, du \\
&\le \sum_{m=1}^{M} \frac{1}{M} \left(\epsilon + \frac{1}{M} X/\!\!\eta \right) = \epsilon + \frac{1}{M} X/\!\!\eta
\end{aligned} \tag{4.47}$$

for all $0 \le x \le X$ and $M > M(\epsilon)$. The latter can be made as small as we like by choosing M sufficiently large; this proves (4.41).

Now consider

$$\begin{aligned}
\left| f(x) - s_M(x) \right| &= \left| \int_0^1 \frac{\varphi'(u)du}{(1+ux)} - \sum_{m=1}^{M} \frac{1}{M} \frac{\varphi'(u_m^M)}{(1+u_m^M x)} \right| \\
&= \left| \sum_{m=1}^{M} \int_{u_{m-1}^M}^{u_m^M} \left(\frac{\varphi'(u)}{(1+ux)} - \frac{\varphi'(u_m^M)}{(1+u_m^M x)} \right) du \right|.
\end{aligned} \tag{4.48}$$

This last quantity has the same form as (4.43), and its uniform convergence to zero for $0 \le x \le X$ is implied by the same reasoning as was used in (4.47), except that this time one relies on the uniform continuity of $\varphi'(u)$ on $0 \le u \le 1$. Equation (4.42) is thus established, and together with (4.41), this completes the proof of (4.39).

We now prove (4.38). We have

$$\begin{aligned}
\left| g(x) \right| &= \left| \sum_{m=1}^{M} \left(\int_{u_{m-1}^M}^{v_{m-1}^M} \frac{\theta'(u)du}{(1+ux)} - \int_{v_{m-1}^M}^{w_{m-1}^M} \frac{\theta'(u)du}{(1+ux)} \right) \right| \\
&\le \sum_{m=1}^{M} \left(\frac{/\!\!\eta_m^M (v_{m-1}^M - u_{m-1}^M)}{(1+u_{m-1}^M x)} - \frac{\measuredangle_m^M (w_{m-1}^M - v_{m-1}^M)}{(1+u_m^M x)} \right)
\end{aligned} \tag{4.49}$$

for $0 \le x \le X$,

where we have used (4.44). Since

$$v_{m-1}^M - u_{m-1}^M = w_{m-1}^M - v_{m-1}^M = \gamma_m^M \le 1/2M, \tag{4.50}$$

we now have

$$\begin{aligned}
\left| g_M(x) \right| &\le \frac{1}{2M} \sum_{m=1}^{M} \left(\frac{(/\!\!\eta_m^M - \measuredangle_m^M)(1+u_m^M x) + (u_m^M - u_{m-1}^M)X/\!\!\eta}{(1+u_{m-1}^M x)(1+u_m^M x)} \right) \\
&\le \frac{1}{2M} \sum_{m=1}^{M} \left((/\!\!\eta_m^M - \measuredangle_m^M) + \frac{1}{M} X/\!\!\eta \right) \\
&\le \tfrac{1}{2}\epsilon + \frac{1}{2M} X/\!\!\eta \text{ for } 0 \le x \le X
\end{aligned} \tag{4.51}$$

for all $0 \le x \le X$ and $M \ge M(\epsilon)$, where we have used (4.45) and (4.46). The last quantity can be made as small as we please by picking M large enough, and hence we have (4.38).

Equations (4.38) and (4.39) taken together yield the desired property (4.19).

It remains only for us to establish the property (4.21) of the sequence $\{\chi_M(u)\}_{M=1}^{\infty}$. We have

$$\begin{aligned}
f_n - f_{nM} &= \sum_{m=1}^{M} \left(\int_{u_{m-1}^M}^{v_{m-1}^M} u^n \theta'(u)du - \int_{v_{m-1}^M}^{w_{m-1}^M} u^n \theta'(u)du \right) \\
&+ \sum_{m=1}^{M} \left(\int_{u_{m-1}^M}^{u_m^M} u^n \varphi'(u)du - \int_{w_{m-1}^M}^{u_m^M} u^n \operatorname{sgn}\{\varphi'(u_m^M)\}\theta'(u)du \right),
\end{aligned} \tag{4.52}$$

and, at fixed n, it can be shown by similar reasoning to that used above, that both sums here tend to zero as $M \to \infty$. In this way (4.21) is proved.

This completes the proof that there exists a sequence $\{\chi_M(u)\}_{M=1}^{\infty}$ with the properties (4.16), (4.19), and (4.21).

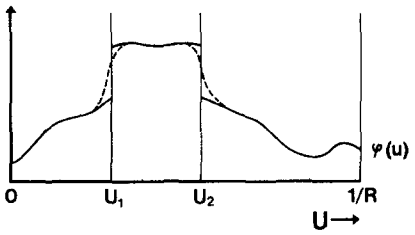

FIG. 1. Sketch of how $\varphi(u)$, posessing discontinuities at u_1 and u_2, might be altered to form a smooth function $\tilde{\varphi}(u)$. The dotted lines indicate the modifications.

Thus our result on the replacement of F_n's by $\tilde{F}_n$'s is established for the case where $\varphi'(u)$ and $\theta'(u)$ are continuous on $0 \leq u \leq 1/R$.

We will now indicate how the above restrictions on $\varphi(u)$ and $\theta(u)$ might be considerably weakened. First, we can certainly allow $\varphi'(u)$ and $\theta'(u)$ to be only piecewise continuous on $0 \leq u \leq 1/R$ provided $\varphi(u)$ and $\theta(u)$ are themselves continuous on the interval. Secondly, if $\varphi(u)$ has discontinuities then, by replacing $\varphi(u)$ by a similar but continuous and piecewise differentiable function $\tilde{\varphi}(u)$ with steep slopes in the neighborhoods of the discontinuities in $\varphi(u)$ (see Fig. 1), we visualize that $f(x)$ may be approximated arbitrarily closely by

$$\tilde{f}(x) = \int_0^{1/R} \frac{d\tilde{\varphi}(u)}{(1+ux)}, \quad 0 \leq x \leq X. \tag{4.53}$$

We now use $\tilde{f}(x)$ in place of $f(x)$, construct PA's and modified correction terms, and then let $\tilde{f}(x)$ approach $f(x)$. Then the condition (4.13) becomes generalized to

$$d\theta(u) \geq |d\varphi(u)|, \quad 0 \leq u \leq 1/R. \tag{4.54}$$

We are led to expect that our result on the replacement of F_n's by $\tilde{F}_n$'s will hold true when $\varphi(u)$ and $\theta(u)$ are related according to (4.54). Finally, with suitable restrictions on the asymptotic behavior of $\varphi(u)$ and $\theta(u)$, we can picture allowing $R \to 0$.

5. EXAMPLES AND DISCUSSION

A. Examples

Functions of the form (1.1) occur in potential theory. The electric potential $V(x)$ due to a charge distribution of line density $\sigma(w)$ on the negative axis, $-b \leq w \leq -a < 0$, is

$$V(x) = \int_{-b}^{-a} \frac{\sigma(w)dw}{(-w+x)}, \quad x \geq 0; \tag{5.1}$$

this can be rewritten

$$V(x) = \int_{1/b}^{1/a} \frac{(1/u)\sigma(-1/u)du}{(1+ux)} \tag{5.2}$$

which is of the form (1.1) with

$$d\varphi(u) = \begin{cases} (1/u)\sigma(-1/u), & 1/b \leq u \leq 1/a, \\ 0, & \text{otherwise.} \end{cases} \tag{5.3}$$

Similar potential functions arise in two-dimensional ideal fluid hydrodynamics, when one has a distribution of sources and sinks on the negative axis, and in certain problems involving a scalar magnetic potential.

Functions of the form (1.1) also arise in scattering theory. Two examples are: (i) S matrix elements in Peres-model field theory,[12] (ii) Kp forward dispersion relations.[13]

Here we look at PA's plus correction terms for the potential $V(x)$ in (5.1) with $a=1$, $b=4$, and

$$\sigma(w) = \begin{cases} -1, & -4 \leq w \leq -3, \\ 0, & -3 < w < -2, \\ +1, & -2 \leq w \leq -1, \end{cases} \tag{5.4}$$

Then

$$V(x) = \ln\left(\frac{(2+x)(3+x)}{(1+x)(4+x)}\right) = \sum_{n=0}^{\infty} (-x)^n f_n, \tag{5.5}$$

where

$$f_n = \begin{cases} \ln(\frac{3}{2}), & n=0, \\ [1-(\frac{1}{2})^n - (\frac{1}{3})^n + (\frac{1}{4})^n]/n, & n=1,2,\cdots. \end{cases} \tag{5.6}$$

The exact F_n's required in the evaluation of the constants in the correction terms are obtained from the expansion of

$$F(x) = \int_{1/4}^{1} \frac{|(1/u)\sigma(-1/u)|\,du}{(1+ux)} = \ln\left(\frac{(2+x)(4+x)}{(1+x)(3+x)}\right). \tag{5.7}$$

A suitable choice for the $\tilde{F}_n$'s is obtained by taking

$$d\theta(u) = \begin{cases} (1/u)du, & 1/4 \leq u \leq 1, \\ 0, & \text{otherwise,} \end{cases} \tag{5.8}$$

corresponding to which we find

$$\tilde{F}(x) = \ln[(4+x)/(1+x)]. \tag{5.9}$$

In Fig. 2 we compare the upper and lower bounds associated with the [1/2] PA to $f(x)$, using a logarithmic scale in x. These are the exact bounds

$$[1/2] - b_2(x) \leq f(x) \leq [1/2] + C_2(x) \tag{5.10}$$

evaluated with the aid of F_0, F_1, F_2, F_3, and F_4. The correction constants themselves are

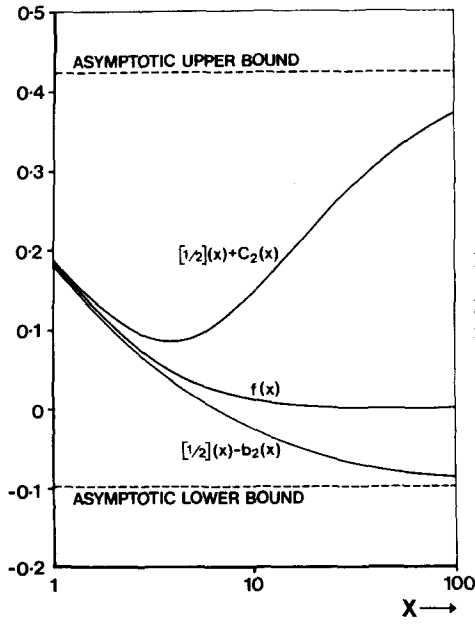

FIG. 2. Upper and lower bounds associated with the [1/2] PA to $V(x)$.

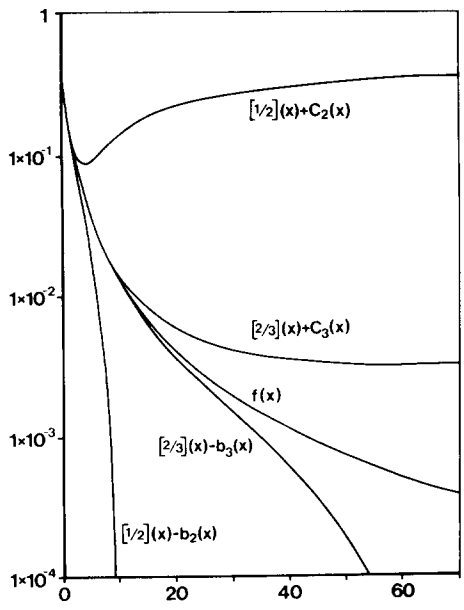

FIG. 3. Comparison of bounds associated with the [1/2] and [2/3] PA's to $V(x)$

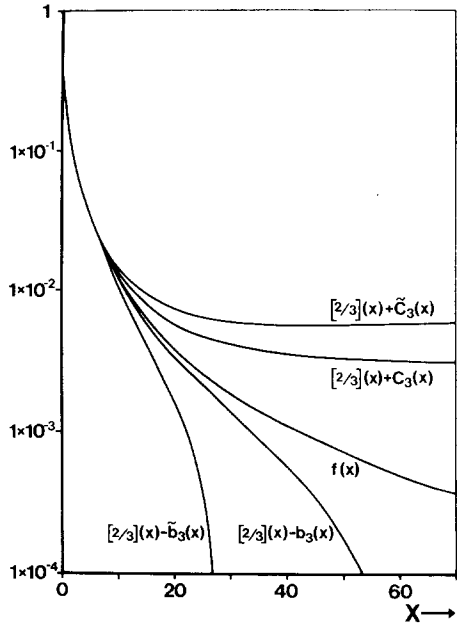

FIG. 4. Comparison between the exact and the modified bounds associated with the [2/3] PA to $V(x)$. The tildes mean modified correction terms.

$$b_2 = 1.962\times10^{-6}, \quad C_2 = 8.281\times10^{-6}, \tag{5.11}$$

and, when $\tilde{F}_n$'s are used in place of F_n's, we obtain the modified constants

$$\tilde{b}_2 = 5.229\times10^{-6}, \quad \tilde{C}_2 = 1.154\times10^{-5}. \tag{5.12}$$

The modified bounds have approximately the same shape as the exact ones. The difference between the upper and lower modified bound is seen to be about sixty per cent greater than the difference between the exact upper and lower bound, and thus here the replacement of F_n's by $\tilde{F}_n$'s does not crucially effect the tightness of the bounds.

The bounds deteriorate rapidly around $x=4$, and for comparison we note that the expansion of $V(x)$, in (5.5) and (5.6), has a radius of convergence $R=1$. Asymptotically the bounds tend to constants, as is easily deduced from the structure of the correction terms.

On increasing N from 2 to 3 we find that the bounds improve considerably, as in illustrated in Fig. 3, where we compare the exact bounds associated with the [1/2] PA with those associated with the [2/3] PA. This time we use a logarithmic scale for the functional values. The range of x over which the bounds may be considered useful is increased from around $x=4$ to around $x=30$. In Fig. 4 we compare the exact bounds associated with the [2/3] PA with the modified ones. Again, the widening of the bounds is not drastic.

The upper and lower bounds corresponding to the [2/2] PA are interesting because the approximant has a simple pole located at $x=7.27$. Accordingly, both correction terms also have poles at this point, but of second order. The resulting bounds become very broad in the vicinity of the pole, as can be seen from Table I. The spurious pole blows up the corrections in its vicinity in such a way as to ensure that the corrected PA's display the desired bounding properties.

In general we expect that PA's plus correction terms will yield bounds which improve with increasing N, provided we omit those PA's with spurious poles.[14]

B. Discussion

In this paper we have found a suitable *structure* for correction terms to $[N-1/N]$ and $[N/N]$ PA's for functions of the form (1.1), such that the resulting corrected PA's impose rigorous bounds on $f(x)$ for all $x>0$. We have further shown how, given appropriate additional information, explicit values for the constants in the correction terms may be evaluated. However, even when such additional information is not available, it is interesting simply to know what such corrections look like both from the point of view of PA theory and of applications.

One may still make progress in applications when neither the F_n's nor $\tilde{F}_n$'s are available. For example, one might estimate the values of the correction constants by using the difference between the PA's and $f(x)$ observed at several x values. Alternatively, assuming that a particular PA has pole locations and residues which mimic the shape of the true distribution, then from these poles and their residues one may construct an approximation to $|d\varphi(u)|$. The latter may then be used to form approximations to the F_n's and hence ap-

TABLE I. Bounds on $V(x)$ associated with the [2/2] PA.

x	$[2/2](x)-B_2(x)$	$[2/2]+C_2(x)$
0	0.40	0.40
1	0.17	0.19
2	0	0.24
3	−0.38	0.66
4	−1.55	2.12
5	−5.74	7.34
6	−28.7	35.6
7	−908	1 103
8	−173	207
9	−40.2	47.8
10	−20.5	24.1
50	−2.67	2.79
100	−1.94	2.81

proximations to the correction constants. The correction constants are not unduely sensitive to inaccuracies in the F_n's because they depend on them only linearly. Both of the above methods have been successfully applied to several different examples.

The idea of forming correction terms to PA's can be extended readily in several directions. With alternative choices of trial functions in the bivariational functionals one can obtain corrections for arbitary $[M/N]$ PA's to $f(x)$. Again, following the method of Epstein and Barnsley,[15] it is possible to develop correction terms for *multipoint* PA's to $f(x)$. The latter would be useful in obtaining bounds on Kp forward dispersion relations,[13] where one has a function of the form (1.1) and the given information, obtained experimentally, is typically $\{f(x_i)\}_{i=1}^{2N}$ with $0 < x_1 < x_2 < \cdots < x_{2N} < \infty$.

ACKNOWLEDGMENT

The author thanks Professor P.D. Robinson for suggesting obtaining PA's from bivariational functionals, and for much assistance.

[1]G.A. Baker, Jr., Advan. Theor. Phys. 1, 1 (1965).
[2]See *Padê Approximants and Their Applications*, edited by P.R. Graves-Morris (Academic, New York and London, 1973).
[3]M.F. Barnsley and P.D. Robinson, "Bivariational Bounds," to appear Proc. Roy. Soc. (1974).
[4]G.A. Baker, Jr., in *The Padê Approximant in Theoretical Physics*, edited by G.A. Baker and J.L. Gammel (Academic, New York and London, 1970), p. 1.
[5]Some discussion of persymmetric determinants and their connection with rational approximations is given by T. Muir, *A Treatise on the Theory of Determinants* (Dover, New York, 1963), p. 419 *et seq.*
[6]A more physical construction in the case of series of Stieltjes has been given by S.T. Epstein and M.F. Barnsley, J. Math. Phys. **14**, 314 (1973), Appendix C.
[7]Detailed considerations of similar Hilbert spaces and operators are given by F. Riesz and B. Sz-Nagy, *Functional Analysis* (Ungar, New York, 1955).
[8]Ref. 7.
[9]Consider the purely discrete case where $d\varphi(u) = \sum_{n=1}^{\infty} v_n \delta(w_n - w)$ with $0 \le w_1 < w_2 \cdots$. Then we may take $\mathfrak{H}$ to be the Hilbert space with orthonormal basis set $\{l_n\}_{n=1}^{\infty}$ with $l_n = (0, 0, \ldots, 1, 0, \ldots)$ having one in the nth place. Putting $L = \sum_{n=0}^{\infty} w_n l_n^* l_n$, $\eta = (|v_1|^{1/2}, |v_2|^{1/2}, \ldots)$, and $\xi = (\mathrm{sgn}\{v_1\}|v_1|^{1/2}, \mathrm{sgn}\{v_2\}|v_2|^{1/2}, \ldots)$, we obtain a representation of $f(x)$ of the desired form. In the combined case we may take $\mathfrak{H} = \mathfrak{H}_{\text{continuous}} \oplus \mathfrak{H}_{0\,\text{discrete}}$, $L = L_{\text{continuous}} \oplus L_{\text{discrete}}$ and so on. This procedure is formally equivalent to the one mentioned in the text. provided we understand, for example, $\int_0^{\infty} g(u)[\delta(w-u)]^{1/2} = 0$, when $0 \le w < \infty$ and $g(u) \in \mathfrak{H}_{\text{continuous}}$.
[10]J. Nuttal, in *The Padê Approximant in Theoretical Physics*, edited by G.A. Baker and J.L. Gammel (Academic, New York and London, 1970), pp. 219—40.
[11]M.F. Barnsley and P.D. Robinson, "Padê Approximant Bounds and Approximate Solutions for Kirkwood—Riseman Integral Equations," to appear J. Inst. Math. Appl. (1974).
[12]Ref. 4, see p. 36.
[13]C. Lopez and F.J. Yndurâin, in *Padê Approximants and Their Applications*, edited by P.R. Graves-Morris (Academic, New York and London, 1973), p. 219—40.
[14]The bounds supplied by PA's plus correction terms will not usually be "best possible on the basis of the given information." For example, with the nomenclature of Sec. 4B one can write $f(x) = f^+(x) - f^-(x)$ where

$$f^{\pm}(x) = \int_0^{1/R} \frac{1/2[d\theta(u) \pm d\phi(u)]}{(1+ux)}$$

are both series of Stieltjes representable functions. The bounds which are "best possible" can now be established to be

$$[N-1/n]_{f^+} - [N/N]_{f^-} \le f(x) \le [N/N]_{f^+} - [N-1/N]_{f^-},$$

in the obvious notation. However, the feature of forming PA's to $f(x)$ itself is lost.
[15]Ref. 6.

From a "laboratory" Galilei-Hilbert bundle to an algebra of observables

Maria C. Abbati, Renzo Cirelli, and Franco Gallone

Istituto di Scienze Fisiche dell'Università, 20133 Milano, Italy
Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Milano, Italy
(Received 4 February 1974)

After a schematic examination of the "physical" representations of the Galilei group, a quantum mechanical description is drawn from a "laboratory" one in the case of a free elementary system with spin, assuming that the kinematical group is the Galilei group. In fact, the "laboratory states" of the system naturally fit in a Galilei-Hilbert bundle. Then, according to the general theory of the unitary representations of groups in the framework of Hilbert bundles which is outlined in this paper, a unitary representation of the Galilei group is constructed which is shown to contain all the physical Galilei representations. The quantum mechanical description which has been obtained in this way gives rise to an algebra of observables by means of a general procedure which connects a unitary representation of a Lie group with a Hilbert representation of the corresponding Lie algebra. The inner energy is shown to be a superobservable for the system under consideration. Moreover, the kinematical properties of such a system are independent of the values of the inner energy.

1. INTRODUCTION

The subject of this paper is the quantum mechanical description of the kinematical properties of an isolated elementary system with spin, namely its behavior under translations, rotations, uniform motions, assuming as kinematical group the Galilei group. However, such properties are completely described by a unitary representation of the group in a Hilbert space, and these representations are very well known.[1] Then what is the novelty of the present work?

Before answering this question, we mention that in Sec. 3 it is shown that successful means in the construction of a unitary representation of a group G is to find a G-Hilbert bundle. Now, we are in the position to expound the somewhat unusual procedure we adopt here. Our starting-point is the remark that the "laboratory states" of an isolated elementary system naturally fit into a Galilei–Hilbert bundle. Then, we are led to construct a representation of the Galilei group, which is shown to contain all the "physical" representations of the the group. Moreover, an "algebra of observables" can be drawn from such a description. Finally, the inner energy is shown to be a superobservable for the system under examination and two such systems have the same kinematical properties also if the relative values of the inner energies are different.

The main physical significance and justification for the the present work are that it furnishes a concrete example of a procedure the extent of which is greater than the definite case which is the object of this work. Such a procedure is to derive, for a physical system, a quantum mechanical description (here this term means that kind of picture involving Hilbert spaces, self-adjoint operators, continuous representations of groups, and so on) from something to be interpreted as a "laboratory" description of the system, inasmuch as it is this phenomenological information which forms in a sense the phenomenological definition of the physical system under consideration. To be definite, such a rather general procedure can be outlined in the following way:

(a) We consider a physical system and a group G as its symmetry group.

(b) The "laboratory" properties of the system lead us to construct in a rather naive way a "set bundle" with an action of G, namely to single out a set (the "base set") whose elements can be interpreted as the "geometric" states of the system and, for any such geometric state, a set (a "fiber") whose elements are to be added to the geometric state to get a "total" state (the fibers then represent the inner variables of the system).[2] Such a state can be called a "laboratory" state as it represents a definite phenomenological situation for the physical system. In addition, we find an action of G on this bundle in a natural way, namely looking at the fashion in which the states transform in connection with G.

(c) We add mathematics (e.g., topological or analytical or Borel structures, measures of the elements of volume, connections among the emerging structures) to the structure of (b).[3] For instance, we can try to construct a G-Hilbert bundle. Suppose we succeed in this purpose.

(d) According to the theory expounded in Sec. 3, a Hilbert space can be constructed as well as a unitary representation of G on it. Therefore we have a quantum mechanical description of the system. Suppose that G is a Lie group. Then we can draw a representation of the Lie algebra of G by essentially self-adjoint operators.[4]

(e) We take the von Neumann algebra generated by the range of the representation of the Lie algebra of G constructed in (d). We are then in the framework of the algebraic approach to quantum mechanics which has been developed by Jauch and others.[5] Therefore we can interpret the mathematical structure that we have got from the standpoint of the algebra of observables. In this way we can reach or recover physically interpretable results, as for instance the presence of superselection rules and the way in which the superselection sectors depend on the values of superobservables.

This procedure is applied in Sec. 4 to a free elementary system with spin (namely the spin is the only inner variable), taking the Galilei group for the kinematical group. Then, in the "set bundle" of (b) the elements of the "base set" are the energy and momentum states and those of the "fibers" are the spin states. To perform the program of (e) it remains necessary to know what are the "physical" representations of the Galilei group. Therefore in Sec. 2 we sketch the arguments which lead to the classification and the construction of these "physical" representations.

In Sec. 3 we expound some theory about G-Hilbert bundles. We show that in this mathematical structure a unitary representation of a group G can be easily constructed. The scope of Sec. 3 is wider than its mere application to the Galilei group which is made in Sec. 4. In fact, Hilbert bundles can be of notable importance in theoretical physics, as can be inferred also from the generality of the scheme outlined above.

2. PHYSICALLY MEANINGFUL REPRESENTATIONS OF THE GALILEI GROUP

In this section we shall outline the chain of arguments which lead to the physically meaningful representations of the proper Galilei group (which will be called the Galilei group in the sequel). Moreover, we shall write a definite expression for any such representation. Since the proof of any assertion of this section will be not even hinted here, to any assertion a definite reference is ascribed wherein the proof can be found.

To avoid unessential complications, we replace the Galilei group with its universal covering group, which can be identified with the group $\mathcal{G} = (\mathbb{R}\times\mathbb{R}^3)\times_\alpha(\mathbb{R}^3 \times_\beta SU(2))$. By $\mathbb{R}^n$ we denote the n-dimensional group of reals. By $SU(2)$ the special unitary group of 2×2 matrices. By $\times_\beta$ the semidirect product relative to the homomorphism β of $SU(2)$ into Aut $\mathbb{R}^3$ defined by $\beta(u)\mathbf{v} = D^{(1)}(u)\mathbf{v}$, where $D^{(1)}$ is the spin 1 representation of $SU(2)$. By $\times_\alpha$ the semidirect product relative to the homorphism α of $\mathbb{R}^3\times_\beta SU(2)$ into Aut$(\mathbb{R}^1\times\mathbb{R}^3)$ defined by $\alpha(\mathbf{v},u)(t,\mathbf{a}) = (t, D^{(1)}(u)\mathbf{a}+\mathbf{v}t)$. The composition law of $\mathcal{G}$ is $(t',\mathbf{a}',\mathbf{v}',u')(t,\mathbf{a},\mathbf{v},u) = (t'+t, \mathbf{a}'+D^{(1)}(u')\mathbf{a}+\mathbf{v}'t,\ \mathbf{v}' + D^{(1)}(u')\mathbf{v}, u'u)$, denoting an element g of $\mathcal{G}$ by $(t,\mathbf{a},\mathbf{v},u)$. The group $\mathcal{G}$ is a locally compact (l.c.), second countable (s.c.), and simply connected Lie group.[6]

The representations of $\mathcal{G}$ of physical interest are projective representations,[7] namely Borel homomorphisms of $\mathcal{G}$ into the quotient group $\mathcal{U}/\mathcal{Z}$. Here $\mathcal{U}$ is the unitary group of a separable Hilbert space endowed with the strong operator topology and $\mathcal{Z}$ is the closed and normal subgroup of the elements of $\mathcal{U}$ which are multiples of the identity operator. The Borel structures we consider on $\mathcal{G}$ and $\mathcal{U}/\mathcal{Z}$ are those generated by the respective topologies.[8]

The study of projective representations can be conveniently performed by the study of ω-representations of $\mathcal{G}$.[8] An ω-representation of $\mathcal{G}$ is a Borel map V of $\mathcal{G}$ into $\mathcal{U}$ for which a multiplier ω for $\mathcal{G}$ exists such that $V_{g'g} = \omega(g',g)V_{g'}V_g$. Similarity classes of multipliers exist, equal in number to the values of a label m which ranges in $\mathbb{R}$. A representative for the class labelled by m is $\omega_m((t',\mathbf{a}',\mathbf{v}',u'),(t,\mathbf{a},\mathbf{v},u)) = \exp[im(\frac{1}{2}\mathbf{v}'^2 t + \mathbf{v}'D^{(1)}\times(u')\mathbf{a})]$.[9] For $m=0$ we have a representation of $\mathcal{G}$ which describes a nonlocalizable Galilei invariant system.[10] Moreover, an ω_{-m}-representation and an ω_m-representation, as antiunitarily equivalent, give two physically equivalent projective representations.[11] Therefore, it is enough to study the ω_m-representations with $m>0$.

The study of the ω_m-representations of $\mathcal{G}$ is conveniently performed by a central extension $\mathcal{G}^m$ of $\mathcal{T}$ by $\mathcal{G}$, where $\mathcal{T}$ denotes the one-dimensional torus and the composition law of $\mathcal{G}^m$ is $(z',g')(z,g) = (z'z\omega_m(g',g)^{-1}, g'g)$, with (z',g') and (z,g) in $\mathcal{T}\times\mathcal{G}$. In fact, if V is a continuous unitary representation (CUR) of $\mathcal{G}^m$ such that $V(z,e) = z\mathbb{1}$ for any z in $\mathcal{T}$, its restriction to $\mathcal{G}$ is an ω_m-representation of $\mathcal{G}$ and any ω_m-representation of $\mathcal{G}$ can be obtained in this way.[12]

With the product topology of $\mathcal{T}$ and $\mathcal{G}, \mathcal{G}^m$ results in a l.c.s.c. Lie group. The group $\mathcal{G}^m$ can be identified with the "regular" semidirect product $(\mathcal{T}\times\mathbb{R}\times\mathbb{R}^3)\times_{\alpha_1}(\mathbb{R}^3\times_\beta SU(2))$, where α_1 is the homomorphism defined by $\alpha_1(\mathbf{v},u)(z,t,\mathbf{a}) = (z\exp[-im(\mathbf{v}D^{(1)}(u)\mathbf{a} + \frac{1}{2}\mathbf{v}^2 t)], t, D^{(1)}(u)\mathbf{a} + \mathbf{v}t)$. Since $\mathcal{G}^m$ is a "regular" semidirect product, Mackey's standard procedure[13] can be applied to obtain all the equivalence classes of irreducible CUR's (CUIR's) of $\mathcal{G}^m$. The results can be summarized in the following way. An action of $\mathcal{G}^m$ can be defined on the dual $\mathbb{Z}\times\mathbb{R}\times\mathbb{R}^3$ (Z denotes the group of integers) of the group $\mathcal{T}\times\mathbb{R}\times\mathbb{R}^3$. Then, take a point $(n,p_0,\mathbf{p})$ of an orbit and a CUIR L of the "little group" $\mathcal{G}^m_{(n,p_0,\mathbf{p})}$ [namely the group of the elements of $\mathcal{G}^m$ which lie in $\mathbb{R}^3\times_\beta SU(2)$ and leave $(n,p_0,\mathbf{p})$ invariant] and construct the representation $U^{(n,p_0,\mathbf{p})L}$ of $\mathcal{G}^m$ induced by the representation $(n,p_0,\mathbf{p})L$ of the subgroup $(\mathcal{T}\times\mathbb{R}\times\mathbb{R}^3)\times_{\alpha_1}\mathcal{G}^m_{(n,p_0,\mathbf{p})}$. As $U^{(n,p_0,\mathbf{p})L}$ is irreducible, this procedure results in the construction of a CUIR of $\mathcal{G}^m$ starting from a CUIR of the little group of a point of an orbit. Moreover, all the CUIR's of $\mathcal{G}^m$ are obtained by this procedure and any one of them once and only once (up to equivalence), if all the orbits are taken and for any orbit all the CUIR's (up to equivalence) of the little group of a (definite but arbitrarily chosen) point of the orbit.[14]

For the case of interest ($m>0$), the $\mathcal{G}^m$-orbits are the sets $\mathcal{O}_{n,\epsilon} = \{(n,p_0,\mathbf{p})\in\mathbb{Z}\times\mathbb{R}\times\mathbb{R}^3;\ \mathbf{p}^2 - 2nmp_0 = \epsilon\}$ with $\epsilon\in\mathbb{R}$ and $n\in\mathbb{Z}$, and $\{(0,p_0,\mathbf{0})\}$ with $p_0\in\mathbb{R}$ (0 and $\mathbf{0}$ are the null elements of Z and $\mathbb{R}^3$, respectively). The little group of a point of the orbit $\mathcal{O}_{n,\epsilon}$ is isomorphic to $SU(2)$ if $n\neq 0$ and to the two-dimensional Euclidean group if $n=0$, while the little group of $\{(0,p_0,0)\}$ is isomorphic to the three-dimensional Euclidean group.

The CUIR's of $\mathcal{G}^m$ which give rise to ω_m-representations of $\mathcal{G}$ are (up to equivalence) just those which can be constructed from the orbits $\mathcal{O}_{1,\epsilon}$, with $\epsilon\in\mathbb{R}$. Therefore, considering the CUIR's $V^{(\epsilon,j)} = U^{(1,\epsilon/2m,0)D^{(j)}}$ [where $D^{(j)}$ denotes the spin j representation of $SU(2)$] of $\mathcal{G}^m$ for any half-integer j and any real number ϵ, we take in fact into account all the physically meaningful representations of $\mathcal{G}$. The representation $V^{(\epsilon,j)}$ can be expressed conveniently in the Hilbert space $L^2_{\mathbb{C}^{2j+1}}(\mathbb{R}^3,\nu^3)$ (ν^3 denotes the Lebesgue measure on $\mathbb{R}^3$)[16] as follows:

$$(V^{(\epsilon,j)}_{(z,\ell)}f)(\mathbf{p})$$

$$= z\exp\, i\left(-\frac{1}{2m}(\mathbf{p}^2-\epsilon)t+\mathbf{pa}\right)\; D^{(j)}(u)f(D^{(1)}(u^{-1})(\mathbf{p}-m\mathbf{v})),$$

$$\forall f\in L^2_{\mathbb{C}^{2j+1}}(\mathbb{R}^3,\nu^3).^{17}$$

In Sec. 4 we shall present a method to get the physically meaningful representations of $\mathcal{G}$ by means of a definite realization of the mathematical structure to be examined in Sec. 3. The important point is that such a realization can be construed from a "laboratory" point of view.

3. G-HILBERT BUNDLES

In the next section we shall draw representations of the Galilei group from a Galilei–Hilbert bundle, which will not be transitive. Since Hilbert bundles with the action of a group are not commonly treated in the literature, at least in the nontransitive case, it is convenient to expound here the elements of this subject which are needed in the next section.

First of all, we prove a theorem which provides us with a tool to construct a Hilbert space out of a field of Hilbert spaces. For the definitions of Borel field and of direct integral of Hilbert spaces and of any other related concept that we use in this paper, see Ref. 16 (hereafter denoted DW).

Proposition 1: Let Z be a Borel space and $\{H(\zeta)\}(\zeta\in Z)$ a field of Hilbert spaces[18] such that [denoting by $d(\zeta)$ the dimension of $H(\zeta)$] $Z_p=\{\zeta\in Z;\ d(\zeta)=p\}$ is a Borel set of any p. For any p let H_p be a define p-dimensional Hilbert space and for any $\zeta\in Z$ let $U(\zeta)$ be a definite unitary isomorphism of $H(\zeta)$ onto $H_{d(\zeta)}$. Denoting by $\Pi_{\zeta\in Z}H(\zeta)$ the complex vector space of the fields of vectors, let

$$\sigma=\{x\in\prod_{\zeta\in Z}H(\zeta);\ Z_p\ni\zeta\to U(\zeta)x(\zeta)\in H_p \text{ is a Borel map for any } p\},$$

where in H_p the Borel structure induced by the norm is considered. Depending on σ, $\{H(\zeta)\}(\zeta\in Z)$ results in a Borel field of Hilbert spaces on Z.

Proof: From Lemma 8.4 in Ref. 19 we have that, for an element x of $\Pi_{\zeta\in Z}H(\zeta)$, $x\in\sigma$ iff $Z_p\ni\zeta\to(u\,|\,U(\zeta)x(\zeta))\in\mathbb{C}$ (where $\mathbb{C}$ denotes the complex plane) is a Borel function, $\forall\ u\in H_p$ and for any p. Then it is easy to show that σ fulfills the conditions of Definition 1 and Rem. 3 in DW-11.1.3. First we notice, in fact, that σ is obviously a linear subspace of $\Pi_{\zeta\in Z}H(\zeta)$. Next, for any $x\in\sigma$, $Z_p\ni\zeta\to\|x(\zeta)\|\in\mathbb{R}$ is a Borel function for any p, as $\|x(\zeta)\|^2=\sum_n|(u_n^{(p)}\,|\,U(\zeta)x(\zeta))|^2$ for any orthonormal basis $\{u_n^{(p)}\}$ in H_p. Hence $\|x(\zeta)\|$ is a Borel function on Z, since the Z_p's are Borel sets whose (countable) union is Z. Let, moreover, $y\in\Pi_{\zeta\in Z}H(\zeta)$ be such that $Z\ni\zeta\to(x(\zeta)\,|\,y(\zeta))\in\mathbb{C}$ is a Borel function, $\forall\ x\in\sigma$. For any p, take then $x^{(p)}$ in H_p and define the field of vectors $x(\zeta)=U(\zeta)^{-1}x^{(d(\zeta))}$. As x is obviously an element of σ, $(x^{(d(\zeta))}\,|\,U(\zeta)y(\zeta))$ is a Borel function on Z, whence $(x^{(p)}\,|\,U(\zeta)y(\zeta))$ is a Borel function on Z_p for any $x^{(p)}$ in H_p and for any p, namely $y\in\sigma$. For any p let finally $\{x_n^{(p)}\}$ be a sequence of elements of H_p which span H_p. Then the field of vectors $x_n(\zeta)=U(\zeta)^{-1}x_n^{(d(\zeta))}$ is obviously an element of σ for any n and $\{x_n(\zeta)\}$ span $H(\zeta)$ for any ζ as $U(\zeta)$ is a unitary isomorphism. This completes the proof.

When the conditions of this theorem hold, we can construct a direct integral $\int_Z^{\oplus}H(\zeta)\,d\mu(\zeta)$ of the $H(\zeta)$'s whenever a σ-finite measure μ is given on Z.[20] Take in fact all the elements $y\in\Pi_{\zeta\in Z}H(\zeta)$ such that the function $Z\ni\zeta\to(y(\zeta)\,|\,x(\zeta))$ is μ-measurable for any $x\in\sigma$. With the set of such elements, $\{H(\zeta)\}(\zeta\in Z)$ results in a μ-measurable field of Hilbert spaces. Therefore, we can define $\int_Z^{\oplus}H(\zeta)\,d\mu(\zeta)$ as the direct integral originating from this μ-measurable field. It is remarkable that any element of $\int_Z^{\oplus}H(\zeta)\,d\mu(\zeta)$ is an equivalence class which contains an element of σ. We shall denote the elements of the direct integral and the representatives thereof with the same notation and, when it will prove useful, we shall choose representatives which lie in σ.

Now we define G-Hilbert bundles, assuming for G a l.c.s.c. group.

Definition 1: A G-Hilbert bundle is a standard Borel space Z on which a field $\{H(\zeta)\}(\zeta\in Z)$ of Hilbert spaces is given, such that, denoting by B the set $B=\cup_{\zeta\in Z}H(\zeta)$ and by π the map

$$\pi: B\to Z,\quad \pi(w)=\zeta \text{ if } w\in H(\zeta),$$

the following conditions hold:

(a) Z is a Borel G-space, namely a homomorphism t of G into the group of the automorphisms of Z exists such that $G\times Z\ni(g,z)\to t(g)\zeta\in Z$ is a Borel map.

(b) B is a G-space, namely a homomorphism T exists of G into the group of the bijections of B with itself.

(c) π is an intertwining map for T and t, namely $t(g)\circ\pi=\pi\circ T(g)$ for each $g\in G$. Moreover, $T(g)$ restricted to $H(\zeta)$ is a unitary isomorphism of $H(\zeta)$ onto $H(t(g)\zeta)$ for each $g\in G$ and $\zeta\in Z$.

(d) Z_p (defined as in Proposition 1) is a Borel set for any p and for each $\zeta\in Z$ a unitary isomorphism $U(\zeta)$ of $H(\zeta)$ onto $H_{d(\zeta)}$ (H_p denotes a definite p-dimensional Hilbert space) exists such that

$$G\times Z_p\ni(g,\zeta)\to U(\zeta)T(g)U(t(g^{-1})\zeta)^{-1}\in U(H_p)$$

is a Borel map for any p, if on the unitary group $U(H_p)$ of H_p the strong operator topology is assumed.

This definition seems somewhat different from the usual ones of G-Hilbert bundles. To recover, for instance, the definition of Ref. 19 (p. 86), we have in fact to replace (d) in the definition above with the following condition: (d′) Z is transitive with respect to t and B is a standard Borel space such that π is a Borel map, B is a Borel G-space with respect to T and, for each $\zeta\in Z$, the natural Borel structure of $H(\zeta)$ is the one induced on it by B. Definition 1 is indeed a generalization of Varadarajan's definition since they are fully equivalent when Z is a transitive G-space. In fact, if (a), (b), and (c) hold, it can be proved that (d) follows from (d′) and that, whenever in (a) Z is transitive and (d) holds,

one and only one (up to isomorphism) Borel structure exists on B such that (d′) holds.[21]

Such an equivalence is really also a motivation to call the structure defined in Definition 1 a G-Hilbert bundle, since this term is the usual one for the structure of Varadarajan's definition. We notice in particular that a result from the previous discussion is that in a transitive G-Hilbert bundle (namely in a G-Hilbert bundle with Z transitive) a Borel structure can be defined on B such that $\{H(\zeta)\}(\zeta \in Z)$ is a Hilbert bundle (in the sense of the definition in Ref. 19, p. 86).

Finally, we construct a CUR of G in a G-Hilbert bundle.

Proposition 2: Let a G-Hilbert bundle be given (whose constituents we denote with the same symbols as in Definition 1) along with a σ-finite measure μ on Z and let μ be invariant with respect to the action t of G. Denoting by H the Hilbert space $\int_Z^{\oplus} H(\zeta)\,d\mu(\zeta)$, for $g \in G$ define the mapping $V_g: H \to H$, $(V_g x)(\zeta) = T(g)x(t(g^{-1})\zeta)$. For each $g \in G$, V_g is a unitary operator and the mapping $V: G \to U(H)$, $V(g) = V_g$ of G into the unitary group $U(H)$ of H is a CUR of G.

Proof: First we notice that the possibility of defining H in the framework of a G-Hilbert bundle derives from Proposition 1 and the remarks following it. Moreover, H results in a separable Hilbert space, as a consequence of the Corollary in DW-11.1.6.

Next we have to prove the consistency of the definition of V_g, namely that $V_g x$ is indeed an element of H, for each $g \in G$ and $x \in H$. Take then $x \in H$. For any p, $G \times Z_p \ni (g, \zeta) \to U(t(g^{-1})\zeta)x(t(g^{-1})\zeta) \in H_p$ [whose definition is correct after (c) in Definition 1] is a Borel map since it is the product of $Z_p \ni \zeta \to U(\zeta)x(\zeta) \in H_p$, which is a Borel map by definition of σ in Proposition 1, and of $G \times Z_p \ni (g, \zeta) \to t(g^{-1})\zeta \ni Z_p$, which is a Borel map since Z_p is a Borel set and (a) in Definition 1 holds. Hence, as a consequence of (d) in Definition 1,

$$G \times Z_p \ni (g, \zeta) \to (U(\zeta)T(g)U(t(g^{-1})\zeta)^{-1},$$

$$U(t(g^{-1})\zeta)x(t(g^{-1})\zeta) \in U(H_p) \times H_p$$

is also a Borel map and this in turn implies that

$$G \times Z_p \ni (g, \zeta) \to U(\zeta)T(g)x(t(g^{-1})\zeta) \in H_p$$

is a Borel map, as $U(H_p) \times H_p \ni (V, u) \to Vu \in H_p$ is easily shown to be a continuous map with respect to the strong operator topology and to the norm of H_p. Therefore, for each $g \in G$, $V_g x$ is an element of $\Pi_{\zeta \in Z} H(\zeta)$ which lies in σ [as follows from (c) in Definition 1]. In fact, it is an element of H, since square integrability follows from

$$\int_Z \|T(g)x(t(g^{-1})\zeta)\|^2 d\mu(\zeta) = \int_Z \|x(\zeta)\|^2 d\mu(\zeta) = \|x\|^2,$$

which is a consequence of (c) in Definition 1 and of the invariance of μ.

For each $g \in G$ it is trivial to show that V_g is an isometric operator on H and that $V_g(V_{g^{-1}}x) = x, \forall\, x \in H$, from which it follows that V_g is indeed a unitary operator. Moreover, $V_{g_1 g_2} = V_{g_1} V_{g_2}, \forall\, g_1, g_2 \in G$, as can be shown by an easy computation. Hence V is a unitary representation of G in H. To complete the proof of the proposition we have to show that V is continuous.

Now, let ν be a finite measure on G equivalent to a Haar measure on G. Such a finite measure exists since in a l.c.s.c. group a Haar measure is σ-finite.[19] We notice also that, for any x and y in H,

$$\varphi: G \times Z \to \mathbb{C}, \quad \varphi(g, \zeta) = ((V_g x)(\zeta) \mid y(\zeta))$$

is a Borel map. In fact, since $G \times Z_p \ni (g, \zeta) \to U(\zeta)(V_g x) \times (\zeta) \in H_p$ has been previously proved to be a Borel map and $G \times Z_p \ni (g, \zeta) \to U(\zeta)y(\zeta) \in H_p$ is a Borel map by definition of σ in Proposition 1, it can be easily shown that φ restricted to $G \times Z_p$ is a Borel map for any p, whence φ itself is a Borel map as the Z_p's are Borel sets whose (countable) union is Z. Then, by Tonelli theorem,[22] the integral

$$I = \int_G \left(\int_Z |\varphi(g, \zeta)|\, d\mu(\zeta) \right) d\nu(\zeta)$$

exists. Moreover, by Schwarz and Hölder inequalities,

$$\int_Z |\varphi(g, \zeta)|\, d\mu(\zeta) \leq \left(\int_Z \|(V_g x)(\zeta)\|^2 d\mu(\zeta) \right)^{1/2} \times \left(\int_Z \|y(\zeta)\|^2 d\mu(\zeta) \right)^{1/2} = \|x\| \|y\|,$$

whence $I \leq \nu(G)\|x\|\|y\|$. Then, again by Tonelli's theorem, φ is $\nu \times \mu$-integrable on $G \times Z$. Therefore, by Fubini's theorem,[23]

$$G \ni g \to \int_Z \varphi(g, \zeta)\, d\mu(\zeta) = (V_g x \mid y)$$

is ν-measurable for all $x, y \in H$. Since this amounts to the continuity of V,[24] the proposition is proved.

To conclude this mathematical section, we point out that Proposition 2 would hold in a similar form also if the measure μ were not actually invariant, but just quasi-invariant. Anyway, since in the quasi-invariant case the proof is slightly more involved than in the invariant one and since the measure we shall use in the next section is invariant, we have preferred to assume μ invariant.

4. A "LABORATORY" GALILEI-HILBERT BUNDLE AND THE INNER ENERGY AS A SUPERSELECTION RULE

In this section we shall be concerned with the description of an isolated elementary system with spin, namely of a free system with no inner variables other than spin. In fact, we shall study its kinematical properties in the framework of Galilean relativity.

We shall present here a way to deduce, from the "laboratory" kinematical properties of a free elementary system of spin j and mass m, its quantum mechanical kinematical properties in the following sense. A triple of values of the energy, the momentum, and the spin can be assumed to be a "laboratory state" of the system, while its quantum kinematical properties are completely described in the framework of a unitary representation of the Galilei group $\mathcal{G}$ in a Hilbert space. Then, we shall deduce a unitary representation of $\mathcal{G}$ from the behavior of the energy, the momentum, and the spin of the system with respect to the transformations of $\mathcal{G}$. In this deduction we shall use the theory expounded in Sec. 3.

From the conclusions of Sec. 2, the "right" group to study the physical representations of $\mathcal{G}$ is the extended group $\mathcal{G}^m$. Then, the approach to Galilean invariance

from the point of view of the Hilbert bundle techniques is to construct a $\mathcal{G}^m$-Hilbert bundle and a CUR of $\mathcal{G}^m$ therein.

With the notations of Definition 1, we assume $Z=\mathbb{R}^4$ and construct on it a field of Hilbert spaces $\{H(p_0,\mathbf{p})\}$ $((p_0,\mathbf{p})\in\mathbb{R}^4)$ setting $H(p_0,\mathbf{p})=\mathbb{C}^{2j+1}$ for each $(p_0,\mathbf{p})\in\mathbb{R}^4$. On $\mathbb{R}^4$ and $\mathcal{G}^m$ we take the standard Borel structures generated by the respective topologies. Moreover, we define a homomorphism t of $\mathcal{G}^m$ into the group of the automorphisms of $\mathbb{R}^4$ setting $t(z,g)(p_0,\mathbf{p})=(p_0',\mathbf{p}')$, where $p_0'=p_0+(m/2)\mathbf{v}^2+D^{(1)}(u)\mathbf{pv}$ and $\mathbf{p}'=D_u^{(1)}\mathbf{p}+m\mathbf{v}$, for each $(z,g)\in\mathcal{G}^m$ and $(p_0,\mathbf{p})\in\mathbb{R}^4$. We also construct a homomorphism T of $\mathcal{G}^m$ into the group of the automorphisms of $B=\cup_{(p_0,\mathbf{p})\in\mathbb{R}^4}H(p_0,\mathbf{p})$, defining $T(z,g)\mathbf{s}$ to be the element $\varphi(p_0,\mathbf{p};z,g)D^{(j)}(u)\mathbf{s}$ of $H(p_0',\mathbf{p}')$, where $\varphi(p_0,\mathbf{p};z,g)=z\exp[i(-p_0't+\mathbf{p}'\mathbf{a})]$, for each $(z,g)\in\mathcal{G}^m$ and each $\mathbf{s}\in B$ which lies in $H(p_0,\mathbf{p})$.[25] Finally, for each $(p_0,\mathbf{p})\in\mathbb{R}^4$, we choose the identity map of $\mathbb{C}^{2j+1}$ to be the unitary isomorphism $U(p_0,\mathbf{p})$ of Definition 1. Then, all the conditions of Definition 1 are easily shown to hold.[26]

The action t we assume on the "base space" $\mathbb{R}^4$ can be easily interpreted from the "laboratory" viewpoint. In fact, $t(z,g)(p_0,\mathbf{p})$ depends only upon the element g of the Galilei group and not upon z and represents the transformation of the laboratory values p_0 of the energy and $\mathbf{p}$ of the momentum of the system for two Galilean observers related by g. The action T we assume on the "total space" B is related to the laboratory behavior of the values of the spin, but it cannot be interpreted as easily as t could. Indeed, the rays in $\mathbb{C}^{2j+1}$ and not the vectors represent the spin states. Therefore, in the "laboratory" determination of an action on B, a phase factor is at our disposal. We have in fact introduced the function φ in the definition of T. A motivation for the "z" part of φ can be found in the link between the representations of $\mathcal{G}^m$ and the projective representations of $\mathcal{G}$, which has been explained in Sec. 1. The convenience of adding to z the exponential part in φ can be understood after the following considerations. In fact, without this exponential part, T would provide a trivial action of time and space translations. Therefore, from the $\mathcal{G}^m$-Hilbert bundle a CUR of $\mathcal{G}^m$ would be drawn in which the translations are represented in a trivial way. This is hardly acceptable since it can be easily shown to lead to a quantum mechanical picture without a position operator and without evolution. Finally, the definite form we have adopted for the exponential part is suggested by the classical relation of energy and momentum with time and space translations.

To draw a CUR of $\mathcal{G}^m$ from the Galilei–Hilbert bundle constructed above, according to Proposition 2 we need a σ-finite invariant measure on $\mathbb{R}^4$. Let ν^4 be the Lebesgue measure on $\mathbb{R}^4$ and α the Borel automorphism of $\mathbb{R}^4$ defined as $\alpha(p_0,\mathbf{p})=(\mathbf{p}^2-2mp_0,\mathbf{p})$. The function μ on the Borel structure of $\mathbb{R}^4$, defined as $\mu(\Delta)=\nu^4(\alpha(\Delta))$ for each Borel set Δ of $\mathbb{R}^4$, is obviously a σ-finite measure on $\mathbb{R}^4$. Moreover, a brief calculation proves that μ is invariant with respect to t, since ν^4 is invariant with respect to the action $\tau(z,g)(p_0,\mathbf{p})=(p_0,D^{(1)}(u)\mathbf{p}+m\mathbf{v})$ of $\mathcal{G}^m$ on $\mathbb{R}^4$ and $\tau=\alpha\circ t\circ\alpha^{-1}$.

Then, from Proposition 2 it follows that

$$V_{(z,g)}:H\to H,\quad (V_{(z,g)}f)(p_0,\mathbf{p})=z\exp[i(-p_0t+\mathbf{pa})]\times D^{(j)}(u)f\left(p_0+\frac{m}{2}\mathbf{v}^2-\mathbf{pv},\ D^{(1)}(u^{-1})(\mathbf{p}-m\mathbf{v})\right),$$

is a unitary operator on $H=\int_{\mathbb{R}^4}^{\oplus}H(p_0,\mathbf{p})\,d\mu(p_0,\mathbf{p})$ for each $(z,g)\in\mathcal{G}^m$ which gives rise to a CUR V of $\mathcal{G}^m$. We shall now show that V contains all the physical representations of $\mathcal{G}$ for the values m for the mass and j for the spin.

Let H_0 denote the Hilbert space $L^2_{\mathbb{C}^{2j+1}}(\mathbb{R}^3,\nu^3)$. Take the field of Hilbert spaces $\{H(\epsilon)\}(\epsilon\in\mathbb{R})$, where $H(\epsilon)=H_0$ for each $\epsilon\in\mathbb{R}$. It is a Borel field with respect to the set of the fields of vectors which are Borel maps from $\mathbb{R}$ into H_0. Then we define $H^{(1)}=\int_{\mathbb{R}}^{\oplus}H(\epsilon)\,d\nu(\epsilon)$, where ν stands for the Lebesgue measure on $\mathbb{R}$. This will result in a Hilbert space where V decomposes into a direct integral of all the CUIR's of $\mathcal{G}^m$ which give rise to physical representations of $\mathcal{G}$. Construct in fact the map

$$W:H\to H^{(1)},\quad (Wf)(\epsilon)=\int_{\mathbb{R}}^{\oplus}f(\alpha^{-1}(\epsilon,\mathbf{p}))\,d\nu^3(\mathbf{p}).$$

It is shown to be a unitary isomorphism of H onto $H^{(1)}$ in the following way. First, after some technicalities the definition of W is shown to be consistent. Next, W is shown to be isometric from the following equalities:

$$\int_{\mathbb{R}}\|(Wf)(\epsilon)\|^2\,d\nu(\epsilon)=\int_{\mathbb{R}}\left(\int_{\mathbb{R}^3}\|f(\alpha^{-1}(\epsilon,\mathbf{p}))\|^2\,d\nu^3(\mathbf{p})\right)d\nu(\epsilon)=\int_{\mathbb{R}^4}\|f(\alpha^{-1}(\epsilon,\mathbf{p}))\|^2\,d\nu^4(\epsilon,\mathbf{p})=\int_{\mathbb{R}^4}\|f(p_0,\mathbf{p})\|^2\,d\mu(p_0,\mathbf{p}),$$

of which the second one follows from Fubini's theorem and the third one from 111.10.8 in Ref. 27. Finally, take three orthonormal bases $\{f_n\}$, $\{g_r\}$ and $\{u_k\}$ for $L^2(\mathbb{R},\nu)$, $L^2(\mathbb{R}^3,\nu^3)$ and $\mathbb{C}^{2j+1}$, respectively. Then $\{f_{n,r,k}\}$, where

$$f_{n,r,k}=\int_{\mathbb{R}}^{\oplus}f_n(\mathbf{p}^2-2mp_0)g_r(\mathbf{p})u_k\,d\mu(p_0,\mathbf{p}),$$

is an orthonormal basis for H.[28] Moreover $\{\psi_{n,r,k}\}$, where $\psi_{n,r,k}=Wf_{n,r,k}$, is an orthonormal basis for $H^{(1)}$, since

$$(Wf_{n,r,k})(\epsilon)=f_n(\epsilon)\int_{\mathbb{R}^3}^{\oplus}g_r(\mathbf{p})u_k\,d\nu^3(\mathbf{p})$$

and $\{g_{r,k}\}$, where

$$g_{r,k}=\int_{\mathbb{R}^3}^{\oplus}g_r(\mathbf{p})u_k\,d\nu^3(\mathbf{p}),$$

is an orthonormal basis for H_0.[28] This completes the proof that W is unitary.

Now, we can determine the form taken by the representation V, when it is transferred in $H^{(1)}$ through the unitary isomorphism W. We have, for each $(z,g)\in\mathcal{G}^m$ and for any $\psi_{n,r,k}$,

$$(WV_{(z,g)}W^{-1}\psi_{n,r,k})(\epsilon)=\int_{\mathbb{R}^3}^{\oplus}(V_{(z,g)}W^{-1}\psi_{n,r,k})(\alpha^{-1}(\epsilon,\mathbf{p}))\,d\nu^3(\mathbf{p})$$

$$= \int_{\mathbb{R}^3}^{\oplus} z \exp[i((-\tfrac{1}{2}m)(\mathbf{p}^2-\epsilon)t+\mathbf{p}\,\mathbf{a})]$$

$$\times D^{(j)}(u)(W^{-1}\psi_{n,r,k})\Big(\frac{1}{2m}(\mathbf{p}^2-\epsilon)+\frac{m}{2}\mathbf{v}^2-\mathbf{p}\mathbf{v},$$

$$D^{(1)}(u^{-1})(\mathbf{p}-m\mathbf{v})\Big)\, d\nu^3(\mathbf{p})$$

$$= V^{(\epsilon)}_{(z,g)} \int_{\mathbb{R}^3}^{\oplus} \psi_{n,r,k}(\epsilon,\mathbf{p})\, d\nu^3(\mathbf{p})$$

$$= V^{(\epsilon)}_{(z,g)}\psi_{n,r,k}(\epsilon) \quad \text{(Ref. 29)}$$

where $V^{(\epsilon)}$ is the CUIR of $\mathcal{G}^m$ introduced in Sec. 2.[30] First of all, from these results it follows that $\epsilon \to V^{(\epsilon)}$ is a ν-measurable field of CUR's of $\mathcal{G}^m$ (for the definition of ν-measurable field of CUR's, see 18.7.1 in Ref. 31, hereafter cited as DC). The field of unitary operators $\epsilon \to V^{(\epsilon)}_{(z,g)}$ is in fact ν-measurable for each $(z,g)\in\mathcal{G}^m$, as $WV_{(z,g)}W^{-1}\psi_{n,r,k}$ is obviously an element of $H^{(1)}$ for any $\psi_{n,r,k}$ and the representatives of $\psi_{n,r,k}$ make up a fundamental sequence of ν-measurable fields of vectors (DW-11.1. Proposition 4, 11.2. Proposition 1). Moreover, $WV_{(z,g)}W^{-1}$ coincides with $\int_{\mathbb{R}}^{\oplus} V^{(\epsilon)}_{(z,g)}\, d\nu(\epsilon)$ for each $(z,g)\in\mathcal{G}^m$, since they are two unitary operators which transform in the same way the vectors of an orthonormal basis of $H^{(1)}$. Therefore, the representation V is unitarily equivalent, by means of W, to the CUR $V^{(1)} = \int_{\mathbb{R}}^{\oplus} V^{(\epsilon)} d\nu(\epsilon)$ of $\mathcal{G}^m$ in $H^{(1)}$.

In fact, the discussion above is the proof of the following theorem.

Theorem: For a Galilei-invariant free elementary system of mass m and spin j it is possible to introduce in a fairly natural way a Galilei–Hilbert bundle with a σ-finite invariant measure, which leads to the construction of a CUR V of $\mathcal{G}^m$ in a Hilbert space H. By a unitary isomorphism of H onto a direct integral of Hilbert spaces $H^{(1)} = \int_{\mathbb{R}}^{\oplus} H(\epsilon)\, d\nu(\epsilon)$, where $H(\epsilon) = L^2_{\mathbb{C}^{2j+1}}(\mathbb{R}^3, \nu^3)$ for each $\epsilon\in\mathbb{R}$, V can be decomposed into the direct integral $\int_{\mathbb{R}}^{\oplus} V^{(\epsilon)}\, d\nu(\epsilon)$ of the CUIR's $V^{(\epsilon)}$, which are all the spin j representations of $\mathcal{G}^m$ whose restrictions to $\mathcal{G}$ are the physical representations of $\mathcal{G}$ for the fixed values of the mass and the spin.

Hence, a representation of $\mathcal{G}^m$ has been constructed which contains any physical representation of $\mathcal{G}$ relative to the values m for the mass and j for the spin. We remark now that in correspondence to the decomposition of V into $\int_{\mathbb{R}}^{\oplus} V^{(\epsilon)}\, d\nu(\epsilon)$ we get a continuous infinity of copies of the same projective representation of $\mathcal{G}$ in H_0, as in $V^{(\epsilon)}$ the index ϵ is completely embodied by the term $\exp[i(\epsilon/2m)t]$ which is of no significance in passing to projective representations. Therefore, the quantum mechanical description of a free elementary system of mass m and spin j which is provided by V splits into a continuous infinity of mutually equivalent quantum mechanical descriptions. We shall now set forth an interpretation of this fact in the framework of the algebraic formulation of the foundations of quantum mechanics.

From a foundational standpoint, the algebraic approach to quantum mechanics based on W^*-algebras[32] is a very good one as it can be drawn in a sense from the logical approach,[33] which in turn is directly inherent in the phenomenological interpretation of the physical experiments.[34] We expound here just the few elements of the algebraic formulation based on W^*-algebras that are used in the sequel. A detailed treatment can be found in Refs. 5 and 33. To a physical system a W^*-algebra $\mathcal{A}$ of operators in a Hilbert space K is assigned, such that the self-adjoint operators affiliated with $\mathcal{A}$ (namely whose spectral projections belong to $\mathcal{A}$) are a representation of the observables of the system; they are briefly called, in fact, observables of $\mathcal{A}$. The observables which are not multiples of the identity operator and are affiliated with the center $C(\mathcal{A})=\mathcal{A}'\cap\mathcal{A}$ of $\mathcal{A}$ are called superobservables.[35] When superobservables exist, namely when $C(\mathcal{A})$ is not trivial, the picture based on $\mathcal{A}$ is said to have superselection rules. In this framework not every W^*-algebra is assumed to be a sensible algebra of observables. It seems in fact necessary to assume that algebra of observables contains a complete system of commuting observables.[36] This assumption seemed to be denied in its generality by the case of parastatistics.[37] On the contrary, a correct interpretation of the algebra of observables in parastatistics shows that no contradiction arises between this case and the general assumption made above about complete systems.[38]

In a W^*-algebra of observables $\mathcal{A}$, the existence of a complete system of commuting observables is equivalent to $\mathcal{A}'\subset\mathcal{A}$. When this condition holds, a unitary isomorphism of K with a direct integral of Hilbert spaces $K^{(1)} = \int_{\Lambda}^{\oplus} K(\lambda)\, d\rho(\lambda)$ (Λ denotes a locally compact space and ρ a measure on it) exists through which $C(\mathcal{A})$ can be identified with the W^*-algebra $D(K^{(1)})$ ($\mathcal{Z}$ in the notation of DW) of the diagonal operators on $K^{(1)}$. In this isomorphism $\mathcal{A}$ is found to correspond to the W^*-algebra $R(K^{(1)})=D(K^{(1)})'$ of the decomposable operators on $\mathcal{A}$. Hence, decomposing $C(\mathcal{A})$, we get in fact a decomposition of $\mathcal{A}$. Moreover, the operator

$$S^{(1)}: D^{(1)} \to K^{(1)}, \quad (S^{(1)}\psi)(\lambda) = \lambda\psi(\lambda),$$

with $D^{(1)} = \{\psi\in K^{(1)};\ \int_{\mathbb{R}} \lambda^2 \|\psi(\lambda)\|^2\, d\rho(\lambda) < \infty\}$, is easily shown to be a self-adjoint operator which generates $D(K^{(1)})$, since the range of its projection-valued measure coincides with the family of the projections of $D(K^{(1)})$. Hence any superobservable is a function of S, denoting by S the operator in K corresponding to $S^{(1)}$. For this reason S can be called "the" superobservable of the system represented by $\mathcal{A}$. The physical interpretation of S depends obviously on the specific situation under consideration. As $\mathcal{A}$ corresponds to $R(K^{(1)})$, it reduces to the family of the algebras of the bounded operators on the $K(\lambda)$'s, which are called superselected sectors relative to the values λ of S.

We shall now associate to V a W^*-algebra in such a way that it will be interpreted in a natural way as the algebra of the observables of the system described by V.

Take the W^*-algebra $\mathcal{A} = V(\mathcal{G}^m)''$ of operators on H.[39] It will be possible to consider $\mathcal{A}$ as an algebra of observables according to the scheme outlined above only if a complete system of commuting observables can be found in $\mathcal{A}$, namely only if $\mathcal{A}'\subset\mathcal{A}$. To state that this is

indeed the case, we need the following proposition as a technical lemma.

Proposition 3: Let ϕ_w be the isomorphism of the algebra $\mathcal{L}(\mathcal{H})$ of the bounded operators on $\mathcal{H}$ with the algebra $\mathcal{L}(\mathcal{H}^{(1)})$ of the bounded operators on $\mathcal{H}^{(1)}$ defined as $\phi_w(A) = WAW^{-1}$ for each $A \in \mathcal{L}(\mathcal{H})$. When restricted to $V(\mathcal{G}^m)'$ it is an isomorphism of $V(\mathcal{G}^m)'$ onto the W^*-algebra $D(\mathcal{H}^{(1)})$ of the diagonal operators on the direct integral of Hilbert spaces $\mathcal{H}^{(1)}$.

Proof: First we notice that $\mathcal{G}^m$ is a group of type I. It is in fact a regular semidirect product whose little groups are $SU(2)$, the two-dimensional and the three-dimensional Euclidean group. Besides, for these Euclidean groups the little groups are, for the two-dimensional case, the one-element group and the group of the rotations in two dimensions and, for the three-dimensional case, the groups of the rotations in two and in three dimensions. Moreover, from DC-15.5.2,4.3.1, and 13.9.4, it follows that a s.c. compact group is of type I. Then, as a consequence of Th. 11.1 in Ref. 40, $\mathcal{G}^m$ results in a group of type I.

We shall now construct a direct integral of Hilbert spaces which will be suitable to study $V(\mathcal{G}^m)'$ in a convenient way. For any positive integer p let H_p be a definite p-dimensional Hilbert space and let $H_\infty = H_0$. Let Rep $\mathcal{G}^m$, Irr $\mathcal{G}^m$, $\hat{\mathcal{G}}^m$ have the same meaning as in DC-18. Take the map.

$$\eta: \mathbb{R} \to \hat{\mathcal{G}}^m, \quad \eta(\epsilon) = \hat{V}^{(\epsilon)},$$

where $\hat{V}^{(\epsilon)}$ denotes the element of $\hat{\mathcal{G}}^m$ which contains $V^{(\epsilon)}$. This is a Borel map, since it results from the composition of the canonical map of Irr $\mathcal{G}^m$ onto $\hat{\mathcal{G}}^m$ with $\mathbb{R} \ni \epsilon \to V^{(\epsilon)} \in \mathrm{Irr}\mathcal{G}^m$, which is a Borel map.[41] Moreover, η is one-to-one as the CUIR's $V^{(\epsilon)}$ of $\mathcal{G}^m$ are mutually inequivalent. As $\mathcal{G}^m$ is of type I, both $\mathbb{R}$ and $\hat{\mathcal{G}}^m$ are standard Borel spaces (see DC-18.5.3, 4.6.1, 13.9.4). Then, from DC-B21 it follows that $\eta(\mathbb{R})$ is a Borel subset of $\hat{\mathcal{G}}^m$ and that η is a Borel isomorphism of $\mathbb{R}$ onto $\eta(\mathbb{R})$. Take now the measure $\tilde{\nu}$ on $\hat{\mathcal{G}}^m$ defined as $\tilde{\nu}(\Delta) = \nu(\eta^{-1}(\Delta))$ for each Borel subset Δ of $\hat{\mathcal{G}}^m$. It is σ-finite as ν is σ-finite. Take also the field of Hilbert spaces $\{\mathcal{H}(\hat{g})\}(\hat{g} \in \hat{\mathcal{G}}^m)$ with $\mathcal{H}(\hat{g}) = H_{d(\hat{g})}$, where $d(\hat{g})$ denotes the common dimension of the representations of $\hat{g}$. As $\{\hat{g} \in \hat{\mathcal{G}}^m;\ d(\hat{g}) = p\}$ is a Borel subset of $\hat{\mathcal{G}}^m$ for any p (as it follows from DC-18.5.1.), the set of the elements of $\Pi_{\hat{g} \in \hat{\mathcal{G}}^m} \mathcal{H}(\hat{g})$ which are Borel maps from $\hat{\mathcal{G}}^m$ into the sum Borel space of the H_p's makes $\{\mathcal{H}(\hat{g})\}(\hat{g} \in \hat{\mathcal{G}}^m)$ a Borel field of Hilbert spaces. Then we can define $\tilde{\mathcal{H}} = \int^{\oplus}_{\hat{\mathcal{G}}^m} \mathcal{H}(\hat{g}) \times d\tilde{\nu}(\hat{g})$.

We shall now construct a direct integral of CUIR's of $\mathcal{G}^m$ on the direct integral of Hilbert spaces $\tilde{\mathcal{H}}$. Such a CUR of $\mathcal{G}^m$ will be found to be unitarily equivalent to $V^{(1)}$. Define then the field $\{\tilde{V}(\hat{g})\}(\hat{g} \in \hat{\mathcal{G}}^m)$ of CUIR's of $\mathcal{G}^m$ setting, for $\tilde{V}(\hat{g})$, $V^{(\eta^{-1}(\hat{g}))}$ if $\hat{g} \in \eta(\mathbb{R})$ and any representation of $\hat{g}$ if $\hat{g} \notin \eta(\mathbb{R})$. This field of representations is $\tilde{\nu}$-measurable as easily follows from ν-measurability of $\epsilon \to V^{(\epsilon)}$ and from the definition of $\tilde{\nu}$. Then it is integrable (DC-18.7) and we can define $\tilde{V} = \int^{\oplus}_{\hat{\mathcal{G}}^m} \tilde{V}(\hat{g})\, d\tilde{\nu}(\hat{g})$. To show the equivalence of $\tilde{V}$ with $V^{(1)}$, construct the map

$$U: \tilde{\mathcal{H}} \to \mathcal{H}^{(1)}, \quad (U\psi)(\epsilon) = \psi(\eta(\epsilon)).$$

This definition makes sense, since $\psi \cdot \eta$ is a Borel map of $\mathbb{R}$ into $\mathcal{H}_0$ whenever $\psi \in \tilde{\mathcal{H}}$ as η is a Borel map and $d(\eta(\epsilon)) = \infty$ for each $\epsilon \in \mathbb{R}$, and since

$$\int_{\mathbb{R}} \|\psi(\eta(\epsilon))\|^2 \, d\nu(\epsilon) = \int_{\eta(\mathbb{R})} \|\psi(\hat{g})\|^2 \, d\tilde{\nu}(\hat{g}) = \int_{\hat{\mathcal{G}}^m} \|\psi(\hat{g})\|^2 \, d\tilde{\nu}(\hat{g}) < \infty,$$

which follows from 111.10.8 in Ref. 27, as η is one-to-one and $\eta(\mathbb{R})$ is a Borel subset of $\hat{\mathcal{G}}^m$, and from $\tilde{\nu}(\hat{\mathcal{G}}^m - \eta(\mathbb{R})) = 0$. Since U is obviously linear, it is an isometric operator of $\tilde{\mathcal{H}}$ into $\mathcal{H}^{(1)}$. Moreover, for each $f \in \mathcal{H}^{(1)}$ construct $\tilde{f} \in \Pi_{\hat{g} \in \hat{\mathcal{G}}^m} \mathcal{H}(\hat{g})$ setting $\tilde{f}(\hat{g}) = f(\eta^{-1}(\hat{g}))$ if $\hat{g} \in \eta(\mathbb{R})$ and $\tilde{f}(\hat{g}) = 0$ if $\hat{g} \notin \eta(\mathbb{R})$. It follows from an easy calculation that $f \in \tilde{\mathcal{H}}$ and $U\tilde{f} = f$. Therefore, U results in a unitary isomorphism of $\tilde{\mathcal{H}}$ onto $\mathcal{H}^{(1)}$. Finally, for each $\psi \in \tilde{\mathcal{H}}$ and $(z,g) \in \mathcal{G}^m$ we have

$$(U\tilde{V}_{(z,g)}\psi)(\epsilon) = (\tilde{V}_{(z,g)}\psi)(\eta(\epsilon)) = \tilde{V}_{(z,g)}(\eta(\epsilon))\psi(\eta(\epsilon)) = V^{(\epsilon)}_{(z,g)}(U\psi)(\epsilon) = (V^{(1)}_{(z,g)}U\psi)(\epsilon), \quad \forall\ \epsilon \in \mathbb{R},$$

whence

$$U\tilde{V}_{(z,g)}U^{-1} = V^{(1)}_{(z,g)}, \quad \forall\ (z,g) \in \mathcal{G}^m.$$

The main point of the present proof is that $\tilde{V}(\mathcal{G}^m)' = D(\tilde{\mathcal{H}})$, where $D(\tilde{\mathcal{H}})$ denotes the W^*-algebra of the diagonal operators on $\tilde{\mathcal{H}}$. In fact, $\mathcal{G}^m$ has been previously proved to be a group of type I and $\tilde{V}(\hat{g})$ belongs to the class $\hat{g}$ for each $\hat{g} \in \hat{\mathcal{G}}^m$, since $V^{(\eta^{-1}(\hat{g}))} \in \hat{g}$ by definition of η. The result then follows from DC-18.7.6, 8.6.4, 13.9.4.

It is now easy to prove that $V^{(1)}(\mathcal{G}^m)' = D(\mathcal{H}^{(1)})$, where $D(\mathcal{H}^{(1)})$ denotes the W^*-algebra of the diagonal operators on $\mathcal{H}^{(1)}$. Since $V^{(1)}$ and $\tilde{V}$ have been proved to be unitarily equivalent through U, we have in fact that $A \in \mathcal{L}(\mathcal{H}^{(1)})$ is an element of $V^{(1)}(\mathcal{G}^m)'$ iff $U^{-1}AU \in D(\tilde{\mathcal{H}})$, namely iff $\lambda \in L^\infty(\hat{\mathcal{G}}^m, \tilde{\nu})$ exists such that $(U^{-1}AU\psi)(\hat{g}) = \lambda(\hat{g})\psi(\hat{g})$ for each $\hat{g} \in \hat{\mathcal{G}}^m$ and $\psi \in \tilde{\mathcal{H}}$, which is equivalent to $(Af)(\epsilon) = \lambda(\eta(\epsilon))f(\epsilon)$ for each $\epsilon \in \mathbb{R}$ and $f \in \mathcal{H}^{(1)}$. Besides, by definition of $\tilde{\nu}$, we have that $\{\lambda \circ \eta;\ \lambda \in L^\infty(\hat{\mathcal{G}}^m, \tilde{\nu})\} = L^\infty(\mathbb{R}, \nu)$. Therefore, we can conclude that $A \in V^{(1)}(\mathcal{G}^m)'$ iff $l \in L^\infty(\mathbb{R}, \nu)$ exists such that $(Af)(\epsilon) = l(\epsilon)f(\epsilon)$ for each $\epsilon \in \mathbb{R}$ and $f \in \mathcal{H}^{(1)}$. This shows that $V^{(1)}(\mathcal{G}^m)'$ and $D(\mathcal{H}^{(1)})$ in fact coincide.

Finally, since V and $V^{(1)}$ are unitarily equivalent through W, a brief calculation leads to $\phi_w(V(\mathcal{G}^m)') = V^{(1)}(\mathcal{G}^m)'$, which, along with the result of the last paragraph, completes the proof of the proposition.

We are now in the position to prove that $\mathcal{A}' \subset \mathcal{A}$. We have in fact $D(\mathcal{H}^{(1)}) \subset R(\mathcal{H}^{(1)}) = D(\mathcal{H}^{(1)})'$ (see the Corollary in DW-11.2.5), whence $\phi_w(V(\mathcal{G}^m)') \subset \phi_w(V(\mathcal{G}^m)'')$ and this in turn amounts to $\mathcal{A}' = (V(\mathcal{G}^m)'')' = V(\mathcal{G}^m)' \subset V(\mathcal{G}^m)'' = \mathcal{A}$ [the second equality holds as $V(\mathcal{G}^m)'$ is a W^*-algebra]. Therfore $\mathcal{A}$ is suitable to be assumed as an algebra of observables.

We shall now show how it is indeed possible to interpret $\mathcal{A}$ as the algebra of the observables of the free elementary system of mass m and spin j described by V. First, we notice that from V a representation of the Lie algebra $L\mathcal{G}^m$ of $\mathcal{G}^m$ can be drawn. For each $\alpha \in L\mathcal{G}^m$ we have in fact a strongly continuous one-parameter group $\mathbb{R} \ni t \to V(\exp t\alpha) \in U(\mathcal{H})$ of unitary operators on

$\mathcal{H}$. By a theorem of Stone there is a unique skew-adjoint operator $T(\alpha)$ in $\mathcal{H}$ such that $V(\exp t\alpha)=\exp[tT(\alpha)]$ for each $t\in\mathbb{R}$.[42] A linear subspace $\mathcal{M}$ of $\mathcal{H}$ exists which is dense in $\mathcal{H}$ and contained in the domain of each $T(\alpha)$[43] The restriction of each $T(\alpha)$ to $\mathcal{M}$ is essentially skew-adjoint.[44] Moreover, $\mathcal{M}$ is invariant with respect to each $T(\alpha)$ and the mapping $L\mathcal{G}^m\ni\alpha\to T(\alpha)_r$ [the restriction of $T(\alpha)$ to $\mathcal{M}$] is a representation of $L\mathcal{G}^m$. Next, as the "right" Lie algebra for a free elementary system of mass m is the mass m extension of the Galilei Lie algebra and this in turn coincides with $L\mathcal{G}^m$,[45] it is sensible to associate with the representation V of $\mathcal{G}^m$ the W^*-algebra $\mathcal{B}$ generated by the self-adjoint operators $(1/i)T(\alpha)$, $\alpha\in L\mathcal{G}^m$, as the algebra of the observables of the elementary system of mass m and spin j. We point out that, since $T(\alpha)$ is not in general bounded, $\mathcal{B}$ is generated in fact by the spectral projections of the operators $(1/i)T(\alpha)$, and these observables are thus affiliated with $\mathcal{B}$. Finally, we can prove that $\mathcal{A}=\mathcal{B}$. In fact, the spectral projections of $(1/i)T(\alpha)$ coincide with the spectral projections of $V(\exp\alpha)$, as $V(\exp\alpha)=\exp T(\alpha)$. Hence they are included in $V(\mathcal{G}^m)''=\mathcal{A}$, whence $\mathcal{B}\subset\mathcal{A}$. Take conversely any element $(z,g)\in\mathcal{G}^m$. Then elements $\alpha_1,\alpha_2,\ldots,\alpha_n$ of $L\mathcal{G}^m$ exist such that $(z,g)=(\exp\alpha_1)(\exp\alpha_2)\cdots(\exp\alpha_n)$,[46] whence $V_{(z,g)}=[\exp\times T(\alpha_1)]\circ\cdots\circ[\exp T(\alpha)]$. Therefore, $V_{(z,g)}\in\mathcal{B}$ for each $(z,g)\in\mathcal{G}^m$, namely $V(\mathcal{G}^m)\subset\mathcal{B}$, whence $\mathcal{A}=V(\mathcal{G}^m)''\subset\mathcal{B}''=\mathcal{B}$.

Thus, we have related in a definite way the algebra of observables $\mathcal{A}=V(\mathcal{G}^m)''$ to the representation V. We notice that $C(\mathcal{A})=V(\mathcal{G}^m)'$, as $\mathcal{A}'\subset\mathcal{A}$. Hence the reducibility of V amounts to the presence of superselection rules in the picture based on $\mathcal{A}$. Therefore, a decomposition of $\mathcal{A}$ through $C(\mathcal{A})$ is possible in the way explained above, with $\mathcal{H}$ in the place of K. From Proposition 3 we get that $\mathcal{H}^{(1)}$ is a direct integral of Hilbert spaces in which $C(\mathcal{A})$ diagonalizes, since $C(\mathcal{A})=V(\mathcal{G}^m)'$. Correspondingly, $\mathcal{A}$ splits into a continuous infinity of algebras of observables. The superobservable which rules this decomposition is $S=W^{-1}S^{(1)}W$, where $S^{(1)}$ is defined as above, with $\mathcal{H}^{(1)}$ in the place of $K^{(1)}$. Its physical interpretation is easily performed by simply looking at its form. It can be shown, in fact, in a rather trivial but lengthy way, that

$$(Sf)(p_0,\mathbf{p})=(\mathbf{p}^2-2mp_0)f(p_0,\mathbf{p})$$

for each f in the domain $W^{-1}(D^{(1)})$ of S. Hence it is natural to interpret S as the "inner energy" observable of the system, since $\mathbf{p}$ and p_0 have been introduced just from the outset as the momentum and the energy [to be definite, the inner energy would be the multiple $-(1/2m)S$ of S]. Therefore, the superselected sectors are in this case relative to the values of the inner energy.

Finally, as to the problem from which our discussion has originated, we can conclude that the continuous family of representations into which V decomposes is in correspondence with all the possible values of the inner energy of the free elementary system of mass m and spin j whose kinematical group has been assumed to be the Galilei group. Therefore, the fact that all these representations generate the same quantum mechanical description for an elementary system amounts to the fact that the kinematical behavior of a system, for fixed values of the mass and of the spin, is independent of the relative values of the inner energy, as long as it can be considered free and elementary.

[1]E. Inönu and E. P. Wigner, Nuovo Cimento **9**, 705 (1952); J.-M. Lévy-Leblond, J. Math. Phys. **4**, 776 (1963); J. Voisin, J. Math. Phys. **6**, 1519 (1965).

[2]We notice that the definite bundle ascribed to a system depends on what we decide to consider relevant among the data that are furnished by the technology (for instance, in the case of elementary particles the fibers have been growing more and more, as at the beginning they contained nothing while now they contain spins and charges of several kinds).

[3]At this point any naivety is usually abandoned. On the contrary, some amount of skill is required to find out "natural" easily interpreted mathematical equipment which will prove useful for the further developments.

[4]D. J. Simms, "Lie Groups and Lie Algebras," Summer School on Group Representations and Quantum Mechanics, Dublin, 1969, Sec. IV.

[5]J. M. Jauch, Helv. Phys. Acta **33**, 711 (1960); J. M. Jauch and B. Misra, Helv. Phys. Acta **34**, 699 (1961); R. Cirelli and F. Gallone, Ann. Inst. H. Poincaré, **19A**, 297 (1974).

[6]J.-M. Lévy-Leblond, "Galilei Group and Galilean Invariance," in *Group Theory and Its Applications*, edited by E. M. Loebl (Academic, New York, 1971), Vol. II.

[7]E. P. Wigner, Ann. Math. **40**, 149 (1939).

[8]K. R. Parthasarathy, Commun. Math. Phys. **15**, 305 (1969); V. S. Varadarajan, *Geometry of Quantum Theory* (Van Nostrand, New York, 1970), Vol. II, Chap. X.

[9]V. Bargmann, Ann. Math. **59**, 1 (1954); see also Voisin's paper of Ref. 1 and Lévy-Leblond's paper of Ref. 6.

[10]The paper of Inönu and Wigner of Ref. 1; M. Hamermesh, Ann. Phys. **9**, 518 (1960); A. S. Wightman, Rev. Mod. Phys. **34**, 845 (1962).

[11]Varadarajan's book of Ref. 8, Chap. XII.

[12]Varadarajan's book of Ref. 8, Chap. X.

[13]G. W. Mackey, "The Theory of Group Representations," Lecture notes, Department of Mathematics, University of Chicago, 1955; G. W. Mackey, *Induced Representations of Group and Quantum Mechanics* (Benjamin, New York, 1968). 1968).

[14]Voisin's paper of Ref. 1 and Lévy-Leblond's paper of Ref. 6.

[15]Voisin's paper of Ref. 1 and Varadarajan's book of Ref. 8.

[16]For the definition of $L^2_{\mathbf{C}^{2j+1}}(\mathbb{R}^3,\nu^3)$, see J. Dixmier, *Les algèbres d'opérateurs dans l'espace Hilbertien (Algèbres de von Neumann)* (Gauthier-Villars, Paris, 1969), Ex. 2 in 11.1.5. Hereafter, this book will be denoted simply by DW.

[17]A similar result can be found in Sec. IV, C of Ref. 6.

[18]By "Hilbert space" we mean here and in the sequel a complex and separable Hilbert space.

[19]Varadarajan's book of Ref. 8.

[20]By "measure" we mean here and in the sequel a positive measure.

[21]The proof of this statement, along with further discussion on G-Hilbert bundles, will be the content of a forthcoming paper.

[22]H. L. Royden, *Real Analysis* (Macmillan, New York, 1963), Chap. 12, Theorem. 22.

[23]Chapter 12, Theorem 21 in Ref. 22.

[24]See p. 55 of Ref. 19 or p. 4 of Mackey's lecture notes of Ref. 13.

[25]As in Sec. 1, g and $(t,\mathbf{a},\mathbf{v},u)$ are two equivalent notations for an element of $\mathcal{G}$.

[26]In particular, the maps in (a) and (d) of Definition 1 are easily shown to be Borel maps, since in the present case they are in fact analytic maps.

[27]N. Dunford and J. T. Schwartz, *Linear Operators*, Part 1 (Interscience, New York, 1958).

[28]The Corollary in DW-11.1.8. together with 11.4-Prop. 2 in

M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic, New York, 1972), Vol. 1.

[29]These equalities hold as, from the definition of $\psi_{n,r,k}$ (namely from $f_{n,r,k} = W^{-1}\psi_{n,r,k}$), it follows that for any $\psi_{n,r,k}$ a representative $\mathbb{R} \ni \epsilon \to \psi_{n,r,k}(\epsilon) \in \mathcal{H}_0$ exists such that for each $\epsilon \in \mathbb{R}$ a representative $\mathbb{R}^3 \ni \mathbf{p} \to \psi_{n,r,k}(\epsilon, \mathbf{p}) \in \mathbb{C}^{2j+1}$ of $\xi_{n,r,k}(\epsilon)$ exists with the property that $\mathbb{R}^4 \ni (p_0, \mathbf{p}) \to \psi_{n,r,k}(\alpha(p_0, \mathbf{p})) \in \mathbb{C}^{2j+1}$ is a representative of $W^{-1}\psi_{n,r,k}$.

[30]We omit here the index j since the value of the spin is fixed through this discussion from the outset, namely from the construction of the "laboratory" Galilei–Hilbert bundle.

[31]J. Dixmier, *Les C*-algèbres et leurs représentations*, (Gauthier-Villars, Paris, 1964). Hereafter, this book will be denoted simply by DC.

[32]See Ref. 5. W^*-algebra is a shortened notation for von Neumann algebra.

[33]R. Cirelli, F. Gallone, and B. Gubbay, "An Algebraic Representation of Continuous Superselection Rules J. Math. Phys. (to be published).

[34]A number of papers have appeared on this subject recently. We mention here only two books: J.M. Jauch, *Foundations of Quantum Mechanics* (Addison-Wesley, Reading, Mass., 1968); V.S. Varadarajan, *Geometry of Quantum Theory* (Van Nostrand, Princeton, 1968), Vol. 1.

[35]Let $\mathcal{L}(H)$ be the set of the bounded operators on a Hilbert space H. By $\mathcal{E}'$ we denot the set of the elements of $\mathcal{L}(H)$ which commute with all the elements of a subset $\mathcal{E}$ of $\mathcal{L}(H)$. By $\mathcal{E}''$ we shall denote $(\mathcal{E}')'$.

[36]P.A.M. Dirac, *The Principles of Quantum Mechanics* (Oxford U.P., London, 1958), 4th ed.

[37]A.M.L. Messiah and O.W. Greenberg, Phys. Rev. **136**, B 248 (1964).

[38]F. Gallone, "Algebra of Observables and Paraparticles," unpublished manuscript.

[39]By $V(\mathcal{G}^m)$ and, in the sequel, by $V^{(1)}(\mathcal{G}^m)$ and $\tilde{V}(\mathcal{G}^m)$ we denote the range of the representations V, $V^{(1)}$ and $\tilde{V}$, respectively.

[40]G.W. Mackey's Appendix in I.E. Segal, *Mathematical Problems of Relativistic Physics* (American Mathematical Society, Providence, R.I., 1963).

[41]From DC-18.7.2 we have indeed that $\epsilon \to V^{(\epsilon)}$ equals a Borel map only ν-almost everywhere, as it is ν-measurable. Anyway, such a Borel map can be replaced by it and the same symbols retained, since we are interested, in fact, just in the direct integral $V^{(1)}$ and not in the field $\epsilon \to V^{(\epsilon)}$ directly.

[42]M. Stone, Ann. Math. **33**, (2), 643 (1932); Theorem VIII 8 in Reed and Simon's book of Ref. 28.

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

[44]I.E. Segal, Duke Math. J. **18**, 221 (1951).

[45]L. O'Raifeartaigh, "Unitary Representations of Lie Groups in Quntum Mechanics," in *Group Representations in Mathematics and Physics* edited by V. Barmann (Springer-Verlag, Berlin, 1970); see also Ref. 6.

[46]A neighbourhood of the unit element of $\mathcal{G}^m$ exists, any element of which equals $\exp\alpha$ for some $\alpha \in L\mathcal{G}^m$. As $\mathcal{G}^m$ is connected, any element of $\mathcal{G}_m$ can be expressed as a finite product of elements of such a neighbourhood.

On the interaction of the electromagnetic field with heat conducting deformable semiconductors

H. G. de Lorenzi and H. F. Tiersten

Mechanics Division, Rensselaer Polytechnic Institute, Troy, New York 12181
(Received 2 October 1974)

The differential equations and boundary conditions describing the behavior of a finitely deformable, polarizable and magnetizable heat conducting and electrically semiconducting continuum in interaction with the electromagnetic field are derived by means of a systematic application of the laws of continuum physics to a well-defined macroscopic model. The model consists of five suitably defined interpenetrating continua. The relative displacement of the bound electronic continuum with respect to the lattice continuum produces electrical polarization, and electrical conduction results from the motion of the charged free electronic and hole fluids. Since partial pressures are taken to act in the conducting fluids, semiconduction boundary conditions arise, which have not appeared previously. The resulting rather cumbersome system of equations is reduced to that for the quasistatic electric field and static homogeneous magnetic field. In the absence of heat conduction, for the n-type semiconductor, nonlinear equations quadratic in the small field variables, for small fields superposed on a bias, are obtained from the latter, more tractable, system of equations. These small field equations reduce to four equations in four dependent variables. The linear portion of the small field equations is applied in the analysis of the propagation of both plane and surface waves in piezoelectric semiconductors subject to a static biasing electric field. On account of the aforementioned semiconduction boundary condition, the assumption of zero electric surface charge employed in previous treatments of the surface wave problem is not employed here.

1. INTRODUCTION

Subsequent to the work of Toupin[1] on the interaction of the electric field with a polarizable and deformable solid in the static case, numerous authors[2–13] have obtained rotationally invariant descriptions of the interaction of the electric, magnetic, and electromagnetic fields with deformable solids under a variety of circumstances. A discussion interrelating much of this work from the viewpoint of the present authors is given in Ref. 12. Although insulators, both electric and magnetic, and ohmic type electrical conductors have been treated in the aforementioned rotationally invariant descriptions of the interaction of the electric and magnetic fields with deformable solids, none of that work treats semiconductors. Existing theoretical descriptions[14–18] of deformable semiconductors simply consist of the equations of linear piezoelectricity coupled to the somewhat nonlinear current density relation from semiconductor physics.[19] Although this theory has been useful in the description of the behavior of piezoelectric semiconductors for small fields under a variety of circumstances, it is not rotationally invariant, lacks consistency in certain other respects also, and does not provide proper electrical boundary conditions, which are required when surfaces are present, as in the case of surface wave propagation among other circumstances. Consequently, only linear deformation can be treated within the framework of the existing theory, and other limitations inherent in the description are unclear.

In this paper the differential equations and boundary conditions describing the behavior of a finitely deformable, polarizable, magnetizable, heat conducting and electrically semiconducting continuum in interaction with the electromagnetic field are determined by means of a systematic application of the laws of continuum physics to a well-defined macroscopic model. The model consists of five suitably defined interpenetrating continua. The five continua consist of the positively charged lattice continuum coupled to four distinct charged continua. The four electrically charged continua are referred to as the bound electronic continuum, the free electronic continuum, the hole continuum, and the impurity continuum, respectively. The negatively charged bound electronic continuum can displace slightly with respect to the positively charged lattice continuum and, thereby, produce the electric polarization. The impurity continuum, which can be positively or negatively charged and is required for the general balance of electric charge in the semiconductor, is rigidly attached to the lattice continuum. Both the free electronic continuum and hole continuum are charged fluids that can move with respect to the lattice continuum while experiencing a force of resistance. Naturally, the two conducting fluids are allowed to interchange charge with each other and with the impurity continuum in order to allow for a variable degree of semiconduction. Electric current arises as a result of the motion of the free electronic and hole fluids and magnetization is taken to arise from a circulating current density as in Ref. 12. Since no material resonance effects are considered, the lattice continuum is assumed to possess all mass, i. e., linear momentum, and all other continua are taken to be massless, i. e., to have negligible linear momentum. The rates of supply of linear momentum and energy from the electromagnetic field to the deformable semiconductor are determined from the Lorentz force in the manner set forth in Ref. 12.

As in all continuum descriptions, the application of the appropriate equations of balance of charge, mass, and momentum to the respective continua yields the

material equations of motion, which, with the electromagnetic field equations, constitutes an underdetermined system. The application of the equation of conservation of energy to the combined material continuum results in the first law of thermodynamics which, with the aid of the second law of thermodynamics[20–22] and the principle of material objectivity,[23,24] enables the determination of the constitutive equations. These constitutive equations along with the aforementioned equations of motion and electromagnetism and the thermodynamic dissipation equation result in a properly determined system, which can readily be reduced to 18 equations in 18 dependent variables. In order to complete the system of equations, jump (or boundary) conditions across moving, not necessarily material, surfaces of discontinuity are determined from the appropriate integral forms of the field equations, which are taken to be valid even when the differential forms from which they were obtained are not. These integral forms result in definitions of electromagnetic quantities, such as the Maxwell stress tensor, which are identical with those employed in Ref. 12. Since the very important fluid pressure terms,[25] which are directly related[26] to the chemical potentials occurring in conventional semiconductor theory, are included in the description of the conducting fluids in a rather fundamental manner, semiconduction boundary conditions occur at the surface of the semiconductor, which have not appeared in other works on this subject. Moreover, previous work[16] in this area tacitly assumes that the electric surface charge density vanishes at an interface between a semiconductor and the surrounding space. Since the material is a semiconductor and not an insulator, this is a restrictive assumption. By virtue of the aforementioned semiconduction boundary condition, this restrictive assumption on electric surface charge density does not exist in the description of the semiconductor presented here.

When the electric field is assumed to be quasistatic,[27] the number of dependent variables, differential equations, and boundary conditions, respectively, is reduced by five. Furthermore, in the special case of an n-type semiconductor, which conducts by means of the free electronic continuum only, in the absence of heat conduction and magnetic effects, the number of differential equations is further reduced to four equations in four dependent variables. From these latter equations nonlinear differential equations and boundary conditions for small dynamic fields superposed on large static biasing fields have been obtained in the same manner as in Ref. 28. The small field equations are nonlinear because they include terms quadratic in the small field variables. The linear version of these small field equations under a homogeneous biasing electric field is applied to the problems of the propagation of plane and surface waves in piezoelectric semiconductors with hexagonal symmetry. The plane wave analysis indicates the existence of a term in the propagation relation not present in previous work[15] on the subject. The term, which is probably small in all practical cases, is due essentially to a mechanical body force caused by the dc electric field and oscillating electric charge density. The surface wave analysis employs the aforementioned semiconduction boundary condition and does not make the assumption of zero electric surface charge density on the surface of the semiconductor, which was made in previous work on this problem.[16–18] Furthermore, previous work[16–18] in this area does not exhibit the dependence of the effective material coefficients on the biasing dc electric field, which arises naturally in this consistent treatment and in principle can serve to change the symmetry properties completely in many cases. However, the formalism presented here requires the measurement of material coefficients for the semiconduction boundary condition, which are not presently available.

Finally, it should be noted that the present theory, which is for a semiconductor with one valence band only, can readily be extended to semiconductors with any number of valence bands simply by increasing the number of hole and free electronic continua. In the absence of deformation this theory should be applicable in the description of high field effects in rigid semiconductors.

2. THE INTERACTING CONTINUA

As stated in the Introduction, the macroscopic model of the deformable semiconductor consists of five interacting, interpenetrating continua. The five identifiable continua consist of the following:

1. The lattice continuum, which has a positive charge density and, since material resonance effects are not taken into account, is assumed to be the only continuum possessing a nonzero mass density. All other continua experience force interactions with this continuum only and not with each other. This continuum is denoted by the superscript l.

2. The bound electronic continuum, which has a negative charge density and a circulating current density and is denoted by the superscript b. In a (finite) motion this continuum can displace slightly with respect to the lattice continuum and thus produce electric polarization. It produces magnetization also by virtue of the circulating current density it possesses.

3. The impurity continuum,[19] which is rigidly bound to the lattice continuum and not allowed to displace at all with respect to it and is denoted by the superscript i. The impurity continuum can have either a positive or negative charge density and for many purposes can be regarded essentially as a part of the lattice continuum. However, since it is a source of electric charge and is required in order that the degree of semiconduction can be variable, it is advisable to treat it as a separate continuum.

4. The free electronic continuum, which has a negative charge density and is denoted by the superscript e. This continuum is a conducting compressible fluid possessing negligible inertia and experiencing a force of resistance from its motion with respect to the lattice continuum.

5. The hole continuum,[19] which has a positive charge density and is denoted by the superscript h. This continuum also is a conducting compressible fluid possessing negligible inertia and experiencing a force of re-

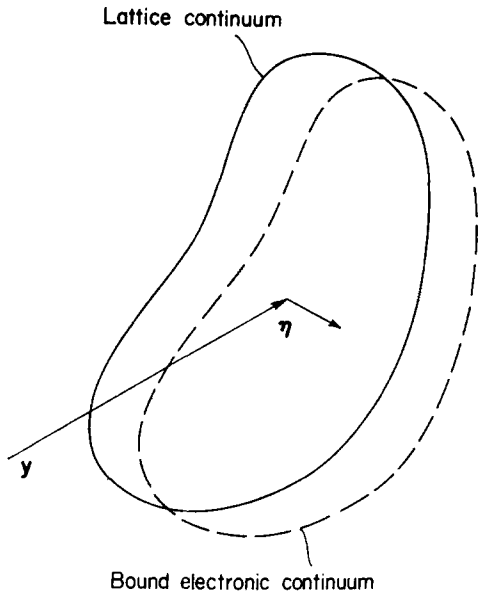

FIG. 1. Schematic diagram showing the relative displacement of the bound electronic continuum with respect to the lattice continuum.

sistance from its motion with respect to the lattice continuum.

Initially, the lattice continuum, the impurity continuum, and the bound electronic continuum all occupy the same region of space and, hence, have the same reference coordinates X_L. The motion of a point of the lattice continuum is described by the mapping

$$y_i = y_i(X_L, t), \quad \mathbf{y} = \mathbf{y}(\mathbf{X}, t), \tag{2.1}$$

which is one-to-one and differentiable as often as required. In (2.1) the y_i denote the present coordinates of material (lattice continuum) points and X_L, the reference coordinates, and t denotes the time. We consistently use the convention that capital indices denote the Cartesian components of **X** and lower case indices, the Cartesian components of **y**. Both dyadic and Cartesian tensor notation are used interchangeably. A comma followed by an index denotes partial differentiation with respect to a coordinate, i. e.,

$$y_{i,L} = \frac{\partial y_i}{\partial X_L}, \quad X_{K,j} = \frac{\partial X_K}{\partial y_j}, \tag{2.2}$$

and the summation convention for repeated tensor indices is employed. In a (finite) motion the bound electronic continuum is permitted to displace with respect to the lattice continuum by an infinitesimal displacement field $\eta = \eta(\mathbf{y}, t)$, which, by virtue of the charge density in the bound electronic continuum, accounts for the electric polarization. A schematic diagram indicating the relative displacement of the bound electronic continuum with respect to the lattice continuum is shown in Fig. 1. Although the bound electronic continuum and lattice continuum can displace with respect to each other, η is constrained to satisfy

$$\eta_{k,k} = 0, \tag{2.3}$$

in order that the two continua have equal volumes at all times and the proper electric charge equation may be obtained[29] from the present bound charge model of the polarization. The lattice continuum is assumed to have a positive charge density μ^l and the bound electronic continuum, a negative charge density μ^b, which differ by a residual lattice charge density μ^r, which in elementary conduction is simply the positive charge density that neutralizes the negative charge density of the free electronic continuum. Since the total lattice charge and bound electronic charge, respectively, are constants, we have the conservation of charge for the lattice and bound electronic continua, which, with (2.3), yields

$$\mu^l(\mathbf{y}) + \mu^b(\mathbf{y} + \eta) = \mu^r(\mathbf{y}). \tag{2.4}$$

In addition to possessing a negative charge density the bound electronic continuum possesses at each point a circulating current density, which in the appropriate limit accounts for the magnetization in the manner set forth in Ref. 12, i. e., we have

$$\lim_{\substack{r\to 0 \\ i'\to\infty \\ C'\to 0 \text{ in a plane}}} \oint_{C'} \mathbf{r}\times i'\,d\mathbf{s} = \lim_{\substack{S\to 0 \\ i'\to\infty \\ n \text{ fixed}}} i'\mathbf{n}S_0' = \mathbf{M}', \tag{2.5}$$

where i' is the current in magnetic units, C' is an arbitrary vanishingly small circulating current loop taken to be stationary with respect to the instantaneous local rest system of inertia,[30] and $\mathbf{M}'$ is the magnetization referred to the same instantaneous rest system. At this point it should be noted that with the exception of the circulating current density i', which is in magnetic units, and Secs. 8 and 9, in which MKS units are employed, Gaussian electromagnetic units are employed throughout this paper. Although the lattice continuum and bound electronic continuum have no charge source densities, the free electronic continuum, the hole continuum, and the impurity continuum all have charge source densities, which are denoted by γ^e, γ^h, and γ^i, respectively. Then, in order to satisfy the overall conservation of charge, we must have

$$\gamma^e + \gamma^h + \gamma^i = 0. \tag{2.6}$$

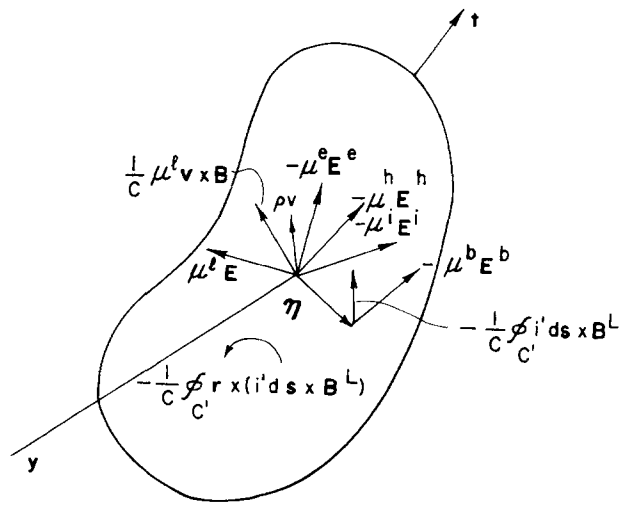

FIG. 2. Schematic diagram showing the linear momentum and force and couple vectors acting in the lattice continuum.

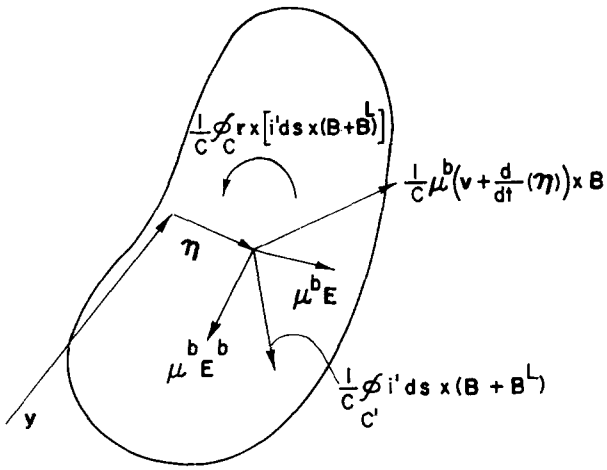

FIG. 3. Schematic diagram showing the force and couple vectors acting in the bound electronic continuum

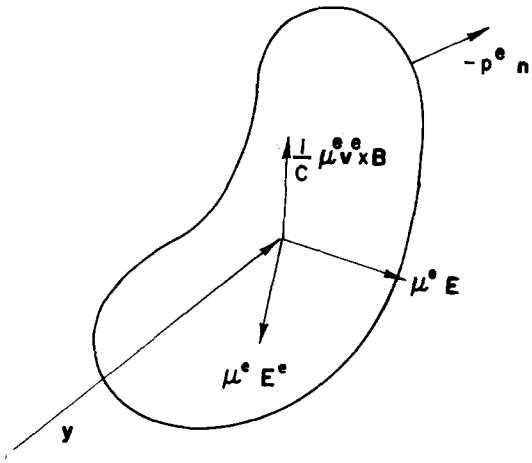

FIG. 5. Schematic diagram showing the force vectors acting in the free electronic continuum.

Since the free electronic and hole continua are fluids, only the present position is meaningful, which naturally is taken to be the present position of the lattice continuum y_i. The charge densities of the free electronic and hole continua are denoted by μ^e and μ^h, respectively. Clearly, the present and reference locations of the impurity continuum, which has charge density μ^i, are identical with those of the lattice continuum.

The free electronic and hole continua interact with the local lattice continuum by means of defined local electric material fields denoted by $\mathbf{E}^e$ and $\mathbf{E}^h$, respectively, which cause equal and opposite forces $\pm \mu^e \mathbf{E}^e$ and $\pm \mu^h \mathbf{E}^h$ to be exerted between the lattice continuum and each of the respective conducting fluids. Each conducting fluid interacts with neighboring elements of the same fluid by means of pressure forces p^e and p^h, which act across the surface of separation in the respective fluids. The impurity and bound electronic continua interact with the local lattice continuum by means of defined local electric material fields $\mathbf{E}^i$ and $\mathbf{E}^b$, respectively, which cause equal and opposite forces $\pm \mu^i \mathbf{E}^i$ and $\pm \mu^b \mathbf{E}^b$ to be exerted between the lattice continuum and each of the two respective continua. No force of interaction is assumed to exist across a surface of separation in either the impurity or bound electronic continuum. While the fields $\mathbf{E}^e$, $\mathbf{E}^h$, and $\mathbf{E}^i$ act through the point y_i, the field $\mathbf{E}^b$ acts through the point $(y_i + \eta_i)$. In addition a defined local magnetic material field $\mathbf{B}^L$ exists, which causes equal and opposite couples $\pm \mathbf{M}' \times \mathbf{B}^L$ to be exerted between the lattice continuum and bound electronic continuum, which contains a circulating current density i' as in Ref. 12. The lattice continuum, which experiences the above mentioned forces and couples from its interaction with the other continua, interacts with neighboring elements of the lattice continuum by means of the usual traction force per unit area $\mathbf{t}$ acting across the surface of separation. As noted in the Introduction, the Maxwell electric field $\mathbf{E}$ and magnetic induction field B exert the usual Lorentz force on all elements of charge and current density. Schematic diagrams illustrating the above-mentioned interactions in the model are shown in Figs. 2–6.

3. THE EQUATIONS OF BALANCE AND ELECTROMAGNETISM

Since, as noted in the Introduction, all mass is considered to reside in the lattice continuum, the equation of the conservation of mass may be written in the form

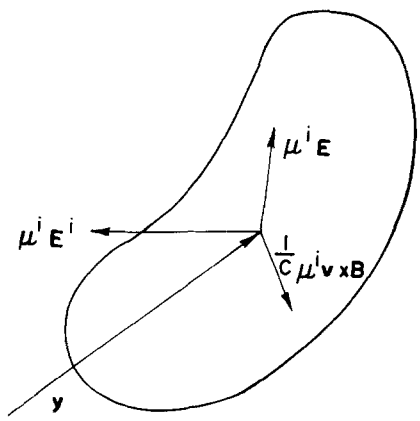

FIG. 4. Schematic diagram showing the force vectors acting in the impurity continuum.

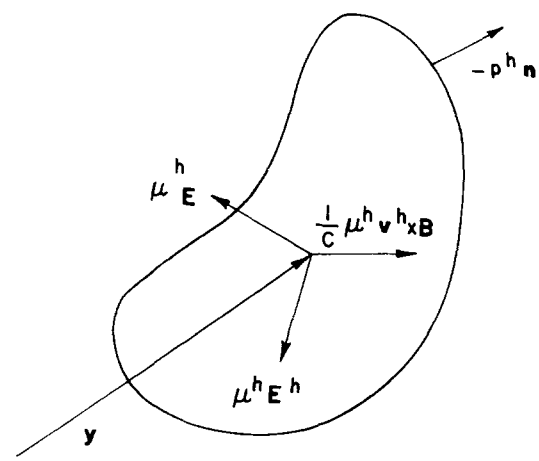

FIG. 6. Schematic diagram showing the force vectors acting in the hole continuum

$$\frac{d}{dt}\int_V \rho\, dV = 0, \tag{3.1}$$

where d/dt denotes the material derivative[31] for the lattice continuum, V is an arbitrary element of material volume of the lattice continuum, and ρ is the mass density. The conservation of electric charge for the lattice and bound electronic continua, which do not interchange charge with the three other continua, has been discussed in Sec. 2, and the result is given in (2.4). Since the remaining constituents of the model consist of two conducting fluids with different velocities and the impurity continuum which moves with a third velocity, all of which interchange charge with each other, the only meaningful way to write the equations of the conservation of charge for the three continua is to consider a stationary element of volume. Accordingly, the equations of the conservation of charge for the impurity, free electronic, and hole continua, respectively, may be written in the integral forms

$$\frac{\partial}{\partial t}\int_V \mu^i\, dV + \int_s \mathbf{n}\cdot\mathbf{v}\mu^i\, ds = \int_V \gamma^i\, dV, \tag{3.2}$$

$$\frac{\partial}{\partial t}\int_V \mu^e\, dV + \int_s \mathbf{n}\cdot\mathbf{v}^e\mu^e\, ds = \int_V \gamma^e\, dV, \tag{3.3}$$

$$\frac{\partial}{\partial t}\int_V \mu^h\, dV + \int_s \mathbf{n}\cdot\mathbf{v}^h\mu^h\, ds = \int_V \gamma^h\, dV, \tag{3.4}$$

where $\mathbf{v} = d\mathbf{y}/dt$ is the velocity of the lattice continuum and $\mathbf{v}^e$ and $\mathbf{v}^h$ denote the velocities of the free electronic and hole continua, respectively. From (3.2)—(3.4), with the aid of the divergence theorem and the arbitrariness of the spatial volume V, we obtain

$$\frac{\partial \mu^i}{\partial t} + \nabla\cdot(\mu^i\mathbf{v}) = \gamma^i, \tag{3.5}$$

$$\frac{\partial \mu^e}{\partial t} + \nabla\cdot(\mu^e\mathbf{v}^e) = \gamma^e, \tag{3.6}$$

$$\frac{\partial \mu^h}{\partial t} + \nabla\cdot(\mu^h\mathbf{v}^h) = \gamma^h, \tag{3.7}$$

where $\nabla = \mathbf{e}_i\partial/\partial y_i$ and $\mathbf{e}_i$ is a unit base vector in the ith Cartesian direction. Equations (3.5)—(3.7) constitute the differential equations of the conservation of charge for the impurity, free electronic, and hole continua, respectively. Since, as noted in Sec. 2, the conservation of charge holds for the bound electronic continuum and lattice continuum separately, we have, with the aid of (2.4), the conservation of residual lattice charge μ^r, which may be written in the form

$$\frac{\partial \mu^r}{\partial t} + \nabla\cdot(\mu^r\mathbf{v}) = 0. \tag{3.8}$$

Since the electric charge equation derived in the Appendix indicates that the total actual electric charge density μ is given by

$$\mu = \mu^r + \mu^i + \mu^e + \mu^h, \tag{3.9}$$

the total electric current density $\mathbf{J}$ is given by

$$\mathbf{J} = \mu^r\mathbf{v} + \mu^i\mathbf{v} + \mu^e\mathbf{v}^e + \mu^h\mathbf{v}^h, \tag{3.10}$$

which, with (3.5)—(3.9) and (2.6), enables us to write

$$\nabla\cdot\mathbf{J} + \partial\mu/\partial t = 0, \tag{3.11}$$

which is the equation of the conservation of total electric charge[32] that must be satisfied for consistency with Maxwells equations. In most cases the material velocity $\mathbf{v}$ is negligible compared with the velocities $\mathbf{v}^e$ and $\mathbf{v}^h$ of the free electronic and hole continua, and, consequently, for practical purposes the current density $\mathbf{J}$ can be written as

$$\mathbf{J} = \mu^e\mathbf{v}^e + \mu^h\mathbf{v}^h. \tag{3.12}$$

The equations of the conservation of linear momentum for the five continua are, respectively,

$$\int_s \mathbf{t}\, ds + \int_V \left[\mu^l\left(\mathbf{E} + \frac{1}{C}\mathbf{v}\times\mathbf{B}\right) - \mu^b\mathbf{E}^b - \mu^e\mathbf{E}^e - \mu^h\mathbf{E}^h - \mu^i\mathbf{E}^i\right] dV = \frac{d}{dt}\int_V \rho\mathbf{v}\, dV, \tag{3.13}$$

$$\int_V \mu^b\left[\mathbf{E}(\mathbf{y}+\boldsymbol{\eta}) + \frac{1}{C}\left(\mathbf{v} + \frac{d\boldsymbol{\eta}}{dt}\right)\times\mathbf{B}(\mathbf{y}+\boldsymbol{\eta}) + \mathbf{E}^b\right] dV + \int_V \oint_{C'} i'\, d\mathbf{s}\times\mathbf{B}\, dV = 0, \tag{3.14}$$

$$\int_V \mu^i\left(\mathbf{E} + \frac{1}{C}\mathbf{v}\times\mathbf{B} + \mathbf{E}^i\right) dV = 0, \tag{3.15}$$

$$-\int_s \mathbf{n}p^e\, ds + \int_V \mu^e\left(\mathbf{E} + \frac{1}{C}\mathbf{v}^e\times\mathbf{B} + \mathbf{E}^e\right) dV = 0, \tag{3.16}$$

$$-\int_s \mathbf{n}p^h\, ds + \int_V \mu^h\left(\mathbf{E} + \frac{1}{C}\mathbf{v}^h\times\mathbf{B} + \mathbf{E}^h\right) dV = 0. \tag{3.17}$$

The equation of the conservation of angular momentum for the bound electronic continuum takes the form

$$\int_V (\mathbf{y}+\boldsymbol{\eta})\times\mu^b\left[\mathbf{E}(\mathbf{y}+\boldsymbol{\eta}) + \frac{1}{C}\left(\mathbf{v} + \frac{d\boldsymbol{\eta}}{dt}\right)\times\mathbf{B}(\mathbf{y}+\boldsymbol{\eta}) + \mathbf{E}^b\right] dV + \int_V (\mathbf{y}+\boldsymbol{\eta})\times\oint_{C'} i'\, d\mathbf{s}\times\mathbf{B}\, dV + \int_V \left(\oint_{C'} \mathbf{r}\times(i'\, d\mathbf{s}\times\mathbf{B}) + \mathbf{M}'\times\mathbf{B}^L\right) dV = 0. \tag{3.18}$$

We do not write the equation of the conservation of angular momentum for the other continua because for three of them—the two conducting fluids and the impurity continuum—the conservation of angular momentum yields the identical information as the conservation of linear momentum and later we impose the condition of invariance of a thermodynamic state function in a rigid rotation, which has been shown to be equivalent to, although more far reaching[33,34] than, the conservation of angular momentum in many circumstances,[1–13] including one[12] considerably more complicated than the one treated here. In the case treated here only the lattice and bound electronic continua are involved in any significant way and the result is well known. We have written the one equation of the conservation of angular momentum in (3.18) because one result of this equation, which is independent of the above considerations, is needed for our purposes. Since $\boldsymbol{\eta}$ is an infinitesimal displacement field, we expand $\mathbf{E}(\mathbf{y}+\boldsymbol{\eta})$ and $\mathbf{B}(\mathbf{y}+\boldsymbol{\eta})$ in a Taylor series about $\mathbf{y}$ and retain the first term to obtain

$$\mathbf{E}(\mathbf{y}+\boldsymbol{\eta}) = \mathbf{E}(\mathbf{y}) + \boldsymbol{\eta}\cdot\nabla\mathbf{E}(\mathbf{y}), \tag{3.19}$$

$$\mathbf{B}(\mathbf{y}+\boldsymbol{\eta}) = \mathbf{B}(\mathbf{y}) + \boldsymbol{\eta}\cdot\nabla\mathbf{B}(\mathbf{y}). \tag{3.20}$$

However, as in Ref. 12, since the infinitesimal dis-

placement field η constitutes an integral part of the model of the polarization, but bears no relation to the model of the magnetization $\mathbf{M}'$, which consists of the circulating current density terms $i'd\mathbf{s}$, the expression (3.20) is employed in charge density terms only and not in current density terms. In Ref. 12 it is shown that

$$\lim_{\substack{i'\to\infty \\ C'\to 0 \text{ in a plane}}} \oint_{C'} i'\,d\mathbf{s}\times\mathbf{B} = \mathbf{M}'\cdot\mathbf{B}\nabla, \tag{3.21}$$

$$\lim_{\substack{r\to 0 \\ i'\to\infty \\ C'\to 0 \text{ in a plane}}} \oint_{C'} \mathbf{r}\times i'\,d\mathbf{s}\times\mathbf{B} = \mathbf{M}'\times\mathbf{B}. \tag{3.22}$$

Application of (3.13) to an elementary tetrahedron in the usual manner yields the definition of the ordinary mechanical stress tensor τ; thus

$$\mathbf{t} = \mathbf{n}\cdot\tau, \quad t_j = n_i\tau_{ij}. \tag{3.23}$$

Substituting from (3.23) into (3.13), taking the material time derivative of (3.13) while employing (3.1), applying the divergence theorem to the surface integral terms in (3.13), (3.16), and (3.17), and employing (3.19)—(3.22) and the arbitrariness of V, we obtain

$$\nabla\cdot\tau + \mu^l\mathbf{E} + \frac{\mu^l}{C}\mathbf{v}\times\mathbf{B} - \mu^b\mathbf{E}^b - \mu^e\mathbf{E}^e - \mu^h\mathbf{E}^h - \mu^i\mathbf{E}^i = \rho\frac{d\mathbf{v}}{dt}, \tag{3.24}$$

$$\mu^b\mathbf{E} + \mu^b\eta\cdot\nabla\mathbf{E} + \frac{\mu^b}{C}\mathbf{v}\times\mathbf{B} + \frac{\mu^b}{C}\mathbf{v}\times(\eta\cdot\nabla\mathbf{B}) + \frac{\mu^b}{C}\frac{d\eta}{dt}\times\mathbf{B} + \mu^b\mathbf{E}^b + \mathbf{M}'\cdot\mathbf{B}\nabla = 0, \tag{3.25}$$

$$\mu^i\mathbf{E} + \frac{\mu^i}{C}\mathbf{v}\times\mathbf{B} + \mu^i\mathbf{E}^i = 0, \tag{3.26}$$

$$-\nabla p^e + \mu^e\mathbf{E} + \frac{\mu^e}{C}\mathbf{v}^e\times\mathbf{B} + \mu^e\mathbf{E}^e = 0, \tag{3.27}$$

$$-\nabla p^h + \mu^h\mathbf{E} + \frac{\mu^h}{C}\mathbf{v}^h\times\mathbf{B} + \mu^h\mathbf{E}^h = 0, \tag{3.28}$$

which constitute the differential equations of motion of the five defined continua consisting of the lattice continuum, the bound electronic, the impurity, the free electronic, and the hole continua, respectively. Substituting from (3.19)—(3.22) into (3.18) and employing (3.25) and the arbitrariness of V and $\mathbf{M}'$, we obtain

$$\mathbf{B}^L = -\mathbf{B}. \tag{3.29}$$

Adding (3.24)—(3.26), defining the electric polarization $\mathbf{P}$ by

$$\mathbf{P} = \mu^b\eta, \tag{3.30}$$

employing (2.4) and the relation[35]

$$\rho\frac{d\pi}{dt} = \mu^b\frac{d\eta}{dt}, \tag{3.31}$$

where π is the polarization per unit mass given by

$$\pi = \mathbf{P}/\rho, \tag{3.32}$$

and retaining terms linear in η only, we obtain

$$\nabla\cdot\tau + \mathbf{P}\cdot\nabla\mathbf{E} + \frac{\mathbf{v}}{C}\times(\mathbf{P}\cdot\nabla\mathbf{B}) + \frac{\rho}{C}\frac{d\pi}{dt}\times\mathbf{B} + \mathbf{M}'\cdot\mathbf{B}\nabla + (\mu^r + \mu^i)\mathbf{E} + (\mu^r + \mu^i)\frac{\mathbf{v}}{C}\times\mathbf{B} - \mu^e\mathbf{E}^e - \mu^h\mathbf{E}^h = \rho\frac{d\mathbf{v}}{dt}, \tag{3.33}$$

which are the stress equations of motion for our deformable solid. The differential equations of linear momentum for the semiconductor system consist of (3.27), (3.28), and (3.33). We now note for later use that adding (3.27), (3.28), and (3.33) and employing (3.9) and (3.10) yields

$$\nabla\cdot\tau - \nabla p^e - \nabla p^h + \mathbf{P}\cdot\nabla\mathbf{E} + \frac{\mathbf{v}}{C}\times(\mathbf{P}\cdot\nabla\mathbf{B}) + \frac{\rho}{C}\frac{d\pi}{dt}\times\mathbf{B} + \mathbf{M}'\cdot\mathbf{B}\nabla + \mu\mathbf{E} + \frac{\mathbf{J}}{C}\times\mathbf{B} = \rho\frac{d\mathbf{v}}{dt}, \tag{3.34}$$

which are the stress equations of motion for the combined semiconductor continuum consisting of the deformable solid and free electronic and hole fluids.

The equations of electromagnetism, which must be included in the theory, consist of the Maxwell field equations, which in Gaussian units take the form[36]

$$C\nabla\times\mathbf{H} = \partial\mathbf{D}/\partial t + 4\pi\mathbf{J}, \tag{3.35}$$

$$C\nabla\times\mathbf{E} = -\partial\mathbf{B}/\partial t, \tag{3.36}$$

where C is the speed of light,

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}, \quad \mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}, \tag{3.37}$$

and

$$\mathbf{M} = \mathbf{M}' - (\mathbf{v}/C)\times\mathbf{P}', \quad \mathbf{P} = \mathbf{P}' + (\mathbf{v}/C)\times\mathbf{M}', \quad \mathbf{J} = \mathbf{J}' + \mu\mathbf{v}, \tag{3.38}$$

are the low velocity limits of the relativistic transformations[37] from one inertial coordinate system to another. In (3.38) $\mathbf{P}'$, $\mathbf{M}'$, and $\mathbf{J}'$ are the polarization, magnetization, and current density, respectively, in the instantaneous local rest system of inertia for the point $\mathbf{y}(\mathbf{X}, t)$ moving with velocity $\mathbf{v}$ relative to *our* rest system of inertia and $\mathbf{P}$, $\mathbf{M}$, and $\mathbf{J}$ are the polarization, magnetization, and current density in *our* rest system of inertia. In addition to (3.35) and (3.36), the auxiliary Maxwell equations

$$\nabla\cdot\mathbf{B} = 0, \quad \nabla\cdot\mathbf{D} = 4\pi\mu \tag{3.39}$$

are satisfied identically. From (3.9), (3.10), and $(3.38)_3$ it is clear that

$$\mathbf{J}' = \mu^e(\mathbf{v}^e - \mathbf{v}) + \mu^h(\mathbf{v}^h - \mathbf{v}). \tag{3.40}$$

Equations (3.35), (3.36), and (3.39), respectively, may properly be regarded as consequences of the integral forms

$$C\oint_C \mathbf{H}\cdot d\mathbf{y} = (\partial/\partial t)\int_S \mathbf{n}\cdot\mathbf{D}\,ds + 4\pi\int_S \mathbf{n}\cdot\mathbf{J}\,ds, \tag{3.41}$$

$$C\oint_C \mathbf{E}\cdot d\mathbf{y} = -(\partial/\partial t)\int_S \mathbf{n}\cdot\mathbf{B}\,ds, \tag{3.42}$$

$$\int_S \mathbf{n}\cdot\mathbf{B}\,ds = 0, \quad \int_S \mathbf{n}\cdot\mathbf{D}\,ds = 4\pi\int_V \mu\,dV, \tag{3.43}$$

which are taken to be valid even when the field vectors are not differentiable, such as across moving surfaces of discontinuity. In (3.41)—(3.43) C denotes a closed curve surrounding an open area s, and S denotes a closed surface surrounding a volume V, all of which are stationary with respect to our inertial reference system.

By means of a procedure essentially identical with the one employed in Sec. 4 of Ref. 12, the electromagnetic body force term

$$f_j = P_k E_{j,k} + e_{jkl}\frac{v_k}{C}P_i B_{i,i} + \frac{\rho}{C}e_{jkl}\frac{d\pi_k}{dt}B_l$$

$$+ M'_k B_{k,j} + \mu E_j + e_{jkl}\frac{J_k}{C}B_l \tag{3.44}$$

in (3.34) may be written in the form

$$f_j = T^{EM}_{ij,i} - \partial g_j/\partial t, \tag{3.45}$$

where

$$T^{EM}_{ij} = (1/4\pi)[4\pi P_i E'_j + E_i E_j + B_i B_j - 4\pi B_i M'_j - \tfrac{1}{2}(E_k E_k + B_k B_k - 8\pi M'_k B_k)\delta_{ij}], \tag{3.46}$$

$$g_j = e_{jil}E_i B_l/4\pi C, \tag{3.47}$$

and

$$E'_j = E_j + e_{jkl}v_k B_l/C. \tag{3.48}$$

The quantity T^{EM}_{ij} is the Maxwell electromagnetic stress tensor for our polarizable, magnetizable, and deformable charged semiconducting continuum and g_j is the linear momentum of the electromagnetic field. Thus, as expected, the Maxwell electromagnetic stress tensor is identical with the one obtained for the insulator in Sec. 4 of Ref. 12. Substituting from (3.44) and (3.45) into (3.34), integrating over an arbitrary material region, and employing the divergence theorem, the transport theorem, [38] and (3.1), we obtain the material integral form

$$\int_s \mathbf{n}\cdot[\boldsymbol{\tau} - (p^e + p^h)\mathbf{I} + \mathbf{T}^{EM} + \mathbf{vg}]\,ds = \frac{d}{dt}\int_V (\rho\mathbf{v} + \mathbf{g})\,dV, \tag{3.49}$$

where I is the idemfactor. Similarly, integrating over a spatial region, which instantaneously coincides with the aforementioned arbitrary material region, we obtain the spatial integral form

$$\int_s \mathbf{n}\cdot[\boldsymbol{\tau} - (p^e + p^h)\mathbf{I} + \mathbf{T}^{EM} - \mathbf{v}\rho\mathbf{v}]\,ds = \frac{\partial}{\partial t}\int_V (\rho\mathbf{v} + \mathbf{g})\,dV, \tag{3.50}$$

which is entirely equivalent to (3.49). We now take either (3.49) or (3.50), it does not matter which, [39] to be valid even when the field variables are not differentiable and the differential form (3.34) cannot be obtained, such as across moving surfaces of discontinuity. As usual in any continuum theory, at this stage the system is underdetermined and constitutive equations are required in order to obtain a determinate system. To this end we consider the conservation of energy for the deformable semiconductor in the next section.

4. THERMODYNAMIC CONSIDERATIONS

The principle of the conservation of energy for the combined semiconducting material medium—consisting of the lattice, the bound electronic, the impurity, the free electronic, and hole continua, respectively—states that, in any *stationary* volume V bounded by a surface s with unit outward normal n, the rate of increase of energy, which consists of the kinetic plus the stored internal energy of the deformable solid (lattice + bound electronic + impurity) plus the stored internal energies of the free electronic and hole fluids, is equal to the rate at which work is done by the mechanical surface tractions and fluid pressures acting across s, less the flux of heat outward across s, less the convective flux of energies of the deformable solid and conducting fluids outward across s, plus the rate at which energy is supplied to the combined semiconducting continuum from the electromagnetic field. Thus

$$\frac{\partial}{\partial t}\int_V (\tfrac{1}{2}\rho\mathbf{v}\cdot\mathbf{v} + \rho\epsilon + \mu^e\epsilon^e + \mu^h\epsilon^h)\,dV = \int_s \Big[\mathbf{t}\cdot\mathbf{v} - p^e\mathbf{n}\cdot\mathbf{v}^e - p^h\mathbf{n}\cdot\mathbf{v}^h - \mathbf{n}\cdot\mathbf{q} - \mathbf{n}\cdot(\mathbf{v}\tfrac{1}{2}\rho\mathbf{v}\cdot\mathbf{v} + \mathbf{v}\rho\epsilon + \mathbf{v}^e\mu^e\epsilon^e + \mathbf{v}^h\mu^h\epsilon^h)\Big]\,ds + \int_V \Sigma\,dV, \tag{4.1}$$

where $\frac{1}{2}\mathbf{v}\cdot\mathbf{v}$ is the kinetic energy per unit mass, ϵ is the stored internal energy per unit mass of the deformable solid (lattice + bound electronic + impurity), ϵ^e is the stored internal energy per unit charge of the free electronic fluid, ϵ^h is the stored internal energy per unit charge of the hole fluid, $\mathbf{t}\cdot\mathbf{v}$ is the rate at which work is done per unit area by the mechanical surface tractions, $-p^e\mathbf{n}\cdot\mathbf{v}^e$ and $-p^h\mathbf{n}\cdot\mathbf{v}^h$ are the rates at which work is done per unit area by the pressures acting in the free electronic and hole fluids, respectively, q is the heat flux vector, $\mathbf{n}\cdot\mathbf{v}\rho(\frac{1}{2}\mathbf{v}\cdot\mathbf{v} + \epsilon)$ is the convective flux of energy of the deformable solid, $\mathbf{n}\cdot\mathbf{v}^e\mu^e\epsilon^e$ and $\mathbf{n}\cdot\mathbf{v}^h\mu^h\epsilon^h$ are the convective fluxes of energy of the free electronic and hole fluids, respectively, and Σ is the rate of supply of energy per unit volume to the entire semiconducting continuum from the electromagnetic field. In order to obtain the expression for Σ, we must return to our model of the combined semiconducting continuum.

From the fundamental electric charge, current, and circulating current model of the continuum, the rate of supply of energy from the Maxwell electromagnetic field is

$$\Sigma = \mu^i\mathbf{E}\cdot\mathbf{v} + \mu^b(\mathbf{E} + \eta\cdot\nabla\mathbf{E})\cdot\left(\mathbf{v} + \frac{d\eta}{dt}\right) + \mu^i\mathbf{E}\cdot\mathbf{v} + \mu^e\mathbf{E}\cdot\mathbf{v}^e + \mu^h\mathbf{E}\cdot\mathbf{v}^h + C\oint_{C'} i'\,d\mathbf{s}\cdot\mathbf{E}, \tag{4.2}$$

in which the entire supply is from the Maxwell electric field **E**. There is no rate of supply of energy from the magnetic induction field B because fundamentally the force exerted on any moving charge element is always normal to the instantaneous total velocity of that charge element. The constant C appears in the last term of (4.2) because i' is in magnetic units. In Sec. 5 of Ref. 12 it is shown that

$$\lim_{\substack{i'\to\infty \\ C'\to 0 \text{ in a plane}}} C\oint_{C'} i'\,d\mathbf{s}\cdot\mathbf{E} = -\mathbf{M}'\cdot\frac{\partial\mathbf{B}}{\partial t}. \tag{4.3}$$

Substituting from (2.4), (3.30), (3.31), and (4.3) into (4.2), we obtain

$$\Sigma = (\mu^r + \mu^i)\mathbf{E}\cdot\mathbf{v} + \mathbf{P}\cdot\nabla\mathbf{E}\cdot\mathbf{v} + \mathbf{E}\cdot\rho\frac{d\pi}{dt} - \mathbf{M}'\cdot\frac{\partial\mathbf{B}}{\partial t} + \mu^e\mathbf{E}\cdot\mathbf{v}^e + \mu^h\mathbf{E}\cdot\mathbf{v}^h. \tag{4.4}$$

Taking the time derivative in (4.1), substituting from (3.23) and (4.4), employing the divergence theorem, (3.6), (3.7), (3.27), (3.28), (3.33), (3.48), the arbi-

trariness of V, and the relations

$$\frac{d}{dt}=\frac{\partial}{\partial t}+v_k\frac{\partial}{\partial y_k},\quad \frac{d^e}{dt}=\frac{\partial}{\partial t}+v_k^e\frac{\partial}{\partial y_k},\quad \frac{d^h}{dt}=\frac{\partial}{\partial t}+v_k^h\frac{\partial}{\partial y_k}, \tag{4.5}$$

and assuming

$$\epsilon^e=\epsilon^e(\mu^e),\quad \epsilon^h=\epsilon^h(\mu^h), \tag{4.6}$$

we obtain

$$\rho\frac{d\epsilon}{dt}+\left(\mu^e\frac{\partial\epsilon^e}{\partial\mu^e}-\frac{p^e}{\mu^e}\right)\frac{d^e\mu^e}{dt}+\left(\mu^h\frac{\partial\epsilon^h}{\partial\mu^h}-\frac{p^h}{\mu^h}\right)\frac{d^h\mu^h}{dt}$$
$$=\tau_{ij}v_{j,i}+\rho\frac{d\pi_i}{dt}E_i'-M_i'\frac{dB_i}{dt}-\mu^eE_i^e(v_i^e-v_i)$$
$$-\mu^hE_i^h(v_i^h-v_i)-\left(\epsilon^e+\frac{p^e}{\mu^e}\right)\gamma^e-\left(\epsilon^h+\frac{p^h}{\mu^h}\right)\gamma^h-q_{i,i}, \tag{4.7}$$

which is the first law of thermodynamics for the deformable semiconducting continuum.

Since we are considering a heat conducting, electrically semiconducting, polarizable and magnetizable, deformable elastic continuum with a first law of thermodynamics of the form shown in (4.7), the mathematical expression of the second law of thermodynamics may be written in the form[40–42]

$$\rho\frac{d\epsilon}{dt}+\left(\mu^e\frac{\partial\epsilon^e}{\partial\mu^e}-\frac{p^e}{\mu^e}\right)\frac{d^e\mu^e}{dt}+\left(\mu^h\frac{\partial\epsilon^h}{\partial\mu^h}-\frac{p^h}{\mu^h}\right)\frac{d^h\mu^h}{dt}-\tau_{ij}v_{j,i}$$
$$-E_i'\rho\frac{d\pi_i}{dt}+M_i'\frac{dB_i}{dt}=\rho\theta\frac{d\eta}{dt}, \tag{4.8}$$

where θ is the absolute temperature and η is the entropy per unit mass. From (4.7) and (4.8), we have the dissipation equation

$$-\mu^eE_i^e(v_i^e-v_i)-\mu^hE_i^h(v_i^h-v_i)-\left(\epsilon^e+\frac{p^e}{\mu^e}\right)\gamma^e$$
$$-\left(\epsilon^h+\frac{p^h}{\mu^h}\right)\gamma^h-q_{i,i}=\rho\theta\frac{d\eta}{dt}, \tag{4.9}$$

and the entropy inequality may be written in the form

$$\rho\frac{d\eta}{dt}+\left(\frac{q_i}{\theta}\right)_{,i}=-\frac{1}{\theta}\left[\frac{q_i\theta_{,i}}{\theta}+\mu^eE_i^e(v_i^e-v_i)+\mu^hE_i^h(v_i^h-v_i)\right.$$
$$\left.+\left(\epsilon^e+\frac{p^e}{\mu^e}\right)\gamma^e+\left(\epsilon^h+\frac{p^h}{\mu^h}\right)\gamma^h\right]=\rho\Gamma\geq 0, \tag{4.10}$$

where Γ is the (positive) rate of entropy production. At this point it should be noted that this theory can readily be *generalized*[43,44] to account for more general functional constitutive response in the manner set forth in Ref. 11.

Before proceeding to a determination of the constitutive equations, we will write the equation of the conservation of energy in a particularly interesting integral form in which no volume source terms appear. To this end we substitute from (3.10) into (4.4) and follow a procedure essentially identical with the one employed in Sec. 5 of Ref. 12 to obtain

$$\Sigma=E_iJ_i+E_i\frac{\partial P_i}{\partial t}-M_i\frac{\partial B_i}{\partial t}+(v_kP_iE_i)_{,k}. \tag{4.11}$$

From (3.35) and (3.36) in the usual way, with the aid of (3.37), we obtain

$$-h_{i,i}=\frac{\partial U^F}{\partial t}+E_iJ_i+E_i\frac{\partial P_i}{\partial t}-M_i\frac{\partial B_i}{\partial t}, \tag{4.12}$$

where

$$h_i=-(C/4\pi)e_{ijk}E_jH_k,\quad U^F=(1/8\pi)(E_kE_k+B_kB_k), \tag{4.13}$$

and U^F may be interpreted as the electromagnetic field energy and h_i is the usual Poynting vector. Equation (4.12) is a particularly interesting and useful form of Poynting's theorem for conducting, polarizable and magnetizable continua. Since the form in (4.12) depends only on the validity of Maxwell's equations [Eqs. (3.35) and (3.36)] and the relations (3.37), and is independent of any particular constitutive assumption, it is always valid. Substituting from (4.11) and (4.12) into (4.1) and employing the divergence theorem and the transport theorem,[38] we obtain

$$\frac{d}{dt}\int_V\left(\tfrac{1}{2}\rho\mathbf{v}\cdot\mathbf{v}+\rho\epsilon+\mu^e\epsilon^e+\mu^h\epsilon^h+U^F\right)dV$$
$$=\int_S\mathbf{n}\cdot[\boldsymbol{\tau}\cdot\mathbf{v}-p^e\mathbf{v}^e-p^h\mathbf{v}^h-\mathbf{h}-\mathbf{q}-(\mathbf{v}^e-\mathbf{v})\mu^e\epsilon^e$$
$$-(\mathbf{v}^h-\mathbf{v})\mu^h\epsilon^h+\mathbf{v}\mathbf{P}\cdot\mathbf{E}+\mathbf{v}U^F]ds, \tag{4.14}$$

which is the particularly interesting integral form of the equation of the conservation of energy we have been after. Similarly, integrating over a spatial region, which instantaneously coincides with the material region considered in (4.14), we obtain the entirely equivalent spatial integral form of the equation of the conservation of energy for our deformable semiconductor

$$\frac{\partial}{\partial t}\int_V\left(\tfrac{1}{2}\rho\mathbf{v}\cdot\mathbf{v}+\rho\epsilon+\mu^e\epsilon^e+\mu^h\epsilon^h+U^F\right)dV$$
$$=\int_S\mathbf{n}\cdot[\boldsymbol{\tau}\cdot\mathbf{v}-p^e\mathbf{v}^e-p^h\mathbf{v}^h-\mathbf{h}-\mathbf{q}-\mathbf{v}\rho(\tfrac{1}{2}\mathbf{v}\cdot\mathbf{v}+\epsilon)$$
$$-\mathbf{v}^e\mu^e\epsilon^e-\mathbf{v}^h\mu^h\epsilon^h+\mathbf{v}\mathbf{P}\cdot\mathbf{E}]ds. \tag{4.15}$$

5. CONSTITUTIVE EQUATIONS

The state function constitutive equations may be determined from the thermodynamic state function equation (4.8), which, by virtue of the relation

$$v_{j,i}=X_{M,i}d(y_{j,M})/dt,$$

may be written in the form

$$\rho\frac{d\epsilon}{dt}+\left(\mu^e\frac{\partial\epsilon^e}{\partial\mu^e}-\frac{p^e}{\mu^e}\right)\frac{d^e\mu^e}{dt}+\left(\mu^h\frac{\partial\epsilon^h}{\partial\mu^h}-\frac{p^h}{\mu^h}\right)\frac{d^h\mu^h}{dt}$$
$$=\tau_{ij}X_{M,i}\frac{d}{dt}(y_{j,M})+E_i'\rho\frac{d\pi_i}{dt}-M_i'\frac{dB_i}{dt}+\rho\theta\frac{d\eta}{dt}. \tag{5.1}$$

Since the entropy inequality is of the form shown in (4.10) and Faraday's law (3.36) contains the electromagnetic field variables **E** and **B** only, it turns out to be convenient to define the thermodynamic state function χ by the Legendre transformation

$$\chi=\epsilon-E_i'\pi_i-\eta\theta. \tag{5.2}$$

The substitution of the material time derivative of (5.2) into (5.1) yields

$$\rho\frac{d\chi}{dt}+\left(\mu^e\frac{\partial\epsilon^e}{\partial\mu^e}-\frac{p^e}{\mu^e}\right)\frac{d^e\mu^e}{dt}+\left(\mu^h\frac{\partial\epsilon^h}{\partial\mu^h}-\frac{p^h}{\mu^h}\right)\frac{d^h\mu^h}{dt}$$

$$= \tau_{ij} X_{M,i} \frac{d}{dt}(y_{j,M}) - \rho\pi_i \frac{dE'_i}{dt} - M'_i \frac{dB_i}{dt} - \rho\eta \frac{d\theta}{dt}. \quad (5.3)$$

Since (5.3) is a state function equation, we must have

$$\chi = \chi(y_{j,M}; E'_i; B_i; \theta). \quad (5.4)$$

Substituting the material time derivative of (5.4) into (5.3), we obtain

$$\left(\tau_{ij} X_{M,i} - \rho \frac{\partial \chi}{\partial (y_{j,M})}\right) \frac{d}{dt}(y_{j,M}) - \rho\left(\pi_i + \frac{\partial \chi}{\partial E'_i}\right) \frac{dE'_i}{dt}$$
$$- \rho\left(\nu'_i + \frac{\partial \chi}{\partial B_i}\right) \frac{dB_i}{dt} - \rho\left(\eta + \frac{\partial \chi}{\partial \theta}\right) \frac{d\theta}{dt}$$
$$- \left(\mu^e \frac{\partial \epsilon^e}{\partial \mu^e} - \frac{p^e}{\mu^e}\right) \frac{d^e \mu^e}{dt} - \left(\mu^h \frac{\partial \epsilon^h}{\partial \mu^h} - \frac{p^h}{\mu^h}\right) \frac{d^h \mu^h}{dt} = 0, \quad (5.5)$$

in which the magnetization per unit mass ν'_i in the instantaneous local rest system of inertia, defined by

$$\nu'_i = M'_i/\rho, \quad (5.6)$$

has been introduced.

Since all the material time derivatives appearing in (5.5) are independent and (5.5) holds for arbitrary $d(y_{j,M})/dt$, dE'_i/dt, dB_i/dt, $d\theta/dt$, $d^e\mu^e/dt$, and $d^h\mu^h/dt$, we have

$$X_{M,i} \tau_{ij} = \rho\, \partial\chi/\partial(y_{j,M}), \quad (5.7)$$

$$\pi_i = -\partial\chi/\partial E'_i, \quad \nu'_i = -\partial\chi/\partial B_i, \quad \eta = -\partial\chi/\partial\theta, \quad (5.8)$$

$$p^e = (\mu^e)^2\, \partial\epsilon^e/\partial\mu^e, \quad p^h = (\mu^h)^2\, \partial\epsilon^h/\partial\mu^h. \quad (5.9)$$

Solving (5.7) for τ, with the aid of the chain rule of differentiation, we find

$$\tau_{ij} = \rho y_{i,M}\, \partial\chi/\partial(y_{j,M}). \quad (5.10)$$

Although ϵ^e and ϵ^h can be arbitrary functions of μ^e and μ^h, respectively, because such functions are automatically invariant in a rigid rotation, χ cannot be an *arbitrary* function of $y_{k,L}$, E_k, B_k, and θ because in order to satisfy the principle of material objectivity,[45,46] ϵ and, hence, χ must be a scalar invariant under rigid rotations[47] of the deformed, polarized and magnetized body, and any arbitrary function of the 16 variables (five vectors and a scalar at the point y_k) will not be so invariant. However, there is a theorem on invariant functions of several vectors due to Cauchy,[48] which says that χ may be an arbitrary single-valued function of the scalar products of the vectors and the determinants of their components taken three at a time.[49] Application of this theorem shows that χ is expressible as an arbitrary function of 15 scalar products and ten determinants, as well as θ, for a total of 26 quantities. However, the 26 quantities are not all functionally independent, and it can be shown, by means of procedures similar to those employed in Sec. 6 of Ref. 4, that the 26 variables are expressible in terms of the 13 arguments consisting of

$$C_{KL} = y_{i,K} y_{i,L}, \quad W_L = y_{i,L} E'_i, \quad N_L = y_{i,L} B_i, \quad \theta. \quad (5.11)$$

Thus we find that χ may be reduced to the form

$$\chi = \chi(E_{KL}, W_L, N_L, \theta), \quad (5.12)$$

in place of the form shown in (5.4), and we have replaced Green's deformation tensor C_{KL}, which does not vanish in the undeformed state, by the entirely equivalent material strain tensor E_{KL}, which does vanish in the undeformed state, and is related to C_{KL} by

$$E_{KL} = \tfrac{1}{2}(C_{KL} - \delta_{KL}). \quad (5.13)$$

From (5.8) and (5.10)–(5.13), we obtain

$$\tau_{ij} = \rho y_{i,L} y_{j,M} \frac{\partial \chi}{\partial E_{LM}} + \rho y_{i,L} \frac{\partial \chi}{\partial W_L} E'_j + \rho y_{i,L} \frac{\partial \chi}{\partial N_L} B_j, \quad (5.14)$$

$$\pi_i = -y_{i,L} \frac{\partial \chi}{\partial W_L}, \quad \nu'_i = -y_{i,L} \frac{\partial \chi}{\partial N_L}, \quad \eta = -\frac{\partial \chi}{\partial \theta}, \quad (5.15)$$

in which we have introduced the convention $\partial\chi/\partial E_{KL} = \partial\chi/\partial E_{LK}$, and it is to be assumed that $\partial E_{RN}/\partial E_{NR} = 0$ in differentiating χ. From (5.14), $(5.15)_{1,2}$, (3.32), and (5.6) note that

$$\tau^A_{ij} = \tfrac{1}{2}(E'_i P_j - P_i E'_j + B_i M'_j - M'_i B_j), \quad (5.16)$$

which is the equation that would have been obtained from the conservation of angular momentum had it been employed.

This brings us to a consideration of the dissipative constitutive equations, which are obtained from the entropy inequality (4.10) which with the aid of (5.9) may be written in the form

$$(q_i \theta_{,i}/\theta) + \mu^e E^e_i (v^e_i - v_i) + \mu^h E^h_i (v^h_i - v_i)$$
$$+ \gamma^e\, \partial(\mu^e \epsilon^e)/\partial\mu^e + \gamma^h\, \partial(\mu^h \epsilon^h)/\partial\mu^h \le 0. \quad (5.17)$$

Motivated by (5.17), we take the dissipative constitutive equations in the form

$$q_i = q_i(\theta_{,i}, \mu^e, \mu^h, E^e_i, E^h_i)$$
$$v^e_i - v_i = V^e_i(\theta_{,i}, \mu^e, \mu^h, E^e_i, E^h_i),$$
$$v^h_i - v_i = V^h_i(\theta_{,i}, \mu^e, \mu^h, E^e_i, E^h_i),$$
$$\gamma^e = \gamma^e(\theta_{,i}, \mu^e, \mu^h, E^e_i, E^h_i),$$
$$\gamma^h = \gamma^h(\theta_{,i}, \mu^e, \mu^h, E^e_i, E^h_i), \quad (5.18)$$

but since the nondissipative constitutive equations (5.14), (5.15) depend on the $y_{i,M}$, E'_i, B_i and θ, there is no logical reason to exclude them from the dissipative constitutive equations.[50] Hence, on account of the chain rule of differentiation, we may write

$$q_i = q_i(\theta_{,M}, \mu^e, \mu^h, E^e_i, E^h_i, y_{i,M}, E'_i, B_i, \theta),$$
$$v^e_i - v_i = V^e_i(\theta_{,M}, \mu^e, E^e_i, y_{i,M}, E'_i, B_i, \theta),$$
$$v^h_i - v_i = V^h_i(\theta_{,M}, \mu^h, E^h_i, y_{i,M}, E'_i, B_i, \theta),$$
$$\gamma^e = \gamma^e(\theta_{,M}, \mu^e, E^e_i, y_{i,M}, E'_i, B_i, \theta),$$
$$\gamma^h = \gamma^h(\theta_{,M}, \mu^h, E^h_i, y_{i,M}, E'_i, B_i, \theta), \quad (5.19)$$

for the general functional dependence of the dissipative constitutive equations. Since the free electronic and hole fluids have been assumed not to interact directly with each other, we have excluded the dependence of V^e_i and γ^e on μ^h and E^h_i and V^h_i and γ^h on μ^e and E^e_i. Now, in order that the dissipative constitutive equations (5.19) may be able to satisfy the principle of material objectivity,[45,46] all variables in (5.19) must be objective,[51] i.e., they must transform as tensors under time-dependent proper orthogonal transformations.[47] All variables in (5.19), save $(v^e_i - v_i)$ and $(v^h_i - v_i)$, satisfy this latter requirement trivially, since they are not time-differentiated quantities, and $(v^e_i - v_i)$ and $(v^h_i - v_i)$ may readily be shown to be objective vectors. To see this, consider

$$y_i^* = Q_{ij}(t)y_j + b_i(t), \quad (y_i^e)^* = Q_{ij}(t)y_j^e + b_i(t), \tag{5.20}$$

where $Q_{ij}(t)$ represents an arbitrary time-dependent proper orthogonal transformation and $b_i(t)$ represents an arbitrary time-dependent translation. In (5.20) the starred quantities represent either the motion as seen from an orthogonal coordinate system in arbitrary rigid motion with respect to ours or the motion plus a superposed rigid motion as seen from our coordinate system. From (5.20), we obtain

$$(v_i^e - v_i)^* = Q_{ij}(v_j^e - v_j) + (dQ_{ij}/dt)(y_j^e - y_j), \tag{5.21}$$

but since at the point under consideration,

$$y_j^e = y_j, \tag{5.22}$$

we have

$$(v_i^e - v_i)^* = Q_{ij}(v_j^e - v_j), \tag{5.23}$$

which shows that $(v_i^e - v_i)$ is an objective vector. In the same way we may readily show that $(v_i^h - v_i)$ is an objective vector. Now, the quantities on the left-hand sides of (5.19) cannot be arbitrary functions of the variables shown because arbitrary functions of the variables shown will not satisfy the principle of material objectivity,[45,46] which requires the constitutive equations to transform appropriately under proper orthogonal transformations. However, if q_i, V_i^e, and V_i^h are expressed in the form

$$q_i = y_{i,K}L_K, \quad V_i^e = y_{i,K}\Omega_K^e, \quad V_i^h = y_{i,K}\Omega_K^h, \tag{5.24}$$

where L_K, Ω_K^e, and Ω_K^h are functions of the variables shown on the respective right-hand sides of (5.19), it may readily be shown using established methods[52] that the principle of material objectivity is satisfied if L_K, Ω_K^e, and Ω_K^h are vector invariants in a rigid motion and γ^e and γ^h are scalar invariants in a rigid motion. Then the previous application of Cauchy's theorem on invariant functions of vectors shows that the required invariance is assured if L_K, Ω_K^e, Ω_K^h, γ^e, and γ^h, respectively, are of the form

$$\begin{aligned}
L_K &= L_K(\theta_{,M}, \mu^e, \mu^h, w_L^e, w_L^h, E_{LM}, W_L, N_L, \theta),\\
\Omega_K^e &= \Omega_K^e(\theta_{,M}, \mu^e, w_L^e, E_{LM}, W_L, N_L, \theta),\\
\Omega_K^h &= \Omega_K^h(\theta_{,M}, \mu^h, w_L^h, E_{LM}, W_L, N_L, \theta),
\end{aligned} \tag{5.25}$$

$$\begin{aligned}
\gamma^e &= \gamma^e(\theta_{,M}, \mu^e, w_L^e, E_{LM}, W_L, N_L, \theta),\\
\gamma^h &= \gamma^h(\theta_{,M}, \mu^h, w_L^h, E_{LM}, W_L, N_L, \theta),
\end{aligned} \tag{5.26}$$

where

$$w_L^e = y_{i,L}E_i^e, \quad w_L^h = y_{i,L}E_i^h, \tag{5.27}$$

and E_{LM}, W_L, and N_L are defined in (5.13) and $(5.11)_{2,3}$, respectively. Now, it must be remembered that, although the dependence of L_K, Ω_K^e, Ω_K^h, γ^e, and γ^h on E_{KL}, W_K, N_L, and θ is arbitrary, there are conditions on their dependence on $\theta_{,M}$, w_L^e, w_L^h, μ^e, and μ^h on account of the Clausius–Duhem inequality (5.17). Thus the dissipative constitutive equations in the general case are given by (5.26) and

$$q_i = y_{i,K}L_K, \quad v_i^e - v_i = y_{i,K}\Omega_K^e, \quad v_i^h - v_i = y_{i,K}\Omega_K^h, \tag{5.28}$$

with L_K, Ω_K^e, and Ω_K^h as given in (5.25).

Equations (5.14), (5.15), (5.26), and (5.28) determine the constitutive equations for our heat conducting, polarizable and magnetizable, deformable semiconducting continuum. Thus, all that remains in the determination of explicit constitutive equations is the selection of specific forms for $\epsilon^e, \epsilon^h, \chi, L_K, \Omega_K^e, \Omega_K^h, \gamma^e$, and γ^h. At this point it should be noted that the generation rates γ^e and γ^h implicitly determine the degree of impurity of the semiconducting continuum. If $\gamma^e + \gamma^h = 0$, we have a pure (intrinsic) semiconductor, but if $\gamma^e + \gamma^h \neq 0$ we have a semiconductor with either a donor or acceptor density. Once the constitutive equations have been determined, we have a determinate theory, which by appropriate substitution can readily be reduced to 18 equations in the 18 dependent variables y_j, θ, E_i, B_i, E_i^e, E_i^h, μ^e, and μ^h. The 18 equations are the three each of (3.27), (3.28), (3.33), (3.35), and (3.36) and (3.6), (3.7), and (4.9). Clearly, the system can be reduced further to 16 equations in 16 dependent variables with the aid of the electromagnetic potentials.[53] In order to have a complete field theory, the boundary (or jump) conditions at moving surfaces of discontinuity have to be adjoined to the aforementioned system of equations. This is done in the next section.

Before proceeding we note that the quantities $\partial(\mu^e\epsilon^e)/\partial\mu^e$ and $\partial(\mu^h\epsilon^h)/\partial\mu^h$ are identical with the chemical potentials φ^e and φ^h for the free electronic and hole continua, respectively, which are used in place of the partial pressures p^e and p^h in most literature[19,54] on semiconductors. Indeed, from (5.9) and

$$\varphi^e = \partial(\mu^e\epsilon^e)/\partial\mu^e, \quad \varphi^h = \partial(\mu^h\epsilon^h)/\partial\mu^h, \tag{5.29}$$

it is relatively easy to show that

$$(1/\mu^e)p_{,i}^e = \varphi_{,i}^e, \quad (1/\mu^h)p_{,i}^h = \varphi_{,i}^h, \tag{5.30}$$

which indicates that in the equations of the conservation of linear momentum (or conductivity equations) for the free electronic continuum (3.27) and hole continuum (3.28), the terms containing the pressure gradients are identical with the gradients of the respective chemical potentials. However, the use of the partial pressures, which are more fundamental than the chemical potentials, indicates the existence and proper form of semiconductor boundary conditions, as shown in the next section, and results in the correct rates of working and attendant thermodynamic description appearing in Sec. 4, which underlies the constitutive equations of this section. Moreover, it should be noted that the substitution of (5.29) in the last two terms on the lhs of the rate of entropy production inequality (5.17), which was obtained from a systematic continuum thermodynamic treatment, results in terms identical with those presented in Section 3.5 of Ref. 54 for the equivalent situation, which terms were obtained in a completely different manner.

6. THE BOUNDARY CONDITIONS

In this section we determine the boundary conditions which must be adjoined to the system of differential equations, as noted in Sec. 5, in order to formulate boundary value problems. As usual, these boundary (or jump) conditions are determined by applying the integral forms of the pertinent field equations to appropriate limiting regions surrounding the moving (not necessarily material) surface of discontinuity[55] with normal velocity u_n, and assuming that certain variables

remain bounded. The pertinent integral forms are (3.1)–(3.4), the integral form associated with (3.8), (3.41)–(3.43), either (3.49) or (3.50), the integral form of (4.10), which takes the form

$$\frac{d}{dt}\int_V \rho\eta\, dV + \int_s \frac{n_i q_i}{\theta} ds = \int_V \rho\Gamma\, dV \geq 0, \tag{6.1}$$

where $\rho\Gamma$ is defined in (4.10) and integral forms are associated with (3.27) and (3.28), neither of which can be used directly to find integral forms for the determination of jump conditions without making some sort of physical assumption about the manner in which the Lorentz force for each conducting fluid and $\mathbf{E}^e$ and $\mathbf{E}^h$ become unbounded. However, before proceeding we observe that since we have the correct integral form (3.50) for the combined semiconducting continuum, any assumptions concerning the integral forms for the conducting fluids must be consistent with (3.50) and, indeed, can be expected to be related to the Maxwell tensor $\mathbf{T}^{EM}$, which results in the force exerted across the surface by the electromagnetic field on the combined semiconducting continuum. Since the conducting fluids possess no polarization or magnetization, the aforementioned surface force on each conducting fluid should be directly related to the Maxwell stress tensor $\mathbf{T}^{ES}$ which contains the terms in $\mathbf{T}^{EM}$ independent of $\mathbf{P}$ and $\mathbf{M}'$, i.e.,

$$T_{ij}^{ES} = (1/4\pi)[E_iE_j + B_iB_j - \tfrac{1}{2}(E_kE_k + B_kB_k)\delta_{ij}]. \tag{6.2}$$

Although the jump in the Maxwell tensor across a surface of discontinuity depends only on the discontinuity in the field vectors and is not directly dependent on the surface charge, from a discrete microscopic viewpoint the resultant macroscopic surface force is due to the sum of the microscopic volumetric forces exerted by the electromagnetic field on the free electrons (and/or holes) and lattice charge in a microscopic volumetric region that can be identified with the macroscopic surface. As a consequence of this reasoning, the surface force on, say, the free electronic continuum and the residual charge of the lattice continuum must be oppositely directed because the above-mentioned microscopic charges are of opposite sign. In fact it can be reasoned that the magnitude of the surface forces on the separate continua can be considerably larger than the magnitude of the resultant force due to the jump in the Maxwell tensor $\mathbf{T}^{ES}$ on the two mentioned continua combined. In view of the above discussion it seems reasonable to assume that there are scalar material coefficients α^e, α^h, and α^s, which are related to appropriate ratios of the above-mentioned microscopic volumetric charge densities within the macroscopic surface of the semiconductor, that when multiplied by the Maxwell tensor $\mathbf{T}^{ES}$ in (6.2) give the forces exerted by the electromagnetic field across the surfaces of the respective continua. Thus, we postulate that the integral forms associated with the differential forms (3.27) and (3.28), respectively, which are valid in the vicinity of a surface of discontinuity are

$$\int_s \mathbf{n}\cdot(-p^e\mathbf{I} + \alpha^e\mathbf{T}^{ES})\, ds + \int_V \mu^e\mathbf{E}^{es}\, dV = \frac{\partial}{\partial t}\int_V \alpha^e\mathbf{g}\, dV, \tag{6.3}$$

$$\int_s \mathbf{n}\cdot(-p^h\mathbf{I} + \alpha^h\mathbf{T}^{ES})\, ds + \int_V \mu^h\mathbf{E}^{hs}\, dV = \frac{\partial}{\partial t}\int_V \alpha^h\mathbf{g}\, dV, \tag{6.4}$$

where $\mathbf{E}^{es} \neq \mathbf{E}^e$ and $\mathbf{E}^{hs} \neq \mathbf{E}^h$ in order that (6.3) and (6.4) be consistent with (3.50), and we have introduced $\mathbf{g}$ in (6.3) and (6.4), even though we deem it to be negligible in actual cases, also for logical consistency with (3.50). Clearly then, in the vicinity of a surface of discontinuity in addition to (6.3), (6.4), and (3.50), we have

$$\int_s \mathbf{n}\cdot[\boldsymbol{\tau} + \mathbf{T}^{EM} + (\alpha^s - 1)\mathbf{T}^{ES} - \mathbf{v}\rho\mathbf{v}]\, ds - \int_V (\mu^e\mathbf{E}^{es} + \mu^h\mathbf{E}^{hs})\, dV = \frac{\partial}{\partial t}\int_V (\rho\mathbf{v} + \alpha^s\mathbf{g})\, dV, \tag{6.5}$$

as the integral form associated with the differential form (3.33), where

$$\alpha^e + \alpha^h + \alpha^s = 1, \tag{6.6}$$

which assures that the sum of (6.3)–(6.5) yields (3.50). The scalar material coefficients α^e, α^h, and α^s can be regarded as either macroscopic quantities to be measured or coefficients to be determined from a microscopic quantum mechanical surface state calculation.[56] In any event in this description they are taken to be known parameters, which may be determined by either of the above mentioned means.

Since the normal component of electric displacement can be discontinuous even across nonmaterial surfaces of discontinuity, the charge density μ and, hence, all the other charge densities, as well as the charge generation rates, can become unbounded at nonmaterial, as well as material, surfaces of discontinuity. However, at nonmaterial surfaces of discontinuity the material fields $\mathbf{E}^{es}$ and $\mathbf{E}^{hs}$ are assumed to remain bounded, while at material surfaces of discontinuity they can become unbounded. For all integral forms considered, except (3.41) and (3.42), a volumetric region is taken in the usual way,[55] and it is assumed that all pertinent variables remain bounded except the aforementioned charge densities and charge generation rates. The jump conditions obtained from the respective integral forms consisting of (3.1)–(3.4), the integral form associated with (3.8), (3.43), either (3.49) or (3.50), (6.1), (6.3), and (6.4) are

$$\mathbf{n}\cdot[\rho\mathbf{v}] - u_n[\rho] = 0, \tag{6.7}$$

$$\mathbf{n}\cdot[\mu^i\mathbf{v}] - u_n[\mu^i] + \partial Q^i/\partial t = \Gamma^i, \tag{6.8}$$

$$\mathbf{n}\cdot[\mu^e\mathbf{v}^e] - u_n[\mu^e] + \partial Q^e/\partial t = \Gamma^e, \tag{6.9}$$

$$\mathbf{n}\cdot[\mu^h\mathbf{v}^h] - u_n[\mu^h] + \partial Q^h/\partial t = \Gamma^h, \tag{6.10}$$

$$\mathbf{n}\cdot[\mu^r\mathbf{v}] - u_n[\mu^r] + \partial Q^r/\partial t = \Gamma^r, \tag{6.11}$$

$$\mathbf{n}\cdot[B] = 0, \quad \mathbf{n}\cdot[\mathbf{D}] = 4\pi Q, \tag{6.12}$$

$$\mathbf{n}\cdot[\boldsymbol{\tau} - (p^e + p^h)\mathbf{I} + \mathbf{T}^{EM} - \mathbf{v}\rho\mathbf{v}] + u_n[\rho\mathbf{v} + \mathbf{g}] = 0, \tag{6.13}$$

$$\mathbf{n}\cdot[(\mathbf{q}/\theta) + \mathbf{v}\rho\eta] - u_n[\rho\eta] \geq 0, \tag{6.14}$$

$$\mathbf{n}\cdot[-p^e\mathbf{I} + \alpha^e\mathbf{T}^{ES}] + u_n[\alpha^e\mathbf{g}] = 0, \tag{6.15}$$

$$\mathbf{n}\cdot[-p^h\mathbf{I} + \alpha^h\mathbf{T}^{ES}] + u_n[\alpha^h\mathbf{g}] = 0, \tag{6.16}$$

where we have introduced the conventional notation $[\mathbf{C}]$ for $\mathbf{C}^+ - \mathbf{C}^-$, $\mathbf{n}$ denotes the unit normal directed from the $-$ to the $+$ side of the surface of discontinuity, Q^i, Q^e, Q^h, and Q^r denote the surface charge densities for the impurity, free electronic, hole and lattice continua, respectively, while Q is the net surface charge density,[57] i.e.,

$$Q = Q^r + Q^i + Q^e + Q^h, \tag{6.17}$$

and Γ^r, Γ^i, Γ^e, and Γ^h are the respective surface charge generation rates, which satisfy

$$\Gamma^r + \Gamma^i + \Gamma^e + \Gamma^h = 0. \tag{6.18}$$

The jump conditions on $\mathbf{H}$ and $\mathbf{E}$, respectively, are determined from (3.41) and (3.42) by considering the circulation around a limiting open surface intersecting the moving surface of discontinuity in the usual way,[58] and are given by

$$\mathbf{n}\times[\mathbf{H}] + (u_n/C)[\mathbf{D}] = 0, \quad \mathbf{n}\times[\mathbf{E}] - (u_n/C)[\mathbf{B}] = 0. \tag{6.19}$$

If the surface of discontinuity is material,

$$u_n = \mathbf{n}\cdot\mathbf{v}^+ = \mathbf{n}\cdot\mathbf{v}^-, \tag{6.20}$$

and (6.7) evaporates, (6.8)—(6.11) and (6.13) reduce to

$$\partial Q^i/\partial t = \Gamma^i, \tag{6.21}$$

$$\mathbf{n}\cdot[\mu^e(\mathbf{v}^e - \mathbf{v})] + \partial Q^e/\partial t = \Gamma^e, \tag{6.22}$$

$$\mathbf{n}\cdot[\mu^h(\mathbf{v}^h - \mathbf{v})] + \partial Q^h/\partial t = \Gamma^h, \tag{6.23}$$

$$\partial Q^r/\partial t = \Gamma^r, \tag{6.24}$$

$$\mathbf{n}\cdot[\boldsymbol{\tau} - (p^e + p^h)\mathbf{I} + \mathbf{T}^{\mathrm{EM}} + \mathbf{vg}] = 0, \tag{6.25}$$

(6.12) remain unchanged, and (6.15) and (6.16) take the respective forms

$$\mathbf{n}\cdot[-p^e\mathbf{I} + \alpha^e\mathbf{T}^{\mathrm{ES}} + \mathbf{v}\alpha^e\mathbf{g}] + \mathcal{J}^e = 0, \tag{6.26}$$

$$\mathbf{n}\cdot[-p^h\mathbf{I} + \alpha^h\mathbf{T}^{\mathrm{ES}} + \mathbf{v}\alpha^h\mathbf{g}] + \mathcal{J}^h = 0, \tag{6.27}$$

where

$$\int_s \mathcal{J}^e\,ds = \lim_{V\to 0}\int_V \mu^e\mathbf{E}^{es}\,dV, \quad \int_s \mathcal{J}^h\,ds = \lim_{V\to 0}\int_V \mu^h\mathbf{E}^{hs}\,dV. \tag{6.28}$$

The vectors $\mathcal{J}^e$ and $\mathcal{J}^h$ denote the surface forces that are exerted by the deformable solid on the free electronic and hole fluids, respectively. Now, from (4.10), (3.27), and (3.28), with the aid of (5.29), (5.30), (3.6), (3.7), the divergence theorem and an integration over an arbitrary volume, we can write

$$\begin{aligned}\int_V \left[\rho\frac{d\eta}{dt} + \frac{1}{\theta}\left(\varphi^e\frac{\partial\mu^e}{\partial t} + \varphi^h\frac{\partial\mu^h}{\partial t}\right)\right]dV \\ + \int_s n_i\frac{1}{\theta}(q_i + \varphi^e\mu^e v_i^e + \varphi^h\mu^h v_i^h)\,ds \\ = \int_V\left(-\frac{1}{\theta^2}(q_i + \varphi^e\mu^e v_i^e + \varphi^h\mu^h v_i^h)\,\theta_{,i} + \frac{1}{\theta}(\mu^e v_i^e + \mu^h v_i^h)E_i \right. \\ \left. + \frac{1}{\theta}(\mu^e E_i^e + \mu^h E_i^h)v_i\right)dV.\end{aligned} \tag{6.29}$$

If θ is continuous, i.e.,

$$[\theta] = 0, \tag{6.30}$$

across the surface of discontinuity, the application of (6.29) to the appropriate limiting region surrounding the moving material surface of discontinuity, along with the assumption that all current terms remain bounded, yields the jump condition

$$\begin{aligned}\mathbf{n}\cdot[\mathbf{q} + \varphi^e\mu^e\mathbf{v}^e + \varphi^h\mu^h\mathbf{v}^h] + \tfrac{1}{2}(\varphi^{e+} + \varphi^{e-})\frac{\partial Q^e}{\partial t} \\ + \tfrac{1}{2}(\varphi^{h+} + \varphi^{h-})\frac{\partial Q^h}{\partial t} = 0,\end{aligned} \tag{6.31}$$

provided we assume that the terms containing $\mathbf{v}$, i.e., $\mu^e\mathbf{E}^e\cdot\mathbf{v}$ and $\mu^h\mathbf{E}^h\cdot\mathbf{v}$ are bounded in the limit even though $\mathbf{E}^e$ and $\mathbf{E}^h$ are not bounded. This is a reasonable physical assumption since $|\mathbf{v}|$ is so much smaller than $|\mathbf{v}^e|$ and $|\mathbf{v}^h|$. This latter situation, consisting of the jump conditions (6.12), (6.19), (6.21)—(6.27), (6.30), and (6.31) along with Eqs. (6.17) and (6.18), is of primary interest to us and these jump conditions are sufficient if the semiconductor abuts free space. However, if the semiconductor abuts another semiconductor, the additional condition

$$[\mathbf{y}] = 0, \tag{6.32}$$

which states that the two bodies are attached, must be satisfied. The normal components of the surface forces $\mathcal{J}^e$ and $\mathcal{J}^h$ exerted by the deformable solid on the respective conducting fluids must be determined from constitutive relations, which, by virtue of considerations discussed in Sec. 5, may be written in the form[59]

$$n_j\mathcal{J}_j^e = n_j y_{j,K}G_K^e, \quad n_j\mathcal{J}_j^h = n_j y_{j,K}G_K^h, \tag{6.33}$$

where

$$\begin{aligned}G_K^e &= G_K^e(\theta_{,M}, \mu^e, w_L^e, E_{LM}, W_L, N_L, \theta), \\ G_K^h &= G_K^h(\theta_{,M}, \mu^h, w_L^h, E_{LM}, W_L, N_L, \theta).\end{aligned} \tag{6.34}$$

Since, by virtue of (5.9), (3.27) and (3.28) constitute first-order differential equations in μ^e and μ^h, respectively, the boundary conditions

$$[-p^e + \alpha^e\mathbf{n}\cdot(\mathbf{T}^{\mathrm{ES}} + \mathbf{vg})\cdot\mathbf{n}] + \mathbf{n}\cdot\mathcal{J}^e = 0, \tag{6.35}$$

$$[-p^h + \alpha^h\mathbf{n}\cdot(\mathbf{T}^{\mathrm{ES}} + \mathbf{vg})\cdot\mathbf{n}] + \mathbf{n}\cdot\mathcal{J}^h = 0, \tag{6.36}$$

which are obtained by taking the normal components of (6.26) and (6.27), respectively, are sufficient when the semiconductor abuts either free space or another semiconductor. The tangential components of the surface forces $\mathcal{J}^e$ and $\mathcal{J}^h$, i.e., $\mathbf{n}\times\mathcal{J}^e$ and $\mathbf{n}\times\mathcal{J}^h$, may be determined *a posteriori* if desired when a solution has been obtained. Now, all terms in boundary expressions, which are not prescribed, may be expressed in terms of the same 18 field variables as the 18 equations mentioned near the end of Sec. 5 by making the appropriate straightforward substitutions.

Thus, at this point we have obtained the nonlinear differential equations and boundary conditions describing the interaction of the electromagnetic field with polarizable and magnetizable, heat conducting, deformable semiconductors. The description consists of the aforementioned 18 equations and 20 boundary conditions, which are the one each of $(6.12)_{1,2}$, (6.21)—(6.24), (6.30), (6.31), (6.35), and (6.36), the two each of $(6.19)_{1,2}$, and the three each of (6.25) and (6.32), all expressed in terms of the 18 field variables y_i, θ, E_i, B_i, E_i^e, E_i^h, μ^e, and μ^h. In addition, at a boundary, Eqs. (6.17) and (6.18) must be satisfied. All that remains is the selection of specific forms for ϵ^e, ϵ^h, L_K, Ω_K^e, Ω_K^h, γ^e, γ^h, G_K^e, G_K^h, Γ^e, and Γ^h.

7. THE QUASISTATIC ELECTRIC FIELD

Since the wavelengths of elastic waves are much shorter than the wavelengths of electromagnetic waves at the same frequency and we are concerned with solutions at the shorter wavelengths, it proves convenient

to reduce the equations that have already been derived to those that hold when the electric field is quasistatic.[27] Although in this section the magnetization **M** is assumed to vanish, the magnetic induction field **B** is permitted to exist but must be static and homogeneous. At this point it should be noted that since the velocity **v** of the lattice continuum is very much smaller than the speed of light C, to this approximation terms containing $\mathbf{v}/C$ may be neglected without loss in accuracy and, from $(3.38)_{1,2}$, (3.48), and (5.6), we have

$$\mathbf{M}=0, \quad \mathbf{P}=\mathbf{P}', \quad \mathbf{E}=\mathbf{E}, \quad \nu=0. \tag{7.1}$$

In this approximation in place of (3.36) we have

$$E_i=-\varphi_{,i}, \tag{7.2}$$

where φ is the electric scalar potential, and the Poynting vector **h** defined in $(4.13)_1$ reduces to

$$h_i=-(\varphi/4\pi)\partial D_i/\partial t. \tag{7.3}$$

Moreover, the electromagnetic momentum **g** defined in (3.47) can be neglected. Under these circumstances the resulting description becomes Galilean invariant.

When the electric field is quasistatic and the magnetic induction is a static homogeneous field, Eqs. (2.6), (3.1), (3.5)—(3.12), (3.23), (3.27)—(3.32), (3.37), $(3.38)_3$, (3.39), (3.40), and (3.43) remain unchanged, Eqs. (3.33) and (3.34) take the respective forms

$$\nabla\cdot\boldsymbol{\tau}+\mathbf{P}\cdot\nabla\mathbf{E}+(\mu^r+\mu^i)\mathbf{E}+\frac{\rho}{C}\frac{d\boldsymbol{\pi}}{dt}\times\mathbf{B}+(\mu^r+\mu^i)\frac{\mathbf{v}}{C}\times\mathbf{B}$$
$$-\mu^e\mathbf{E}^e-\mu^h\mathbf{E}^h=\rho\frac{d\mathbf{v}}{dt}, \tag{7.4}$$

$$\nabla\cdot\boldsymbol{\tau}-\nabla p^e-\nabla p^h+\mathbf{P}\cdot\nabla\mathbf{E}+\mu\mathbf{E}+\frac{\rho}{C}\frac{d\boldsymbol{\pi}}{dt}\times\mathbf{B}+\frac{\mathbf{J}}{C}\times\mathbf{B}=\rho\frac{d\mathbf{v}}{dt}, \tag{7.5}$$

and it is understood that the *prescribed* homogeneous magnetic induction field **B** has a character in the description mathematically analogous to that of a *prescribed* gravitational field in mechanical systems. In this description, primarily because of (7.2), Eq. (3.35) may be replaced by

$$\nabla\cdot[(\partial\mathbf{D}/\partial t)+4\pi\mathbf{J}]=0. \tag{7.6}$$

Equations (3.41), (3.42), (3.44)—(3.46), (3.49), and (3.50), respectively, are replaced by

$$(\partial/\partial t)\int_s\mathbf{n}\cdot\mathbf{D}\,ds+\int_s\mathbf{n}\cdot\mathbf{J}\,ds=0, \tag{7.7}$$

$$\oint_C\mathbf{E}\cdot d\mathbf{y}=0, \tag{7.8}$$

$$f_j=P_kE_{j,k}+\mu E_j+\frac{\rho}{C}e_{jkl}\frac{d\pi_k}{dt}B_l+e_{jkl}\frac{J_k}{C}B_l, \tag{7.9}$$

$$P_kE_{j,k}+\mu E_j=T^E_{ij,i}, \tag{7.10}$$

$$T^E_{ij}=\frac{1}{4\pi}(4\pi P_iE_j+E_iE_j-\tfrac{1}{2}E_kE_k\delta_{ij}), \tag{7.11}$$

$$\int_s\mathbf{n}\cdot[\boldsymbol{\tau}-(p^e+p^h)\mathbf{I}+\mathbf{T}^E]\,ds+\int_V\frac{1}{C}\mathbf{J}\times\mathbf{B}\,dV$$
$$=\frac{d}{dt}\int_V\rho\left(\mathbf{v}-\frac{1}{C}\boldsymbol{\pi}\times\mathbf{B}\right)dV, \tag{7.12}$$

$$\int_s\mathbf{n}\cdot\left(\boldsymbol{\tau}-(p^e+p^h)\mathbf{I}+\mathbf{T}^E-\mathbf{v}\rho\mathbf{v}+\frac{\mathbf{v}}{C}\mathbf{P}\times\mathbf{B}\right)ds$$
$$+\int_V\frac{1}{C}\mathbf{J}\times\mathbf{B}\,dV=\frac{\partial}{\partial t}\int_V\rho\left(\mathbf{v}-\frac{1}{C}\boldsymbol{\pi}\times\mathbf{B}\right)dV. \tag{7.13}$$

Except for the fact that the magnetic terms in Sec. 4 are dropped and h_i in $(4.13)_1$ is replaced by (7.3), all equations in Sec. 4 are unchanged. Aside from the fact that the magnetic terms are dropped in Sec. 5 also and **E′** is replaced by **E**, the constitutive equations in Sec. 5 are unchanged. The resulting theory in this section can readily be reduced by appropriate substitutions to 13 equations in the 13 dependent variables y_j, θ, φ, E^e_i, E^h_i, μ^e, and μ^h. The 13 equations are the three each of (3.27), (3.28), and (7.4) and (3.6), (3.7), (4.9), and (7.6).

At a moving nonmaterial surface of discontinuity the jump conditions (6.7)—(6.12) and (6.14) remain unchanged, (6.13), (6.15), and (6.16), respectively, are replaced by

$$\mathbf{n}\cdot[\boldsymbol{\tau}-(p^e+p^h)\mathbf{I}+\mathbf{T}^E-\mathbf{v}\rho\mathbf{v}+(\mathbf{v}/C)\mathbf{P}\times\mathbf{B}]$$
$$+u_n[\rho\mathbf{v}-(1/C)\mathbf{P}\times\mathbf{B}]=0, \tag{7.14}$$

$$\mathbf{n}\cdot[-p^e\mathbf{I}+\alpha^e\mathbf{T}^{EQ}]=0, \tag{7.15}$$

$$\mathbf{n}\cdot[-p^h\mathbf{I}+\alpha^h\mathbf{T}^{EQ}]=0, \tag{7.16}$$

where

$$T^{EQ}_{ij}=(1/4\pi)(E_iE_j-\tfrac{1}{2}E_kE_k\delta_{ij}). \tag{7.17}$$

Equations (6.17) and (6.18) remain in effect, $(6.19)_1$ is nonexistent, and $(6.19)_2$ is replaced by

$$[\varphi]=0. \tag{7.18}$$

At a material surface of discontinuity Eqs. (6.20)—(6.24) remain in effect and (6.25)—(6.27), respectively, are replaced by

$$\mathbf{n}\cdot[\boldsymbol{\tau}-(p^e+p^h)\mathbf{I}+\mathbf{T}^E]=0, \tag{7.19}$$

$$\mathbf{n}\cdot[-p^e\mathbf{I}+\alpha^e\mathbf{T}^{EQ}]+\mathcal{J}^e=0, \tag{7.20}$$

$$\mathbf{n}\cdot[-p^h\mathbf{I}+\alpha^h\mathbf{T}^{EQ}]+\mathcal{J}^h=0. \tag{7.21}$$

The remaining equations, i.e., (6.28)—(6.34) are unchanged except for the fact that the dependence on N_L in (6.34) is omitted and the vector **g** in (6.35) and (6.36) is omitted.

8. NONLINEAR EQUATIONS FOR SMALL FIELDS SUPERPOSED ON A BIAS

In this section we obtain the nonlinear equations in the small field variables for small dynamic fields superposed on a static bias for the n-type semiconductor from the equations for the quasistatic electric field presented and discussed in Sec. 7. For an n-type semiconductor $\mu^h=\gamma^h=0$ and since the semiconductor is intrinsic, $\gamma^i=0$ and, hence, from (2.6) $\gamma^e=0$. We ignore all temperature effects and thus eliminate θ and the dissipation equation (4.9) and take the static homogeneous magnetic field **B** to vanish. Under these circumstances from (3.6), (3.9), (3.27), $(3.38)_3$, $(3.39)_2$, (3.40), (5.14), $(5.15)_1$, (5.30), $(7.1)_3$, (7.5), and (7.10), we may write the governing differential equations in the form

$$\partial\mu^e/\partial t+(\mu^ev^e_i)_{,i}=0, \tag{8.1}$$

$$(\tau^S_{ij}+T^{ES}_{ij}-p^e\delta_{ij})_{,i}=\rho\,dv_j/dt, \tag{8.2}$$

$$E^e_i=(\varphi+\varphi^e)_{,i}, \quad D_{i,i}=\mu, \quad \mu=\mu^r+\mu^e, \tag{8.3}$$

$$J_i = \mu v_i + \mu^e (v_i^e - v_i), \tag{8.4}$$

where

$$\tau_{ij}^S = \rho y_{i,K} y_{j,L}\, \partial\chi/\partial E_{KL}, \tag{8.5}$$

$$T_{ij}^{ES} = \epsilon_0 E_i E_j - \tfrac{1}{2}\epsilon_0 E_k E_k \delta_{ij}, \tag{8.6}$$

$$D_i = \epsilon_0 E_i - \rho y_{i,L}\, \partial\chi/\partial W_L, \tag{8.7}$$

$$v_i^e - v_i = V_i^e = y_{i,K}\Omega_K^e, \quad J\mu^r = {}_0\mu^r, \tag{8.8}$$

$$\Omega_K^e = \Omega_K^e(\mu^e, w_L^e, E_{LM}, W_L), \quad J = \det y_{i,K}, \tag{8.9}$$

and in this section we employ MKS units in place of Gaussian units, ϵ_0 is the permittivity of free space,[60] and ${}_0\mu^r$ is a constant for a given material. From (3.11), $(8.3)_{2,3}$, and (8.4) we obtain

$$[\mu^e(v_i^e - v_i) + (\partial D_i/\partial t) + D_{k,k} v_i]_{,i} = 0, \tag{8.10}$$

which with (8.2) constitute four governing differential equations for the n-type semiconductor. From $(5.9)_1$, $(5.11)_2$, (5.13), $(5.27)_1$, (5.29), $(7.1)_3$, (7.2), (8.3), and (8.5)—(8.9) it is clear that the four differential equations can readily be expressed in terms of the four dependent variables y_j and φ. At a moving material surface of discontinuity the pertinent boundary conditions that remain are

$$\frac{\partial Q^e}{\partial t} + n_i[\mu^e(v_i^e - v_i)] = \Gamma^e, \quad \frac{\partial Q^r}{\partial t} = \Gamma^r, \tag{8.11}$$

$$n_i[\tau_{ij}^S + T_{ij}^{ES} - p^e \delta_{ij}] = 0, \tag{8.12}$$

$$[-p^e + \alpha^e n_i T_{ij}^{ES} n_j] + n_i \mathcal{J}_i^e = 0, \tag{8.13}$$

$$n_i[D_i] = Q, \quad n_i[J_i] + \partial Q/\partial t = 0, \quad [\varphi] = 0, \tag{8.14}$$

where

$$Q = Q^e + Q^r, \quad \Gamma^e + \Gamma^r = 0. \tag{8.15}$$

Clearly, the boundary conditions (8.11)—(8.14) can readily be expressed in terms of the same four dependent variables as the differential equations.

At this point we note that in obtaining the equations for small fields superposed on a bias, certain results and equations contained in Secs. I—III of Ref. 28 are employed here. In fact the content of Secs. I—III of Ref. 28 is assumed known in this section and the notation is the same. As in Ref. 28, ξ_α denotes the intermediate coordinates of material points and is related to the reference coordinates X_L and present coordinates y_i as shown in Eqs. (35) and (36) of Ref. 28. The small mechanical displacement field u_β and small dynamic increment of electric potential $\tilde{\varphi}$ are defined in Eqs. (37) and (38), respectively, of Ref. 28. Equations (39)—(59), (61), and (62) of Ref. 28 and the discussion associated therewith apply here without essential change, and in place of (60) and (63) we have

$$\kappa_{\alpha j,\alpha} - \rho_{\alpha j,\alpha} = \rho^1 dv_j/dt, \tag{8.16}$$

$$\Delta_{\alpha,\alpha} = \tilde{J}\mu, \tag{8.17}$$

where

$$\kappa_{\alpha j} = \rho^1 \xi_{\alpha,L} y_{j,M}(\partial\chi/\partial E_{LM}) + \tilde{J}\xi_{\alpha,i} T_{ij}^{ES}, \tag{8.18}$$

$$\rho_{\alpha j} = \tilde{J}\xi_{\alpha,j} p^e. \tag{8.19}$$

We now define the intermediate relative velocity U_α^e of the free electronic fluid by

$$U_\alpha^e = \xi_{\alpha,i} V_i^e, \tag{8.20}$$

from which, with (3.11), (8.4), the chain rule of differentiation and the identity

$$(\tilde{J}\xi_{\alpha,i})_{,\alpha} = 0, \tag{8.21}$$

we may write

$$(\mu^e \tilde{J} U_\alpha^e)_{,\alpha} + (\mu\tilde{J}\xi_{\alpha,i} v_i)_{,\alpha} + \tilde{J}\,\partial\mu/\partial t = 0, \tag{8.22}$$

which, with (8.3), (8.17), the chain rule of differentiation, (8.21), (4.5), and

$$v_{i,i} = (1/J)\,dJ/dt = (1/\tilde{J})\,d\tilde{J}/dt, \tag{8.23}$$

enables us to write

$$[(\Delta_{\beta,\beta} - \mu^{r1}) U_\alpha^e]_{,\alpha} + d(\Delta_{\alpha,\alpha})/dt = 0, \tag{8.24}$$

where

$$\mu^{r1} = \tilde{J}\mu^r. \tag{8.25}$$

Referred to the known intermediate coordinates, the jump (or boundary) conditions (8.12)—$(8.14)_1$ at moving material surfaces of discontinuity take the respective forms

$$\nu_\alpha[\kappa_{\alpha j} - \rho_{\alpha j}] + f_j^a = 0, \tag{8.26}$$

$$[-\nu_\alpha \rho_{\alpha j} n_j + \alpha^e \nu_\alpha \tilde{J}\xi_{\alpha,i} T_{ij}^{ES} n_j] + F_j^e n_j = 0, \tag{8.27}$$

$$\nu_\alpha[\Delta_\alpha] = q, \tag{8.28}$$

where f_j^a and q are defined in Eq. (97) of Ref. 28, $d\sigma$ and ν_α denote the magnitude of and unit normal to the differential element of material area in the intermediate configuration, the relation between n_i and ν_α is given in Eq. (94) of Ref. 28, and F_j^e is defined by

$$\mathcal{J}_j^e\, ds = F_j^e\, d\sigma. \tag{8.29}$$

In order to refer the boundary condition on current $(8.14)_{1,2}$ to the *known* intermediate configuration, it is advantageous to consider the integral from of the conservation of charge

$$\int_s n_i J_i\, ds = -(\partial/\partial t)\int_V \mu\, dV, \tag{8.30}$$

where V is an element of volume fixed in space and J_i is given in (8.4). With the aid of the transport theorem,[38] Eq. (8.30) can be written in the form

$$\int_s n_i J_i\, ds = -(d/dt)\int_V \mu\, dV + \int_s n_i \mu v_i\, ds, \tag{8.31}$$

where V in (8.31) is an element of volume, which instantaneously coincides with V in (8.30) but is moving with the velocity $\mathbf{v}$ of the lattice continuum. Substituting from Eq. (89) of Ref. 28 into (8.31), employing (8.4) and (8.20) and defining the surface charge densities Q and q, we obtain

$$\int_\sigma \nu_\alpha \tilde{J}\mu^e U_\alpha^e\, d\sigma = -(d/dt)\int_\sigma q\, d\sigma. \tag{8.32}$$

The application of (8.32) to a limiting region surrounding the moving material surface of discontinuity, with the aid of $(8.3)_2$, (8.17), (8.25), and the material derivative of (8.28), yields

$$\nu_\alpha[(\Delta_{\beta,\beta} - \mu^{r1}) U_\alpha^e + d\Delta_\alpha/dt] = 0, \tag{8.33}$$

which is the most appropriate form of the jump condition on current for the electroelastic semiconductor.

Since the equilibrium intermediate state is assumed known, we have Eqs. (64)—(70) of Ref. 28 along with

$$\mu^e = \mu^{e1} + \tilde{\mu}^e, \quad p^e = p^{e1} + \tilde{p}^e, \tag{8.34}$$

$$p_{\alpha j} = p^1_{\alpha j} + \tilde{p}_{\alpha j}, \quad U^e_\alpha = U^{e1}_\alpha + \tilde{U}^e_\alpha, \tag{8.35}$$

where

$$p^{e1} = (\mu^{e1})^2\, \partial\epsilon^e/\partial\mu^{e1}, \quad p^1_{\alpha j} = p^{e1}\delta_{\alpha j}, \quad U^{e1}_\alpha = \delta_{\alpha i} V^{e1}_i, \tag{8.36}$$

and μ^{e1} denotes the static intermediate free electronic charge density and p^{e1} the associated pressure, and $\tilde{\mu}^e$ and $\tilde{p}^e$ denote the small dynamic increments of free electronic charge density and pressure, respectively, $\tilde{p}_{\alpha j}$ is the small dynamic increment of intermediate Piola–Kirchhoff traction due to the free electronic pressure, V^{e1}_i is the steady relative velocity of the free electronic fluid, $\tilde{U}^e_\alpha$ is the small dynamic increment of the relative velocity of the free electronic fluid in the intermediate configuration, and ξ_α and E^1_α are known and $t^1_{\alpha\beta}$, Δ^1_α, $p^1_{\alpha\beta}$, p^{e1}, and U^{e1}_α satisfy

$$t^1_{\alpha\beta,\,\alpha} - p^1_{\alpha\beta,\,\alpha} = 0, \quad \Delta^1_{\alpha,\,\alpha} = \mu^{r1} + \mu^{e1}, \quad (\mu^{e1} V^{e1}_\alpha)_{,\,\alpha} = 0, \tag{8.37}$$

$$\nu_\alpha[t^1_{\alpha\beta} - p^1_{\alpha\beta}] + t^{a1}_\beta = 0, \quad [-p^{e1} + \alpha^e \nu_\alpha T^{ES1}_{\alpha\beta}\nu_\beta] + F^{e1}_\alpha \nu_\alpha = 0,$$

$$\nu_\alpha[\Delta^1_\alpha] = q^1, \quad [\varphi^1] = 0, \quad \nu_\alpha[\mu^{e1} V^{e1}_\alpha] = 0, \tag{8.38}$$

and the quantities not defined here are defined in Sec. II of Ref. 28. The small field dynamic variables satisfy the dynamic differential equations

$$\tilde{\kappa}_{\alpha j,\,\alpha} - \tilde{p}_{\alpha j,\,\alpha} = \rho^1 \delta_{j\gamma}\, \partial^2 u_\gamma/\partial t^2, \tag{8.39}$$

$$\tilde{\Delta}_{\alpha,\,\alpha} = (\tilde{J} - 1)\mu^{e1} + \tilde{J}\tilde{\mu}^e, \tag{8.40}$$

$$[(\mu^{e1} + \tilde{\Delta}_{\beta,\,\beta})(V^{e1}_\alpha + \tilde{U}^e_\alpha)]_{,\,\alpha} + (\partial/\partial t)\tilde{\Delta}_{\alpha,\,\alpha} = 0. \tag{8.41}$$

The small field constitutive equations for $\tilde{\kappa}_{\alpha j}$ and $\tilde{\Delta}_\alpha$ are given in Eqs. (75) and (76) with the coefficients defined in Eqs. (77) and (78) of Ref. 28. The small field constitutive equations for $p_{\alpha j}$ and $\tilde{U}^e_\alpha$ may be written in the form

$$\tilde{p}_{\alpha j} = \delta_{j\gamma}[\overset{1}{l}_{\alpha\gamma}\tilde{\mu}^e + \overset{2}{l}_{\alpha\gamma\beta\delta}\tilde{\mu}^e u_{\beta,\,\delta} + \overset{3}{l}_{\alpha\gamma}(\tilde{\mu}^e)^2], \tag{8.42}$$

$$\begin{aligned}\tilde{U}^e_\alpha = {} & \overset{1}{m}_{\alpha\beta\gamma} u_{\beta,\,\gamma} + \overset{2}{m}_{\alpha\beta}\tilde{\varphi}_{,\,\beta} + \overset{3}{m}_{\alpha}\tilde{\mu}^e + \overset{4}{m}_{\alpha\beta}\tilde{\mu}^e_{,\,\beta} + \overset{5}{m}_{\alpha\beta\gamma\delta\epsilon} u_{\beta,\,\gamma} u_{\delta,\,\epsilon} \\ & + \overset{6}{m}_{\alpha\beta\gamma}\tilde{\varphi}_{,\,\beta}\tilde{\varphi}_{,\,\gamma} + \overset{7}{m}_{\alpha}(\tilde{\mu}^e)^2 + \overset{8}{m}_{\alpha\beta}\tilde{\mu}^e\tilde{\mu}^e_{,\,\beta} + \overset{9}{m}_{\alpha\beta\gamma}\tilde{\mu}^e_{,\,\beta}\tilde{\mu}^e_{,\,\gamma} \\ & + \overset{10}{m}_{\alpha\beta\gamma\delta} u_{\beta,\,\gamma}\tilde{\varphi}_{,\,\delta} + \overset{11}{m}_{\alpha\beta\gamma} u_{\beta,\,\gamma}\tilde{\mu}^e + \overset{12}{m}_{\alpha\beta\gamma\delta} u_{\beta,\,\gamma}\tilde{\mu}^e_{,\,\delta} \\ & + \overset{13}{m}_{\alpha\beta}\tilde{\varphi}_{,\,\beta}\tilde{\mu}^e + \overset{14}{m}_{\alpha\beta\gamma}\tilde{\varphi}_{,\,\beta}\tilde{\mu}^e_{,\,\gamma},\end{aligned} \tag{8.43}$$

where

$$\begin{aligned}
\overset{1}{l}_{\alpha\gamma} &= \delta_{\alpha\gamma}\left[(\mu^{e1})^2\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + 2\mu^{e1}\frac{\partial\epsilon^e}{\partial\mu^e}\Big)_1\Big], \\
\overset{2}{l}_{\alpha\beta\gamma\delta} &= (\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\beta}\delta_{\gamma\delta})\mu^{e1}\left[\mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + 2\frac{\partial\epsilon^e}{\partial\mu^e}\Big)_1\Big], \\
\overset{3}{l}_{\alpha\gamma} &= \delta_{\alpha\gamma}\left[\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 + 2\mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1 + \tfrac{1}{2}(\mu^{e1})^2\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big],
\end{aligned} \tag{8.44}$$

$$\begin{aligned}
\overset{1}{m}_{\alpha\beta\gamma} &= \xi_{\alpha,\,K}\xi_{\beta,\,L}\xi_{\gamma,\,M}\frac{\partial\Omega^e_K}{\partial E_{LM}}\Big)_1, \\
\overset{2}{m}_{\alpha\beta} &= -\,\xi_{\alpha,\,K}\xi_{\beta,\,L}\left[\frac{\partial\Omega^e_K}{\partial W_L}\right)_1 - \frac{\partial\Omega^e_K}{\partial w^e_L}\Big)_1\Big], \\
\overset{3}{m}_{\alpha} &= \mu^{e1}_{,\,\beta}\left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big]\xi_{\alpha,\,M}\xi_{\beta,\,K}\frac{\partial\Omega^e_M}{\partial w^e_K}\Big)_1 \\
&\quad + \xi_{\alpha,\,M}\frac{\partial\Omega^e_M}{\partial\mu^e}\Big)_1, \\
\overset{4}{m}_{\alpha\beta} &= \left[2\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 + \mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1\Big]\xi_{\beta,\,K}\xi_{\alpha,\,M}\frac{\partial\Omega^e_M}{\partial w^e_K}\Big)_1, \\
\overset{5}{m}_{\alpha\beta\gamma\delta\epsilon} &= \tfrac{1}{2}\delta_{\beta\delta}\xi_{\gamma,\,K}\xi_{\epsilon,\,L}\xi_{\alpha,\,M}\frac{\partial\Omega^e_M}{\partial E_{KL}}\Big)_1 \\
&\quad + \tfrac{1}{2}\xi_{\beta,\,K}\xi_{\gamma,\,L}\xi_{\delta,\,R}\xi_{\epsilon,\,S}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial E_{KL}\partial E_{RS}}\Big)_1, \\
\overset{6}{m}_{\alpha\beta\gamma} &= \tfrac{1}{2}\xi_{\beta,\,L}\xi_{\gamma,\,K}\xi_{\alpha,\,M}\left[\frac{\partial^2\Omega^e_M}{\partial W_L\partial W_K}\right)_1 + \frac{\partial^2\Omega^e_M}{\partial w^e_L\partial w^e_K}\Big)_1 \\
&\quad - 2\frac{\partial^2\Omega^e_M}{\partial W_L\partial w^e_K}\Big)_1\Big], \\
\overset{7}{m}_{\alpha} &= \mu^{e1}_{,\,\beta}\left[2\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\right)_1 + \tfrac{1}{2}\mu^{e1}\frac{\partial^4\epsilon^e}{\partial(\mu^e)^4}\Big)_1\Big]\xi_{\beta,\,K}\xi_{\alpha,\,M}\frac{\partial\Omega^e_M}{\partial w^e_K}\Big)_1 \\
&\quad + \tfrac{1}{2}\mu^{e1}_{,\,\beta}\mu^{e1}_{,\,\gamma}\left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big]\xi_{\beta,\,K}\xi_{\gamma,\,L}\xi_{\alpha,\,M} \\
&\quad \times\frac{\partial^2\Omega^e_M}{\partial w^e_L\partial w^e_K}\Big)_1 + \mu^{e1}_{,\,\beta}\left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big] \\
&\quad \times\xi_{\beta,\,K}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial w^e_K\partial\mu^e}\Big)_1 + \tfrac{1}{2}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial(\mu^e)^2}\Big)_1, \\
\overset{8}{m}_{\alpha\beta} &= \left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big]\xi_{\beta,\,K}\xi_{\alpha,\,M}\frac{\partial\Omega^e_M}{\partial w^e_K}\Big)_1 \\
&\quad + \mu^{e1}_{,\,\gamma}\left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big]\left[2\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 \\
&\quad + \mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1\Big]\xi_{\beta,\,K}\xi_{\gamma,\,L}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial w^e_L\partial w^e_K}\Big)_1 + \left[2\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 \\
&\quad + \mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1\Big]\xi_{\beta,\,K}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial w^e_K\partial\mu^e}\Big)_1, \\
\overset{9}{m}_{\alpha\beta\gamma} &= \frac{1}{2}\left[2\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 + \mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1\Big]^2\xi_{\beta,\,L}\xi_{\gamma,\,K}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial w^e_L\partial w^e_K}\Big)_1, \\
\overset{10}{m}_{\alpha\beta\gamma\delta} &= \xi_{\beta,\,L}\xi_{\gamma,\,N}\xi_{\delta,\,K}\xi_{\alpha,\,M}\left[\frac{\partial^2\Omega^e_M}{\partial E_{LN}\partial w^e_K}\right)_1 - \frac{\partial^2\Omega^e_M}{\partial E_{LN}\partial W_K}\Big)_1\Big], \\
\overset{11}{m}_{\alpha\beta\gamma} &= \mu^{e1}_{,\,\delta}\left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big]\xi_{\beta,\,L}\xi_{\gamma,\,N}\xi_{\delta,\,K}\xi_{\alpha,\,M} \\
&\quad \times\frac{\partial^2\Omega^e_M}{\partial E_{LN}\partial w^e_K}\Big)_1 + \xi_{\beta,\,L}\xi_{\gamma,\,N}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial E_{LN}\partial\mu^e}\Big)_1, \\
\overset{12}{m}_{\alpha\beta\gamma\delta} &= \left[2\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 + \mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1\Big]\xi_{\beta,\,L}\xi_{\gamma,\,N}\xi_{\delta,\,K}\xi_{\alpha,\,M}\frac{\partial^2\Omega^e_M}{\partial E_{LN}\partial w^e_K}\Big)_1, \\
\overset{13}{m}_{\alpha\beta} &= \mu^{e1}_{,\,\gamma}\left[3\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\right)_1 + \mu^{e1}\frac{\partial^3\epsilon^e}{\partial(\mu^e)^3}\Big)_1\Big]\xi_{\gamma,\,K}\xi_{\beta,\,L}\xi_{\alpha,\,M}\left[\frac{\partial^2\Omega^e_M}{\partial w^e_L\partial w^e_K}\right)_1 \\
&\quad - \frac{\partial^2\Omega^e_M}{\partial W_L\partial w^e_K}\Big)_1\Big] + \xi_{\beta,\,K}\xi_{\alpha,\,M}\left[\frac{\partial^2\Omega^e_M}{\partial w^e_K\partial\mu^e}\right)_1 - \frac{\partial^2\Omega^e_M}{\partial W_K\partial\mu^e}\Big)_1\Big], \\
\overset{14}{m}_{\alpha\beta\gamma} &= \left[2\frac{\partial\epsilon^e}{\partial\mu^e}\right)_1 + \mu^{e1}\frac{\partial^2\epsilon^e}{\partial(\mu^e)^2}\Big)_1\Big]\xi_{\beta,\,L}\xi_{\gamma,\,K}\xi_{\alpha,\,M}\left[\frac{\partial^2\Omega^e_M}{\partial w^e_L\partial w^e_K}\right)_1 \\
&\quad - \frac{\partial^2\Omega^e_M}{\partial W_L\partial w^e_K}\Big)_1\Big],
\end{aligned} \tag{8.45}$$

where it is to be noted that Eqs. $(5.25)_2$, $(5.27)_1$, $(5.28)_2$, (5.29), (7.2), $(8.3)_2$, and (8.20) were employed in obtaining the results presented in (8.45). From (8.40), with the aid of Eqs. (54) and (76) of Ref. 28, $\tilde{\mu}^e$ can be expressed in terms of the four dependent variables u_α and $\tilde{\varphi}$. Now, the substitution of this latter

relation obtained from (8.40) into (8.42) and (8.43), which are then substituted into (8.39) and (8.41) along with Eqs. (75) and (76) of Ref. 28 yields four differential equations in the four dependent variables u_α and $\tilde{\varphi}$.

The small field dynamic boundary conditions across moving material surfaces of discontinuity are obtained by substituting from Eqs. (64), (65), and (94) of Ref. 28 and (8.35) into (8.26), (8.27), and (8.33) and employing $(8.37)_2$ and (8.38), with the result

$$\nu_\alpha[\tilde{\kappa}_{\alpha j} - \tilde{\rho}_{\alpha j}] + \tilde{f}^a_\beta \delta_{\beta j} = 0, \tag{8.46}$$

$$[-\nu_\alpha \rho^1_{\alpha j}(n_j - \nu_\beta \delta_{\beta j}) - \nu_\alpha \tilde{\rho}_{\alpha j} n_j + \alpha^e \nu_\alpha T^{\mathrm{ESI}}_{\alpha\beta} \delta_{\beta j}(n_j - \nu_\gamma \delta_{\gamma j}) + \alpha^e \nu_\alpha \tilde{M}_{\alpha j} n_j] + F^{e1}_\alpha \delta_{\alpha j}(n_j - \nu_\beta \delta_{\beta j}) + \tilde{F}^e_j n_j = 0, \tag{8.47}$$

$$\nu_\alpha[(\mu^{e1} + \tilde{\Delta}_{\beta,\beta})(V^{e1}_\alpha + \tilde{U}^e_\alpha) + (\partial/\partial t)\tilde{\Delta}_\alpha] = 0, \tag{8.48}$$

where

$$M_{\alpha j} = \tilde{J} \xi_{\alpha,i} T^{\mathrm{ES}}_{ij} = T^{\mathrm{ESI}}_{\alpha\beta} \delta_{\beta j} + \tilde{M}_{\alpha j}, \tag{8.49}$$

and

$$\tilde{M}_{\alpha j} = \delta_{\gamma j}[h_{1\alpha\gamma\delta\beta} u_{\delta,\beta} + h_{2\delta\gamma\alpha} \tilde{\varphi}_{,\delta} + h_{3\alpha\gamma\epsilon\delta\beta} u_{\delta,\beta} \tilde{\varphi}_{,\epsilon} + h_{4\alpha\gamma\delta\epsilon} \tilde{\varphi}_{,\delta} \tilde{\varphi}_{,\epsilon} + h_{5\alpha\gamma\delta\beta\epsilon\zeta} u_{\delta,\beta} u_{\epsilon,\zeta}], \tag{8.50}$$

in which the $h_N \cdots$ may be obtained by taking only those portions of the respective $H_N \cdots$ given in Eq. (77) of Ref. 28, containing ϵ_0, e.g.,

$$h_{2\delta\gamma\alpha} = \epsilon_0(E^1_\delta \delta_{\alpha\gamma} - E^1_\alpha \delta_{\gamma\delta} - E^1_\gamma \delta_{\alpha\delta}),$$
$$h_{4\alpha\gamma\delta\epsilon} = \epsilon_0(\delta_{\gamma\delta}\delta_{\alpha\epsilon} - \tfrac{1}{2}\delta_{\alpha\gamma}\delta_{\delta\epsilon}). \tag{8.51}$$

The small field dynamic surface force $\tilde{F}_j n_j$ may be written in the form

$$\tilde{F}^e_j n_j + F^{e1}_\alpha \delta_{\alpha j}(n_j - \nu_\beta \delta_{\beta j}) = \Gamma_{1\alpha\beta}[u_{\alpha,\beta}] + \Gamma_{2\alpha}[\tilde{\varphi}_{,\alpha}] + \Gamma_{3\alpha\beta\gamma\delta}[u_{\alpha,\beta} u_{\gamma,\delta}] + \Gamma_{4\alpha\beta\gamma}[u_{\beta,\gamma}\tilde{\varphi}_{,\alpha}] + \Gamma_{5\alpha\beta}[\tilde{\varphi}_{,\alpha}\tilde{\varphi}_{,\beta}], \tag{8.52}$$

where the $\Gamma_N \cdots$ are effective surface coefficients in this description which is quadratic in the small field variables u_α and $\tilde{\varphi}$. Although the effective surface coefficients $\Gamma_N \cdots$ can be expressed in terms of the fundamental material surface constants with the aid of (6.33), (6.34), and Eq. (94) of Ref. 28, we do not bother to do this here. Moreover, we have simply assumed the static surface force $\nu_\alpha F^{e1}_\alpha$ to be known and not even bothered to give a representation. At this point it should be noted that the tangential components of F^{e1}_α and $\tilde{F}^e_j$, i.e., $\nu \times \mathbf{F}^{e1}$ and $\mathbf{n} \times \tilde{\mathbf{F}}^e$, can be determined *a posteriori* if desired. The substitution of the constitutive equations (8.42), (8.43), (8.52), and (75) and (76) of Ref. 28 into (8.46)—(8.48) enables the eight boundary equations consisting of (8.46)—(8.48) and (104) and (121) of Ref. 28 to be expressed in terms of the four dependent variables u_α and $\tilde{\varphi}$ on each side of the surface of discontinuity.

Since the points of free-space remain fixed in a motion, the *known* intermediate coordinates may be taken as the independent variables and we have[28,61]

$$\psi^1_{,\alpha\alpha} = 0, \quad \tilde{\psi}_{,\alpha\alpha} = 0, \tag{8.53}$$

as the intermediate static and dynamic small field equations for points of freespace, where

$$\varphi = \psi^1 + \tilde{\psi}, \tag{8.54}$$

as in Eq. (81) of Ref. 28. Moreover, since the values of the variables immediately on the free-space side of the *unknown* present position of a material surface may be obtained by means of a Taylor expansion about their values at the *known* intermediate position of the surface in the *unknown* displacement u_α of the material surface, Eqs. (105)—(118) of Ref. 28 hold and in place of (119) and (120), we have

$$\nu_\alpha(\tilde{\kappa}^f_{\alpha j} - \tilde{\kappa}_{\alpha j} + \tilde{\rho}_{\alpha j}) + \tilde{f}^a_\beta \delta_{\beta j} = 0, \tag{8.55}$$

$$\nu_\alpha[(\partial/\partial t)\tilde{\Delta}^f_\alpha - (\mu^{e1} + \tilde{\Delta}_{\beta,\beta})(V^{e1}_\alpha + \tilde{U}^e_\alpha) - (\partial/\partial t)\tilde{\Delta}_\alpha] = 0. \tag{8.56}$$

Equation (8.56) is the counterpart of (8.48) at a free surface. The counterpart of (8.47) at a free surface may be written in the form

$$[\alpha^e \nu_\alpha T^{\mathrm{ESf1}}_{\alpha\beta} \delta_{\beta j}(n_j - \nu_\gamma \delta_{\gamma j}) + \alpha^e \nu_\alpha \tilde{\kappa}^f_{\alpha j} n_j + \nu_\alpha \rho^1_{\alpha j}(n_j - \nu_\beta \delta_{\beta j}) + \nu_\alpha \tilde{\rho}_{\alpha j} n_j - \alpha^e \nu_\alpha T^{\mathrm{ESI}}_{\alpha\beta} \delta_{\beta j}(n_j - \nu_\gamma \delta_{\gamma j}) - \alpha^e \nu_\alpha \tilde{M}_{\alpha j} n_j] + F^{e1}_\alpha \delta_{\alpha j}(n_j - \nu_\beta \delta_{\beta j}) + \tilde{F}^e_j n_j = 0, \tag{8.57}$$

where $T^{\mathrm{ESf1}}_{\alpha\beta}$ denotes the static intermediate Maxwell stress tensor immediately on the free-space side of the intermediate position of the free surface and $\tilde{\kappa}^f_{\alpha j}$ and $\tilde{\Delta}^f_\alpha$ are dynamic small field variables in free space defined in Eqs. (115) and (116) of Ref. 28. Since matter exists on only one side of a free surface, the jump symbols in (8.52) are omitted when substituted in (8.57).

9. BULK AND SURFACE WAVE PROPAGATION

In this section we consider the propagation of both bulk and surface waves in n-type semiconductors, which have hexagonal symmetry and are subject to a static homogeneous biasing electric field along the hexagonal axis. Both the plane and surface waves are propagating in the direction of the applied dc field. The linear version of the equations obtained in Sec. 8 are applied in the analysis. In the problems under consideration, for simplicity we ignore the explicit representation of the static deformation gradients under the applied dc electric field. When the static deformation gradients are ignored, we have

$$\xi_{\alpha,M} = \delta_{\alpha M}, \quad \rho^0 \approx \rho^1 \approx \rho. \tag{9.1}$$

For linear electroelastic wave propagation the simplest polynomial approximation for χ that can be assumed is of the form

$$\chi = (1/2\rho^0) c_{KLMN} E_{KL} E_{MN} - (1/\rho^0) e_{KLM} W_K E_{LM} - (1/2\rho^0) \chi_{LM} W_L W_M, \tag{9.2}$$

in which the elastic, piezoelectric and dielectric constants c_{KLMN}, e_{KLM}, and χ_{LM} must be functions of the applied dc field $\mathbf{E}^1$. On account of the use of the simplified expression for χ and the fact that we do not provide the explicit representation for the static deformation gradients, a portion of the dependence of the resulting effective material constants on the biasing electric field is exhibited explicitly and a portion is not. With somewhat greater effort the entire dependence of the effective material constants on the biasing electric

field can be exhibited explicitly. However, this is not of particular interest here and, consequently, we do not take the trouble to provide the relation.

The functions ϵ^e and Ω_M^e are taken in the restricted forms

$$\epsilon^e = a^e \mu^e, \tag{9.3}$$

$$\Omega_M^e = m_{MN} u_N^e, \tag{9.4}$$

where m_{MN}, the electronic mobility, and a^e, which could quite properly be called the electronic pressure coefficient, are functions of the biasing electric field. It should be noted that since the entropy inequality (4.10) holds for any process and μ^e is negative, positivity conditions are imposed on m_{MN}.

Now, from (8.37) we see that the static intermediate equations are satisfied if we assume that all bias quantities are homogeneous. Hence we have to be concerned only with the dynamic small field equations (8.39)–(8.41), which in the linear case reduce to

$$\begin{aligned}(e_{\pi\alpha\beta} - \epsilon_0 E^1_\alpha \delta_{\pi\beta})\frac{\partial}{\partial t}(u_{\alpha,\beta\pi}) - [(e_{\alpha\epsilon\beta} - \epsilon_0 E^1_\epsilon \delta_{\alpha\beta}) m_{\pi\gamma} E^1_\gamma \\ + 2a^e(\mu^{1e})^2 m_{\pi\beta}\delta_{\alpha\epsilon}]u_{\epsilon,\alpha\beta\pi} + 2a^e\mu^{1e} m_{\pi\alpha}(e_{\gamma\epsilon\beta} - \epsilon_0 E^1_\epsilon \delta_{\gamma\beta}) u_{\epsilon,\gamma\beta\alpha\pi} \\ - \epsilon_{\alpha\beta}\frac{\partial}{\partial t}(\tilde{\varphi}_{,\alpha\beta}) + \mu^{1e} m_{\alpha\beta}\tilde{\varphi}_{,\alpha\beta} + \epsilon_{\alpha\beta} m_{\pi\gamma} E^1_\gamma \tilde{\varphi}_{,\alpha\beta\pi} \\ - 2a^e\mu^{1e} m_{\alpha\beta}\epsilon_{\gamma\delta}\tilde{\varphi}_{,\alpha\beta\gamma\delta} = 0,\end{aligned} \tag{9.5}$$

$$\begin{aligned}[c_{\nu\delta\alpha\beta} - e_{\eta\delta\beta}E^1_\eta\delta_{\alpha\nu} - \epsilon_0 E^1_\nu E^1_\alpha \delta_{\delta\beta} + 2a^e(\mu^{1e})^2\delta_{\delta\nu}\delta_{\alpha\beta}]u_{\alpha,\beta\delta} \\ - 2a^e\mu^{1e}(e_{\alpha\epsilon\beta} - \epsilon_0 E^1_\epsilon\delta_{\alpha\beta})u_{\epsilon,\alpha\beta\nu} + (e_{\alpha\delta\nu} - \epsilon_0 E^1_\nu\delta_{\alpha\delta})\tilde{\varphi}_{,\alpha\delta} \\ + 2a^e\mu^{1e}\epsilon_{\alpha\beta}\tilde{\varphi}_{,\alpha\beta\nu} = \rho\frac{\partial^2 u_\nu}{\partial t^2},\end{aligned} \tag{9.6}$$

where we have introduced the dielectric constant $\epsilon_{\alpha\beta}$, which is defined by

$$\epsilon_{\alpha\beta} = \epsilon_0\delta_{\alpha\beta} + \chi_{\alpha\beta}. \tag{9.7}$$

The linear dynamic small field boundary conditions for a semiconductor abutting free-space can similarly be reduced to

$$\begin{aligned}\nu_\pi\{(e_{\pi\alpha\beta} - \epsilon_0 E^1_\alpha\delta_{\pi\beta})(\partial/\partial t)(u_{\alpha,\beta}) - [m_{\pi\gamma}E^1_\gamma(e_{\alpha\epsilon\beta} - \epsilon_0 E^1_\epsilon\delta_{\alpha\beta}) \\ + 2a^e(\mu^{1e})^2 m_{\pi\alpha}\delta_{\beta\epsilon}]u_{\epsilon,\alpha\beta} + 2a^e\mu^{1e}m_{\pi\gamma}(e_{\alpha\epsilon\beta} - \epsilon_0 E^1_\epsilon\delta_{\alpha\beta})u_{\epsilon,\alpha\beta\gamma} \\ - \epsilon_{\pi\alpha}(\partial/\partial t)(\tilde{\varphi}_{,\alpha}) + \mu^{1e}m_{\pi\alpha}\tilde{\varphi}_{,\alpha} + \epsilon_{\alpha\beta}m_{\pi\gamma}E^1_\gamma\tilde{\varphi}_{,\alpha\beta} \\ - 2a^e\mu^{1e}m_{\pi\gamma}\epsilon_{\alpha\beta}\tilde{\varphi}_{,\alpha\beta\gamma}\}^- = -\nu_\pi\{\epsilon_0\partial\tilde{\psi}_{,\pi}/\partial t\}^+\end{aligned} \tag{9.8}$$

$$\begin{aligned}\nu_\delta\{[\tfrac{1}{2}\epsilon_0 E^1_\epsilon E^1_\epsilon(\delta_{\beta\nu}\delta_{\alpha\delta} - \delta_{\delta\nu}\delta_{\alpha\beta}) + \epsilon_0 E^1_\nu(E^1_\delta\delta_{\alpha\beta} - E^1_\beta\delta_{\delta\alpha} - E^1_\alpha\delta_{\delta\beta}) \\ + \epsilon_0 E^1_\alpha(E^1_\beta\delta_{\delta\nu} - E^1_\delta\delta_{\beta\nu}) + c_{\nu\delta\alpha\beta} - e_{\eta\delta\beta}E^1_\eta\delta_{\alpha\nu} \\ + a^e(\mu^{1e})^2(\delta_{\alpha\delta}\delta_{\beta\nu} + \delta_{\alpha\beta}\delta_{\delta\nu})]u_{\alpha,\beta} - 2a^e\mu^{1e}(e_{\alpha\epsilon\beta} \\ - \epsilon_0 E^1_\epsilon\delta_{\alpha\beta})\delta_{\delta\nu}u_{\epsilon,\alpha\beta} + [(e_{\alpha\delta\nu} - \epsilon_0 E^1_\delta\delta_{\alpha\nu}) + \epsilon_0 E^1_\alpha\delta_{\delta\nu} \\ - \epsilon_0 E^1_\nu\delta_{\alpha\delta}]\tilde{\varphi}_{,\alpha} + 2a^e\mu^{1e}\epsilon_{\alpha\beta}\tilde{\varphi}_{,\alpha\beta}\delta_{\delta\nu}\}^- \\ = \nu_\delta\epsilon_0\{[E^1_\nu(E^1_\delta\delta_{\alpha\beta} - E^1_\beta\delta_{\alpha\delta}) + \tfrac{1}{2}E^1_\pi E^1_\pi(\delta_{\delta\alpha}\delta_{\beta\nu} \\ - \delta_{\delta\nu}\delta_{\alpha\beta})]u_{\alpha,\beta} + (E^1_\alpha\delta_{\delta\nu} - E^1_\delta\delta_{\alpha\nu} - E^1_\nu\delta_{\delta\alpha})\tilde{\varphi}_{,\alpha}\}^+,\end{aligned} \tag{9.9}$$

$$\begin{aligned}\nu_\delta\{-a^e(\mu^{1e})^2(\delta_{\alpha\delta}\delta_{\beta\nu} + \delta_{\alpha\beta}\delta_{\delta\nu})u_{\alpha,\beta} - \epsilon_0\alpha^e[E^1_\alpha(E^1_\beta\delta_{\delta\nu} - E^1_\delta\delta_{\beta\nu}) \\ + E^1_\nu(E^1_\delta\delta_{\alpha\beta} - E^1_\beta\delta_{\delta\alpha} - E^1_\alpha\delta_{\delta\beta}) + \tfrac{1}{2}E^1_\epsilon E^1_\epsilon(\delta_{\beta\nu}\delta_{\alpha\delta} - \delta_{\delta\nu}\delta_{\alpha\beta})]u_{\alpha,\beta} \\ + 2a^e\mu^{1e}(e_{\alpha\epsilon\beta} - \epsilon_0 E^1_\epsilon\delta_{\alpha\beta})\delta_{\delta\nu}u_{\epsilon,\alpha\beta} - \epsilon_0\alpha^e(E^1_\alpha\delta_{\delta\nu} - E^1_\delta\delta_{\alpha\nu} \\ - E^1_\nu\delta_{\alpha\delta})\tilde{\varphi}_{,\alpha} - 2a^e\mu^{1e}\epsilon_{\alpha\beta}\delta_{\delta\nu}\tilde{\varphi}_{,\alpha\beta}\}^-\nu_\nu \\ = \Gamma_{1\,\alpha\beta}u_{\alpha,\beta} + \Gamma_{2\,\alpha}\tilde{\varphi}_{,\alpha} - \epsilon_0\alpha^e\nu_\delta\{[E^1_\nu(E^1_\delta\delta_{\alpha\beta} - E^1_\beta\delta_{\alpha\delta}) \\ + \tfrac{1}{2}E^1_\pi E^1_\pi(\delta_{\delta\alpha}\delta_{\beta\nu} - \delta_{\delta\nu}\delta_{\alpha\beta})]u_{\alpha,\beta} \\ + (E^1_\alpha\delta_{\delta\nu} - E^1_\delta\delta_{\alpha\nu} - E^1_\nu\delta_{\delta\alpha})\tilde{\varphi}_{,\alpha}\}^+\nu_\nu,\end{aligned} \tag{9.10}$$

$$(\tilde{\varphi})^- = (\tilde{\psi} - E^1_\alpha u_\alpha)^+. \tag{9.11}$$

We now apply these equations to the propagation of both plane and surface waves in a hexagonal crystal in class $C_{6\nu} = 6$ mm with the axis of symmetry in the X_3 direction. The static biasing electric field is in the direction of the axis of symmetry and, in the surface wave problem where there is a surface, of equal magnitude on both sides of the boundary, i.e.,

$$(E^1_1)^* = (E^1_2)^* = 0, \quad (E^1_3)^* = E. \tag{9.12}$$

Since in the surface wave problem the surface is taken normal to X_2, all variables are taken to be independent of X_1. The four differential equations then take the form

$$\begin{aligned}(\partial/\partial t)\{(e_{15} + e_{31})u_{2,32} + e^*_{15}u_{3,22} + e^*_{33}u_{3,33}\} - m_{33}[(e_{15} + e_{31})E \\ + 2a^e(\mu^{1e})^2]u_{2,233} - 2a^e(\mu^{1e})^2 m_{11}u_{2,222} - [m_{33}e^*_{15}E \\ + 2a^e(\mu^{1e})^2 m_{11}]u_{3,322} - m_{33}[e^*_{33}E + 2a^e(\mu^{1e})^2]u_{3,333} \\ + 2a^e\mu^{1e}[m_{11}(e_{15} + e_{31})u_{2,2223} + m_{33}(e_{15} + e_{31})u_{2,2333} \\ + m_{11}e^*_{15}u_{3,2222} + (m_{11}e^*_{33} + m_{33}e^*_{15})u_{3,2233} \\ + m_{33}e^*_{33}u_{3,3333}] - (\partial/\partial t)\{\epsilon_{11}\tilde{\varphi}_{,22} + \epsilon_{33}\tilde{\varphi}_{,33}\} \\ + \mu^{1e}m_{11}\tilde{\varphi}_{,22} + \mu^{1e}m_{33}\tilde{\varphi}_{,33} + \epsilon_{11}m_{33}E\tilde{\varphi}_{,223} + \epsilon_{33}m_{33}E\tilde{\varphi}_{,333} \\ - 2a^e\mu^{1e}[m_{11}\epsilon_{11}\tilde{\varphi}_{,2222} + (m_{11}\epsilon_{33} + m_{33}\epsilon_{11})\tilde{\varphi}_{,2233} \\ + m_{33}\epsilon_{33}\tilde{\varphi}_{,3333}] = 0,\end{aligned} \tag{9.13}$$

$$c^*_{66}u_{1,22} + c^*_{44}u_{1,33} = \rho\,\partial^2 u_1/\partial t^2, \tag{9.14}$$

$$\begin{aligned}c^{**}_{11}u_{2,22} + c^*_{44}u_{2,33} + (c^*_{13} + c_{44})u_{3,23} + (e_{15} + e_{31})\tilde{\varphi}_{,23} \\ - 2a^e\mu^{1e}[(e_{15} + e_{31})u_{2,223} + e^*_{15}u_{3,222} + e^*_{33}u_{3,233} \\ - \epsilon_{11}\tilde{\varphi}_{,222} - \epsilon_{33}\tilde{\varphi}_{,233}] = \rho\,\partial^2 u_2/\partial t^2,\end{aligned} \tag{9.15}$$

$$\begin{aligned}(c^*_{13} + c_{44})u_{2,23} + c^{**}_{44}u_{3,22} + c^{**}_{33}u_{3,33} + e^*_{15}\tilde{\varphi}_{,22} + e^*_{33}\tilde{\varphi}_{,33} \\ - 2a^e\mu^{1e}[(e_{15} + e_{31})u_{2,233} + e^*_{15}u_{3,223} + e^*_{33}u_{3,333} \\ - \epsilon_{11}\tilde{\varphi}_{,223} - \epsilon_{33}\tilde{\varphi}_{,333}] = \rho\,\partial^2 u_3/\partial t^2,\end{aligned} \tag{9.16}$$

where

$$e^*_{15} = e_{15} - \epsilon_0 E, \tag{9.17}$$

$$e^*_{33} = e_{33} - \epsilon_0 E, \tag{9.18}$$

$$c^*_{11} = c_{11} - Ee_{31}, \quad c^{**}_{11} = c^*_{11} + 2a^e(\mu^{1e})^2, \tag{9.19}$$

$$c^*_{33} = c_{33} - Ee_{33}, \quad c^{**}_{33} = c^*_{33} + 2a^e(\mu^{1e})^2 - \epsilon_0 E^2, \tag{9.20}$$

$$c^*_{44} = c_{44} - Ee_{33}, \quad c^{**}_{44} = c_{44} - Ee_{31} - \epsilon_0 E^2, \tag{9.21}$$

$$c^*_{66} = c_{66} - Ee_{31}, \tag{9.22}$$

$$c^*_{13} = c_{13} + 2a^e(\mu^{1e})^2, \tag{9.23}$$

and the compressed notation for tensor indices[62] has been employed.

Since the boundary is normal to X_2, we have

$$\nu_\alpha = \delta_{2\alpha}, \tag{9.24}$$

and the jump conditions (9.8)—(9.11) can similarly be reduced to

$$\{(\partial/\partial t)[e_{15}u_{2,3}+e_{15}^{*}u_{3,2}-\epsilon_{11}\tilde{\varphi}_{,2}]-2a^{e}(\mu^{1e})^{2}m_{11}(u_{2,22}+u_{3,23})+\mu^{1e}m_{11}\tilde{\varphi}_{,2}+2a^{e}\mu^{1e}m_{11}[(e_{15}+e_{31})u_{2,223}+e_{15}^{*}u_{3,222}+e_{33}^{*}u_{3,233}-\epsilon_{11}\tilde{\varphi}_{,222}-\epsilon_{33}\tilde{\varphi}_{,233})\}^{-}=-\epsilon_{0}\{(\partial/\partial t)(\tilde{\psi}_{,2})\}^{+}, \tag{9.25}$$

$$(u_{1,2})^{-}=0, \tag{9.26}$$

$$\{c_{11}^{**}u_{2,2}+c_{13}^{**}u_{3,3}+e_{31}^{*}\tilde{\varphi}_{,3}-2a^{e}\mu^{1e}[(e_{15}+e_{31})u_{2,23}+e_{15}^{*}u_{3,22}+e_{33}^{*}u_{3,33}-\epsilon_{11}\tilde{\varphi}_{,22}-\epsilon_{33}\tilde{\varphi}_{,33}]\}^{-}=\{\epsilon_{0}E\tilde{\psi}_{,3}\}^{+}, \tag{9.27}$$

$$\{c_{44}^{**}u_{2,3}+c_{44}^{**}u_{3,2}+e_{15}^{*}\tilde{\varphi}_{,2}\}^{-}=\{-\epsilon_{0}E\tilde{\psi}_{,2}\}^{+}, \tag{9.28}$$

$$\{-2a^{e}(\mu^{1e})^{2}u_{2,2}-[a^{e}(\mu^{1e})^{2}+\epsilon_{0}\alpha^{e}E^{2}]u_{3,3}-\epsilon_{0}\alpha^{e}E\tilde{\varphi}_{,3}+2a^{e}\mu^{1e}\times[(e_{15}+e_{31})u_{2,23}+e_{15}^{*}u_{3,22}+e_{33}^{*}u_{3,33}-\epsilon_{11}\tilde{\varphi}_{,22}-\epsilon_{33}\tilde{\varphi}_{,33}]\}^{-}=\Gamma_{1}^{11}u_{2,2}+\Gamma_{1}^{33}u_{3,3}+\Gamma_{2}^{3}\tilde{\varphi}_{,3}-\{\epsilon_{0}\alpha^{e}E\tilde{\psi}_{,3}\}^{+}, \tag{9.29}$$

$$\{\tilde{\varphi}\}^{-}=\{\tilde{\psi}-Eu_{3}\}^{+}, \tag{9.30}$$

where

$$c_{13}^{**}=c_{13}+\epsilon_{0}E^{2}+a^{e}(\mu^{1e})^{2}, \tag{9.31}$$

$$c_{44}^{**}=c_{44}+a^{e}(\mu^{1e})^{2}, \tag{9.32}$$

$$e_{31}^{*}=e_{31}+\epsilon_{0}E. \tag{9.33}$$

From Eqs. (9.13)—(9.16) and (9.25)—(9.30) it is readily seen that the u_1 displacement completely uncouples from the three other variables. The solution for u_1 is elementary, and we are concerned only with the solutions containing u_2, u_3, and $\tilde{\varphi}$. For a plane wave traveling in the direction of the applied dc electric field in an infinite solid there is no dependence on X_2, and in this case u_2 uncouples from u_3 and $\tilde{\varphi}$. Consequently, we take the plane wave solution of interest in the form

$$u_{3}=\mathrm{Re}\{A_{1}\exp[i(kX_{3}-\omega t)]\},\quad \tilde{\varphi}=\mathrm{Re}\{A_{2}\exp[i(kX_{3}-\omega t)]\}, \tag{9.34}$$

and substitute into (9.13) and (9.16) to obtain

$$A_{1}[\omega e_{33}^{*}+m_{33}k(e_{33}^{*}E+2a^{e}(\mu^{1e})^{2})-i2a^{e}\mu^{1e}m_{33}e_{33}^{*}k^{2}]+A_{2}[-\omega\epsilon_{33}-Em_{33}k\epsilon_{33}+i(2a^{e}\mu^{1e}m_{33}\epsilon_{33}k^{2}+\mu^{1e}m_{33})]=0, \tag{9.35}$$

$$A_{1}[\rho\omega^{2}-c_{33}^{**}k^{2}+i2a^{e}\mu^{1e}k^{3}e_{33}^{*}]+A_{2}[-e_{33}^{*}k^{2}-i2a^{e}\mu^{1e}k^{3}\epsilon_{33}]=0.$$

For a nontrivial solution the determinant of the coefficients of A_1 and A_2 vanishes, i. e.,

$$\begin{vmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{vmatrix}=0, \tag{9.36}$$

where

$$\begin{aligned}a_{11}&=\omega e_{33}^{*}+m_{33}k(Ee_{33}^{*}+2a^{e}(\mu^{1e})^{2})+i\mathcal{D}_{33}e_{33}^{*}k^{2},\\ a_{12}&=-\omega\epsilon_{33}-Em_{33}k\epsilon_{33}-i(\mathcal{D}_{33}\epsilon_{33}k^{2}+\sigma_{33}),\\ a_{21}&=\rho\omega^{2}-c_{33}^{**}k^{2}-i(\mathcal{D}_{33}/m_{33})k^{3}e_{33}^{*},\\ a_{22}&=-e_{33}^{*}k^{2}+i(\mathcal{D}_{33}/m_{33})k^{3}\epsilon_{33},\end{aligned} \tag{9.37}$$

and we have introduced the conductivity tensor $\sigma_{\alpha\beta}$ and the diffusivity tensor $\mathcal{D}_{\alpha\beta}$, which are defined by

$$\sigma_{\alpha\beta}=-\mu^{1e}m_{\alpha\beta},\quad \mathcal{D}_{\alpha\beta}=-2a^{e}\mu^{1e}m_{\alpha\beta}. \tag{9.38}$$

Equation (9.36) determines the dispersion relationship for our plane wave. It has four complex roots k_n ($n=1,2,3,4$) for each value of ω and has to be solved numerically in each specific instance. However, if we write (9.36) in the form

$$\rho\left(\frac{\omega}{k}\right)^{2}=c_{33}^{**}\left(1+K^{2}\left[\Gamma+i\frac{\omega}{\omega_{D}}\left[1-\frac{\omega^{2}}{\omega_{D}\omega_{C}}\left(\frac{\sigma_{33}}{km_{33}e_{33}^{*}}\right)^{2}\right]\times\left[\Gamma+i\left(\frac{\omega}{\omega_{D}}+\frac{\omega_{C}}{\omega}\right)\right]^{-1}\right)\right), \tag{9.39}$$

where

$$K^{2}=(e_{33}^{*})^{2}/c_{33}^{**}\epsilon_{33},\quad \omega_{C}=\sigma_{33}/\epsilon_{33},\quad \omega_{D}=\omega^{2}/k^{2}\mathcal{D}_{33},\quad \Gamma=1+m_{33}Ek/\omega, \tag{9.40}$$

we see that, except for the last term on the right-hand side, we get the same form White[15] obtained using a simplified theory. Another difference between White's result and the result obtained here by this more general theory is that we have taken into account the modification in the elastic and piezoelectric constants caused by the static electric field bias. However, as noted earlier in this section, we have not bothered to obtain the full explicit dependence of the effective material constants on the biasing dc field. Consequently, the dependence considered here is essentially implicit. Nevertheless, as noted earlier, the full explicit dependence can readily be obtained from the general description, with some effort if desired.

For a surface wave propagating in the X_3 direction of the semiconductor occupying the region $X_2 \le 0$ the three variables u_2, u_3, and $\tilde{\varphi}$ remain coupled on account of the three equations (9.13), (9.15), and (9.16) and the boundary conditions (9.25) and (9.27)—(9.30). In this case we consider as a solution of (9.13), (9.15), and (9.16)

$$\begin{aligned}u_{2}&=\mathrm{Re}\{A_{1}\exp(\beta X_{2})\exp[i(kX_{3}-\omega t)]\},\\ u_{3}&=\mathrm{Re}\{A_{2}\exp(\beta X_{2})\exp[i(kX_{3}-\omega t)]\},\\ \tilde{\varphi}&=\mathrm{Re}\{A_{3}\exp(\beta X_{2})\exp[i(kX_{3}-\omega t)]\},\end{aligned} \tag{9.41}$$

which satisfies (9.13), (9.15), and (9.16) provided

$$A_{1}\{(e_{15}+e_{31})k\beta[\omega\Gamma-i(\mathcal{D}_{11}\beta^{2}-\mathcal{D}_{33}k^{2})]+\beta\mu^{1e}(\mathcal{D}_{11}\beta^{2}-\mathcal{D}_{33}k^{2})\}+A_{2}\{(e_{33}^{*}k^{2}-e_{15}^{*}\beta^{2})[\mathcal{D}_{11}\beta^{2}-\mathcal{D}_{33}k^{2}+i\omega\Gamma]+ik\mu^{1e}(\mathcal{D}_{11}\beta^{2}-\mathcal{D}_{33}k^{2})\}+A_{3}\{(\epsilon_{11}\beta^{2}-\epsilon_{33}k^{2})\times[\mathcal{D}_{11}\beta^{2}-\mathcal{D}_{33}k^{2}+i\omega\Gamma]-(\sigma_{11}\beta^{2}-\sigma_{33}k^{2})\}=0, \tag{9.42}$$

$$A_{1}\{\rho\omega^{2}+c_{11}^{**}\beta^{2}-c_{44}^{*}k^{2}-i2a^{e}\mu^{1e}(e_{15}+e_{31})k\beta^{2}\}+A_{2}\{-2a^{e}\mu^{1e}\beta(e_{15}^{*}\beta^{2}-e_{33}^{*}k^{2})+i(c_{13}^{*}+c_{44})\beta k\}+A_{3}\{2a^{e}\mu^{1e}\beta(\epsilon_{11}\beta^{2}-\epsilon_{33}k^{2})+i(e_{15}+e_{31})\beta k\}=0, \tag{9.43}$$

$$A_{1}\{2a^{e}\mu^{1e}(e_{15}+e_{31})\beta k^{2}+i(c_{13}^{*}+c_{44})\beta k\}+A_{2}\{\rho\omega^{2}+c_{44}^{**}\beta^{2}-c_{33}^{**}k^{2}-i2a^{e}\mu^{1e}k(e_{15}^{*}\beta^{2}-e_{33}^{*}k^{2})\}+A_{3}\{e_{15}^{*}\beta^{2}-e_{33}^{*}k^{2}+i2a^{e}\mu^{1e}k(\epsilon_{11}\beta^{2}-\epsilon_{33}k^{2})\}=0. \tag{9.44}$$

For a nontrivial solution the determinant of the coefficients of A_1, A_2, and A_3 in (9.42)—(9.44) vanishes, which leads to an algebraic equation of fourth degree in β^2, which has eight complex roots that may be written

in the form

$$\pm\beta^{(n)} = \pm\beta^{(n)}(k,\omega), \quad n=1,2,3,4. \tag{9.45}$$

However, in order that the solution not become unbounded as $X_2 \to \infty$ only the $\beta^{(n)}$'s with a positive real part are admissible. For each of these four roots we can then find the corresponding amplitude ratios from any two of the three equations in (9.42)—(9.44)

$$A_1^{(n)} : A_2^{(n)} : A_3^{(n)}, \quad n=1,2,3,4. \tag{9.46}$$

At the surface $X_2 = 0$ the five boundary conditions (9.25) and (9.27)—(9.30) must be satisfied. Now, the electric field at $X_2 > 0$ must satisfy the equation

$$\tilde{\psi}_{,\alpha\alpha} = 0, \tag{9.47}$$

which is satisfied by

$$\tilde{\psi} = \mathrm{Re}\{B\exp(-\hat{k}X_2)\exp[i(kX_3-\omega t)]\}, \tag{9.48}$$

where $\hat{k} = \pm k$ must have a positive real part. In order to satisfy the five boundary conditions at $X_2 = 0$, all four solutions of the semiconductor equations are required in addition to the solution (9.48) in free space. Accordingly, we write

$$\begin{aligned}
u_2 &= \mathrm{Re}\left(\exp[i(kX_3-\omega t)\sum_{n=1}^{4} C^{(n)}A_1^{(n)}\exp(\beta^{(n)}X_2)\right),\\
u_3 &= \mathrm{Re}\left(\exp[i(kX_3-\omega t)\sum_{n=1}^{4} C^{(n)}A_2^{(n)}\exp(\beta^{(n)}X_2)\right),\\
\tilde{\varphi} &= \mathrm{Re}\left(\exp[i(kX_3-\omega t)\sum_{n=1}^{4} C^{(n)}A_3^{(n)}\exp(\beta^{(n)}X_2)\right).
\end{aligned} \tag{9.49}$$

Substituting from (9.48) and (9.49) into the boundary conditions (9.25) and (9.27)—(9.30), we obtain

$$\begin{aligned}
&\sum_{n=1}^{4} C^{(n)}\{A_1^{(n)}[e_{15}\omega k + \mu^{1e}\mathcal{D}_{11}(\beta^{(n)})^2 - i(e_{15}+e_{31})\mathcal{D}_{11}(\beta^{(n)})^2 k]\\
&\quad + A_2^{(n)}[\mathcal{D}_{11}\beta^{(n)}(e_{33}^{*}k^2 - e_{15}^{*}(\beta^{(n)})^2) + i\beta^{(n)}(\mu^{1e}\mathcal{D}_{11}k - e_{15}^{*}\omega)]\\
&\quad + A_3^{(n)}[\mathcal{D}_{11}\beta^{(n)}(\epsilon_{11}(\beta^{(n)})^2 - \epsilon_{33}k^2) - \sigma_{11}\beta^{(n)}\\
&\quad + i\epsilon_{11}\omega\beta^{(n)}]\} + i\epsilon_0\omega\hat{k}B = 0,
\end{aligned} \tag{9.50}$$

$$\begin{aligned}
&\sum_{n=1}^{4} C^{(n)}\{A_1^{(n)}\beta^{(n)}[c_{11}^{**} - i2a^e\mu^{1e}(e_{15}+e_{31})k] + A_2^{(n)}[2a^e\mu^{1e}(e_{33}^{*}k^2\\
&\quad - e_{15}^{*}(\beta^{(n)})^2) + ic_{13}^{**}k] + A_3^{(n)}[2a^e\mu^{1e}(\epsilon_{11}(\beta^{(n)})^2 - \epsilon_{33}k^2)\\
&\quad + ie_{31}^{*}k]\} - i\epsilon_0 EkB = 0,
\end{aligned} \tag{9.51}$$

$$\sum_{n=1}^{4} C^{(n)}\{A_1^{(n)}ic_{44}^{***}k + A_2^{(n)}c_{44}^{**}\beta^{(n)} + A_3^{(n)}e_{15}^{*}\beta^{(n)}\} - \epsilon_0\hat{k}B = 0, \tag{9.52}$$

$$\begin{aligned}
&\sum_{n=1}^{4} C^{(n)}\{A_1^{(n)}[2a^e\mu^{1e}\beta^{(n)}(-\mu^{1e} + i(e_{15}+e_{31})k) - \Gamma_{11}\beta^{(n)}]\\
&\quad + A_2^{(n)}[2a^e\mu^{1e}(e_{15}^{*}(\beta^{(n)})^2 - e_{33}^{*}k^2) - i(a^e(\mu^{1e})^2\\
&\quad + \epsilon_0\alpha^e E^2 - \Gamma_{33})k] + A_3^{(n)}[-2a^e\mu^{1e}(\epsilon_{11}(\beta^{(n)})^2 - \epsilon_{33}k^2)\\
&\quad - i\epsilon_0\alpha^e Ek - \Gamma_3 ik]\} + i\epsilon_0\alpha^e EkB = 0,
\end{aligned} \tag{9.53}$$

$$\sum_{n=1}^{4} C^{(n)}\{A_3^{(n)} + EA_2^{(n)}\} - B = 0, \tag{9.54}$$

which constitute five linear homogeneous algebraic equations in the five constants $C^{(1)}$, $C^{(2)}$, $C^{(3)}$, $C^{(4)}$, and B. This system yields nontrivial solutions when the determinant of the coefficients vanishes, which leads to an algebraic equation in k. The values of k at a given ω satisfying the system must be determined numerically. In the absence of conduction, i.e., in the purely piezoelectric case, at least one surface wave almost always exists,[63] and it is nondispersive. If in a calculation the imaginary part of k turns out to be negative, the surface wave is being amplified by the dc field E. The coefficients Γ_{11}, Γ_{33}, and Γ_3, which appear in Eq. (9.53), have never been measured. On account of the use of the normal force boundary condition on the free-electronic fluid, the condition of no electrical surface charge on the semiconductor assumed in earlier work on this problem[16-18] has not been employed in this treatment. Indeed, after a solution has been obtained numerically, the resulting surface charge can be determined *a posteriori* from the small field counterpart of (8.28).

ACKNOWLEDGMENTS

One of the authors (H. F. T.) wishes to thank P. Das and M. Araghi for a fruitful discussion. This work was supported in part by the Office of Naval Research under Contract No. N00014-67-A-0117-0007 and the National Science Foundation under Grant No. GK-38118.

APPENDIX

The charge equation of electrostatics for the model, consisting of the five charged continua, may be written in the form

$$E_{i,i} = 4\pi[\mu^{l}(\mathbf{y}) + \mu^{b}(\mathbf{y}) + \mu^{i}(\mathbf{y}) + \mu^{e}(\mathbf{y}) + \mu^{h}(\mathbf{y})]. \tag{A1}$$

The substitution of (2.4) into (A1) yields

$$E_{i,i} = 4\pi[\mu^{r}(\mathbf{y}) - \mu^{b}(\mathbf{y}+\boldsymbol{\eta}) + \mu^{b}(\mathbf{y}) + \mu^{i}(\mathbf{y}) + \mu^{e}(\mathbf{y}) + \mu^{h}(\mathbf{y})]. \tag{A2}$$

Expanding $\mu^{b}(\mathbf{y}+\boldsymbol{\eta})$ in a Taylor series about $\mathbf{y}$, retaining the first term and substituting in (A2), we find

$$E_{i,i} = 4\pi[\mu^{r} - \eta_i\mu^{b}_{,i} + \mu^{i} + \mu^{e} + \mu^{h}]. \tag{A3}$$

Employing (3.30), (2.3), (3.9), and (3.37), we obtain

$$D_{i,i} = 4\pi\mu, \tag{A4}$$

which is identical with $(3.39)_2$, the charge equation of electrostatics for the electrically polarized continuum.

[1] R. A. Toupin, J. Ratl. Mech. Anal. **5**, 848 (1956).
[2] R. A. Toupin, Int. J. Eng. Sci. **1**, 101 (1963).
[3] A. C. Eringen, Int. J. Eng. Sci. **1**, 127 (1963).
[4] H. F. Tiersten, J. Math. Phys. **5**, 1298 (1964).
[5] W. F. Brown, Jr., J. Appl. Phys. **36**, 994 (1965).
[6] N. F. Jordan and A. C. Eringen, Int. J. Eng. Sci. **2**, 59 (1964).
[7] H. F. Tiersten, J. Math. Phys. **6**, 779 (1965).
[8] R. C. Dixon and A. C. Eringen, Int. J. Eng. Sci. **3**, 359 (1965).
[9] R. A. Grot and A. C. Eringen, Int. J. Eng. Sci. **4**, 611 (1966).
[10] L. Bragg, J. Math. Phys. **11**, 318 (1970).
[11] H. F. Tiersten, Int. J. Eng. Sci. **9**, 587 (1971).
[12] H. F. Tiersten and C. F. Tsai, J. Math. Phys. **13**, 361 (1972).
[13] M. Lax and D. F. Nelson, Phys. Rev. B **4**, 3694 (1971).
[14] A. R. Hutson and D. L. White, J. Appl. Phys. **33**, 40 (1962).
[15] D. L. White, J. Appl. Phys. **33**, 2547 (1962).
[16] K. M. Lakin and H. J. Shaw, IEEE Trans. Microwave Theory Tech. MTT-**17**, 912 (1969).
[17] G. S. Kino and T. M. Reeder, IEEE Trans. Electron Devices ED-**18**, 909 (1971).
[18] P. S. Ramakrishna, "Amplification of Acoustic Surface and

Layer Waves," Master's Thesis submitted to McGill University, Montreal, 1971.
[19]W. Shockley, *Electrons and Holes in Semiconductors* (Van Nostrand, Princeton, N.J., 1950).
[20]B. A. Boley and J. H. Weiner, *Theory of Thermal Stresses* (Wiley, New York, 1967).
[21]S. R. DeGroot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1963).
[22]A. C. Eringen, *Nonlinear Theory of Continuous Media* (McGraw-Hill, New York, 1962).
[23]C. Truesdell and W. Noll, "The Nonlinear Field Theories of Mechanics," in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin 1965), Vol. III/2, Secs. 17 and 19.
[24]Ref. 22, Secs. 27 and 44.
[25]The fluid pressure terms were employed in this manner in H. F. Tiersten, Physica **37**, 504 (1967).
[26]C. Truesdell, J. Chem. Phys. **37**, 2336 (1962).
[27]H. F. Tiersten, *Linear Piezoelectric Plate Vibrations* (Plenum, New York, 1969), Chap. 4, Sec. 4.
[28]J. C. Baumhauer and H. F. Tiersten, J. Acoust. Soc. Am. **54**, 1017 (1973).
[29]See the Appendix.
[30]C. Moller, *The Theory of Relativity* (Oxford U. P., London, 1952), Sec. 29.
[31]Ref. 22, Sec. 17.
[32]M. Mason and W. Weaver, *The Electromagnetic Field* (The University of Chicago Press, Chicago, 1929) (also Dover, New York), Sec. 52, p. 261.
[33]A. E. Green and R. S. Rivlin, Arch. Ratl. Mech. Anal. **16**, 325 (1964).
[34]H. F. Tiersten, "Surface Coupling in Magnetoelastic Insulators," *Surface Mechanics, A Symposium Volume*, American Society of Mechanical Engineers, New York, 120 (1969).
[35]Ref. 11, Sec. 3.
[36]R. Becker and F. Sauter, *Electromagnetic Fields and Interactions* (Blaisdell, New York, 1964), Vol. 1, Sec. 53.
[37]Ref. 36, Secs. 86-87.
[38]C. Truesdell and R. A. Toupin, "The Classical Field Theories," in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1960), Vol. III/1, Sec. 81.
[39]Either the spatial or material integral forms of the equations of balance can be taken as fundamental, since either yields the same jump conditions across moving not necessarily material surfaces of discontinuity.
[40]Ref. 20, Secs. 1.8-1.12.
[41]Ref. 21, Chap. III, Secs. 1 and 2.
[42]Ref. 22, Secs. 36-40.
[43]B. D. Coleman and W. Noll, Arch. Ratl. Mech. Anal. 13, 167 (1963).
[44]B. D. Coleman, Arch Ratl. Mech. Anal. 17, 1 (1964).
[45]Ref. 23.
[46]Ref. 24.
[47]See Ref. 50 of Ref. 12. For the recoverable or state function constitutive equations being treated here the statement applies directly. For the dissipative consitutive equations treated later in this section the point of view mentioned in Ref. 50 of Ref. 12 is adopted.
[48]A. L. Cauchy, Mem. Acad. Sci. XXII, 615 (1850) [Oevres (1), 2, 351].
[49]A proof may be found in, A. J. M. Spencer, "Theory of Invariants," *Continuum Physics*, Vol. 1, Part III (Academic, New York, 1972), 239, Sec. 2.1.
[50]This procedure was given the name "Principle of Equipresence" by Truesdell. See Ref. 38, Sec. 293.
[51]Ref. 22, Sec. 27.
[52]A. E. Green and J. E. Adkins, *Large Elastic Deformations and Nonlinear Continuum Mechanics* (Oxford U. P., London, 1960), Chap. 8.
[53]J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill, New York, 1941), Sec. 1.9.
[54]A. C. Smith, J. F. Janak, and R. B. Adler, *Electronic Conduction in Solids* (McGraw-Hill, New York, 1967), Sec. 3.4.
[55]Ref. 38, Secs. 192 and 193.
[56]J. A. Appelbaum and D. R. Hamann, Phys. Rev. Lett. **32**, 225 (1974).
[57]The surface charge densities are defined from the volumetric charge densities in the usual way. See Ref. 53, Sec. 1.4.
[58]H. H. Woodson and J. R. Melcher, *Electromechanical Dynamics* (Wiley, New York, 1968), Sec. 6.21.
[59]Surface constitutive equations must satisfy the principle of material objectivity as well as volumetric ones. See Ref. 232, Sec. 5.
[60]Ref. 53, Appendix I.
[61]H. F. Tiersten and J. C. Baumhauer, J. Appl. Phys. **45**, 4272 (1974).
[62]Ref. 27, Chapter 7.
[63]In the purely piezoelectric case it can be shown that a surface wave almost always exists. G. A. Coquin, private communication, 1967. Also K. A. Ingebrigtsen and A. Tonning, Phys. Rev. **184**, 942 (1969).

Exact solutions to Einstein field equations

Jorge Melnick*

Departamento de Astronomia, Universidad de Chile, Santiago, Chile

Romualdo Tabensky

Departamento de Fisica, Universidad de Chile, Santiago, Chile

(Received 2 December 1974)

A method of generating static and isotropic solutions of the Einstein field equations is presented for the case in which the source of the field is a perfect fluid. A special case is exhibited. The general solution for vacuum is derived.

I. INTRODUCTION

It is the purpose of this paper to give a method of obtaining solutions of the Einstein equations for the case where the source of the field is a perfect fluid described by the energy momentum tensor[1] $T^{\mu\nu}=(p+\omega)u^\mu u^\nu - pg^{\mu\nu}$, (greek indices range from 0 to 3, italic indices from 1 to 3) where p is the pressure and ω the rest energy density. In the comoving frame the only nonvanishing components of the energy—momentum tensor for our metric [see Eq. (1) below] are

$$T^1_1=T^2_2=T^3_3=-p, \quad T^0_0=\omega.$$

The metric considered in this paper will be static and isotropic, that is,

$$ds^2=\exp[2\phi(x,y,z)]\,dt^2-\exp[2\psi(x,y,z)](dx^2+dy^2+dz^2), \tag{1}$$

where $\phi(x,y,z)$ and $\psi(x,y,z)$ are arbitrary functions of their arguments. No symmetry group is assumed in (1).

It is useful to introduce the three dimensional trace-free Einstein tensor[2] $\tilde{G}^i_j=G^i_j-G\delta^i_j$ (here $G=G^i_i$) which vanishes in the comoving frame for our metric and energy—momentum tensor, allowing us to separate the field equations as

$$\tilde{G}^i_j=0 \tag{2}$$

and

$$-8\pi p=\tfrac{1}{3}\exp(-2\psi)\{2\nabla^2\psi+(\nabla\psi)^2-2(\nabla\phi)^2\}, \tag{3}$$

$$8\pi\omega=\exp(-2\psi)\{2\nabla^2\psi+(\nabla\psi)^2\}. \tag{4}$$

This enables us to compute the pressure and rest energy density once (2) is solved for the functions $\phi(x,y,z)$ and $\psi(x,y,z)$ since neither p nor ω appear in (2).

In Sec. II we describe a general method for solving Eq. (2), which is applied in obtaining a physically reasonable solution[3] to Einstein's equations.

In Sec. III the method is applied to obtain the general vacuum solution to the field equations for the spacetime given by (1).

II. THE SOLUTION

Writing Eq. (2) explicitly, we get

$$\Lambda_{,ik}=\Lambda\lambda_{,i}\lambda_{,k}-\Sigma\delta_{ik}, \tag{5}$$

where we have defined $\lambda=\sqrt{2}\,\phi$, $\Lambda=\exp[-(\psi+\phi)]$, and $\Sigma=-\frac{1}{3}\{\nabla^2\Lambda-2\Lambda(\nabla\phi)^2\}$. The notation $\Gamma_{,i}=\partial\Gamma/\partial x_i$ is used. The differential form of (5) is

$$d\Lambda_{,i}=\Lambda\lambda_{,i}\,d\lambda-\Sigma\,dx_i, \tag{6}$$

which implies the functional relations

$$\Lambda,x=F(\lambda,x)=-\Sigma$$

$$\Lambda,y=G(\lambda,y)=-\Sigma$$

$$\Lambda,z=H(\lambda,z)=-\Sigma,$$

from which it can be seen that Σ depends on λ alone, $\Sigma=\Sigma(\lambda)$.

Now (6) takes the form

$$d(\Lambda_{,i}+\Sigma x_i)=(\Lambda\lambda_{,i}+x_i\dot{\Sigma})\,d\lambda, \tag{7}$$

where $\dot{\Sigma}=d\Sigma/d\lambda$. Equation (7) implies that $F_i=\Lambda_{,i}+\Sigma x_i$ depends on λ alone, $F_i=F_i(\lambda)$.

Equation (5) written in terms of F_i takes the form

$$x_i-\dot{F}_i/\dot{\Sigma}=-(\Lambda/\dot{\Sigma})\lambda_i. \tag{8}$$

Multiplying this equation by dx_i, we can write it as

$$d(\mathbf{x}-\mathbf{R}_0(\lambda))^2=\left(\frac{dR_0^2}{d\lambda}-2\mathbf{x}\cdot\dot{\mathbf{R}}-\frac{2\Lambda}{\dot{\Sigma}}\right)d\lambda,$$

where $\mathbf{R}_0(\lambda)=\dot{\mathbf{F}}/\dot{\Sigma}$. From here it follows that

$$(\mathbf{x}-\mathbf{R}_0(\lambda))^2=R^2(\lambda), \tag{9}$$

where

$$\frac{dR^2(\lambda)}{d\lambda}=\frac{dR_0^2}{d\lambda}-2\mathbf{x}\cdot\dot{\mathbf{R}}-\frac{2\Lambda}{\dot{\Sigma}}. \tag{10}$$

Equation (9) is that of a sphere centered at $\mathbf{R}_0(\lambda)$ with radius $R(\lambda)$, that is, the surfaces $\lambda=\text{const}$ are spheres. (We have assumed here that $\dot{\Sigma}\neq 0$; It can be shown that the surfaces $\lambda=\text{constant}$ are planes in the case where $\dot{\Sigma}$ vanishes, but we do not consider this case here.)

Equation (10) implies that Λ has the functional form

$$\Lambda=A(\lambda)+\mathbf{B}(\lambda)\cdot\mathbf{x}, \tag{11}$$

where $A(\lambda)=\frac{1}{2}\dot{\Sigma}\,d/d\lambda\,\{R_0^2-R^2(\lambda)\}$, and $\mathbf{B}(\lambda)=-\dot{\Sigma}\dot{\mathbf{R}}_0$.

Replacing (11) in (5), after a long calculation we obtain that $A(\lambda)$ and $\mathbf{B}(\lambda)$ must have the form

$$A(\lambda)=A_0\Gamma(\lambda)\dot{\Sigma}$$

and (12)

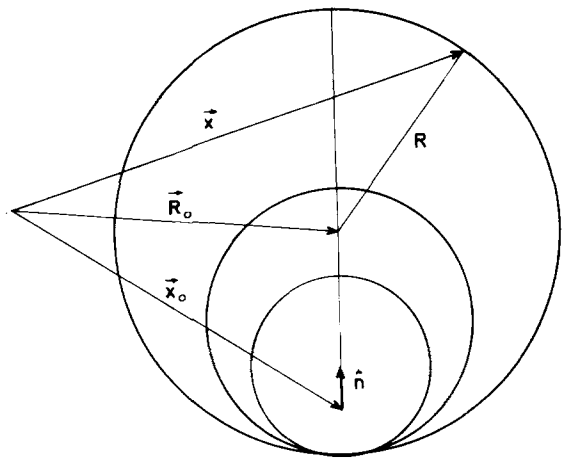

FIG. 1. The distribution of spheres $\lambda = \text{const}$ associated with the solutions of Eq. (5). $m = q = 1$ has been used in the formula for the radii.

$$\mathbf{B}(\lambda) = \mathbf{B}_0 \Gamma(\lambda) \dot{\Sigma}$$

with $\Gamma(\lambda) = 1/\dot{\Sigma} \exp(\int \Sigma/\dot{\Sigma}\, d\lambda)$. Rewriting (12) in terms of $R(\lambda)$ and $\mathbf{R}_0(\lambda)$, we get

$$\mathbf{R}_0(\lambda) = C_0 + \mathbf{B}_0 \int \Gamma(\lambda)\, d\lambda$$

and (13)

$$\frac{d}{d\lambda}(R_0^2 - R^2) = 2A_0 \int \Gamma(\lambda)\, d\lambda + D_0,$$

where A_0, B_0, C_0, and D_0 are constants.

Equations (13) imply that the centers of the spheres $\lambda = \text{const}$ must lie along a straight line, that is

$$\mathbf{R}_0 = \mathbf{x}_0 + \hat{n}s, \tag{14}$$

and that the radii are distributed along the line according to the law (see Fig. 1).

$$R^2(\lambda) = s^2 + 2ms + q, \tag{15}$$

where $s = \int \Gamma(\lambda)\, d\lambda$. Combining (14), (15), and (9), the formula for s is

$$S = \frac{1}{2} \frac{(\mathbf{x} - \mathbf{x}_0)^2 - q}{\hat{n} \cdot (\mathbf{x} - \mathbf{x}_0) + m}. \tag{16}$$

Finally, introducing (14) and (15) in (11), we get

$$\Lambda(s) = \gamma(s)[\hat{n} \cdot (\mathbf{x} - \mathbf{x}_0) + m], \tag{17}$$

where the function $\gamma(s)$ satisfies the ordinary differential equations

$$-\Sigma(s) = \frac{d\gamma(s)}{ds}$$

and

$$\frac{d^2\gamma(s)}{ds^2} = \gamma(s)\left(\frac{d\lambda}{ds}\right)^2. \tag{18}$$

To generate solutions to Einstein field equations we procede as follows: Pick an arbitrary function of one variable $\gamma(s)$ such that $\gamma^{-1} d^2\gamma/ds^2 \geq 0$, integrate (18) to get $\lambda = \sqrt{2}\,\phi(s)$; then from (17) we get $\Lambda(s)$ and thus ψ. With the help of Eq. (16) we express ϕ and ψ in terms of x, y, and z. Therefore, the solution depends on one arbitrary function of one variable and two parameters q, m. p and ω are computed from (3) and (4).

As a particular example we choose $\gamma(s) = s^2$. The metric we get is

$$ds^2 = \left(\frac{x^2 - q}{z}\right)^2 dt^2 - \frac{z^4}{(x^2 - q)^6}(dr^2 + r^2\, d\phi^2 + dz^2). \tag{19}$$

From (3) and (4) we find

$$8\pi p = -2ms^5 - 3qs^4,$$

and

$$8\pi\omega = 12s^5 m + 15s^4 q.$$

The Hawking–Penrose[4] energy condition $-R^{\mu\nu} v_\mu v_\nu \geq 0$ for any timelike vector v_μ is satisfied for all values for m and q, showing that the solution (19) is physically reasonable.

III. THE VACUUM SOLUTION

Up to here we have derived a general method of solving the field equations that reduces the problem of solving Einstein's equations to that of integrating a second order ordinary differential equation, and specifying a distribution of spheres in space. We shall show in this section that for the vacuum there is a unique $\gamma(s)$ and a unique distribution of spheres that correspond to solutions of Einstein field equations.

By combining (8) with (3) and (4) for $p = \omega = 0$, we get

$$\tfrac{4}{3} f_\pm(s) + \frac{df_\pm(s)}{ds}(m + s) + \frac{d^2 f_\pm(s)}{dt^2}(s^2 + 2ms + q) = 0 \tag{20}$$

where $f_\pm(s) = \exp(\pm\phi/2)/\sqrt{\gamma(s)}$.

It is convenient to introduce the new variable $s' = s + m/2\sqrt{m^2 - q} + 1/2$. In terms of s' (20) can be written as

$$s'(s' - 1)\frac{d^2 f_\pm(s')}{ds'^2} - 3(s' - \tfrac{1}{2})\frac{df_\pm(s')}{ds'} - \tfrac{3}{4} f_\pm(s') = 0. \tag{21}$$

The most general solution to (2) is[5]

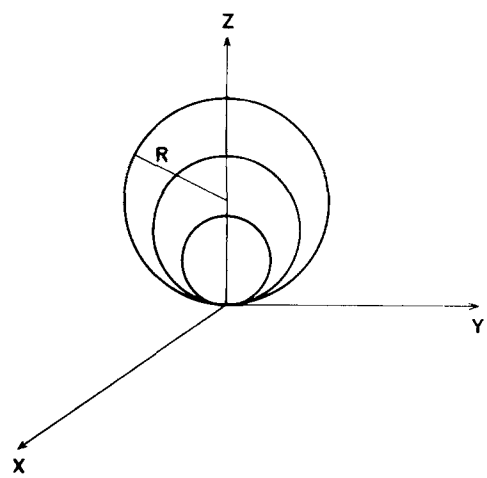

FIG. 2. Distribution of spheres $\lambda = \text{const}$ associated with the vacuum solution.

$$f_+ = A_+/\sqrt{s} + B_+/\sqrt{1-s}$$

and

$$f_- = A_-/\sqrt{s} + B_-/\sqrt{1-s}.$$

Replacing $\gamma(s) = (f_+ f_-)^{-2}$ and $\phi = \ln(f_+/f_-)$ in (18), we get for consistency $m = q = 0$. In solving equation (20) with $m = q = 0$ we get $\gamma(s) = s^2$. Thus the metric for vacuum is (19) with $m = q = 0$, that is,

$$ds^2 = \frac{x^4}{z^2}dt^2 - \frac{z^4}{x^{12}}(dr^2 + r^2 d\phi^2 + dz^2).$$

The associated distribution of spheres is shown in Fig. 2.

Schwarzchild's solution is a degenerate case of our calculation, the distribution of spheres is concentric and therefore s has no meaning. It can be obtained from (5) by assuming spherical symmetry for λ and Λ.

*Present address: Astronomy Department, California Institute of Technology, Pasadena, California 91109

[1]R. C. Tolman, *Relativity, Thermodynamics and Cosmology* (Oxford U. P., Oxford, 1934), p. 239.
[2]D. Eardley, E. Liang, and R. Sachs, J. Math. Phys. 13, 1 (1972).
[3]S. W. Hawking and G. F. R. Ellis, *The Large Scale Structure of Space-Time* (Cambridge U. P., Cambridge, 1973), p. 263.
[4]S. W. Hawking and R. Penrose, Proc. Roy. Soc. A 314, 529 (1970).
[5]G. Korn and T. Korn, *Mathematical Handbook for Scientists and Engineers* (McGraw-Hill, New York, 1968), p. 260.

Scattering by singular potentials with a perturbation—Theoretical introduction to Mathieu functions

H. H. Aly

Department of Physics, Southern Illinois University at Edwardsville, Illinois

H. J. W. Müller-Kirsten

Fachbereich Physik, Universitat Trier–Kaiserslautern In Kaiserslautern

N. Vahedi-Faridi

Aria Mehr University–Tehran, Iran

(Received 1 May 1974)

Different treatments of the important potential $1/r^4$ are correlated to understand their interrelations and to clear up the connection between the eigenvalues of Mathieu's equation and the poles of the S matrix. We also derive a new solution of the modified Mathieu equation. Mathematical and physical implications are also discussed.

1. INTRODUCTION

Considerable attention has recently been paid to the scattering by singular potentials.[1] This interest arose mainly from the hope of gaining some deeper insight into the infinities which plague nonrenormalizable field theory, and for using it as a testing ground for regularization and peratization techniques. Although a nonrelativistic potential can hardly be compared with (say) a nonrenormalizable 4-fermion interaction, there is a definite analogy between them insofar as a neutrino-antineutrino loop Feynman diagram[2] (for instance) behaves like a "singular potential" $1/r^5$ near the origin of coordinate space or like a correspondingly divergent quantity in momentum space. Particular attention[3–8] has always been paid to the potential $1/r^4$, since in this case the radial Schrödinger equation may be transformed into the reasonably well-known modified Mathieu equation, for which standard texts such as Meixner and Schäfke[9] (the most rigorous one, hereafter referred to as MS) are available.

The present investigation was motivated on the one hand by a desire to correlate different treatments[3–5] of the potential $1/r^4$ given in the literature, to understand their interrelation and to clear up the connection between the eigenvalues of Mathieu's equation and the poles of the scattering matrix. On the other hand, our study received impetus from the new trend in semi-empirical Regge pole analysis of favouring linearly rising, unitarity-violating trajectories which are believed[7,8] to be more like those for singular potentials than for regular Yukawa-like interactions.[10] We wanted to understand in particular the relation between expressions for the S matrix as given by Spector,[3] Bertocchi *et al.*,[5] and Challifour and Eden,[4] the relation between its poles and the eigenvalues of Mathieu's equation or its auxilliary parameters, and finally to see the behavior of the Regge trajectories. Moreover, since Mathieu functions are by no means as popular as, e.g., Bessel functions (or more generally functions of hypergeometric type), we considered it profitable to rederive all required solutions as a means of opening the way for generalization to potentials $1/r^m$, $m \neq 4$. However, our derivations are different from those given in the literature—also the solutions differ formally in important aspects. We derive the solutions by using a powerful perturbation approach[11,12] which has proved (e.g., in application to Yukawa[13] and Gauss[14] potentials) to be superior to customary straightforward power (or equivalent function) expansion. This program is carried out in Sec. 2. In Sec. 3 we derive various expressions of the S matrix, in Sec. 4 we calculate the low-energy behavior of Regge poles, and in Sec. 5 the behavior of the phase shift. The corresponding high-energy solutions have been discussed elsewhere.[4–6] The calculations show that the Regge trajectories rise into the first quadrant of the complex 1-plane. Finally, in Sec. 6, we derive an interesting new solution of the modified Mathieu equation which could also be used in the present context—in fact, it is this solution which corresponds to the solution of the scattering problem for the potential $1/r^m$, $m \neq 4$.

2. SOLUTIONS OF THE SCHRÖDINGER EQUATION FOR THE POTENTIAL $1/r^4$

We start by considering the repulsive potential

$$V(r) = g^2/r^4. \tag{2.1}$$

The radial Schrödinger equation may then be written

$$y'' + \left\{k^2 - \frac{l(l+1)}{r^2} - g^2/r^4\right\} y = 0, \tag{2.2}$$

where $E = k^2$, $m = \frac{1}{2}$, and $\hbar = c = 1$. It is useful to introduce the following substitutions:

$$y = r^{1/2}\varphi, \quad r = \gamma e^z, \quad \gamma = ig/h, \quad h^2 = +ikg. \tag{2.3}$$

The Schrödinger equation then assumes the form

$$\frac{d^2\varphi}{dz^2} + \{2h^2 \cosh 2z - (l+\tfrac{1}{2})^2\}\varphi = 0. \tag{2.4}$$

In the literature this equation is known as the modified Mathieu equation. We now develop a simple procedure for solving this equation for sufficiently small values of $|h^2|$ so that the expansions exist. First we make the additional substitution

$$\omega = 2h\cosh z, \tag{2.5}$$

so that (2.4) becomes

$$\frac{d^2\varphi}{d\omega^2} + \frac{1}{\omega}\frac{d\varphi}{d\omega} + \left\{1 - \frac{(l+\frac{1}{2})^2}{\omega^2}\right\}\varphi = \frac{2h^2}{\omega^2}\left\{\varphi + 2\frac{d^2\varphi}{d\omega^2}\right\}. \tag{2.6}$$

Next we define a parameter ν by the relation

$$\nu^2 = (l+\tfrac{1}{2})^2 - 2\Delta h^2. \tag{2.7}$$

Thus ν^2 is to be a parameter possessing a power series expansion in h^2 such that its zeroth-order approximation is $(l+\frac{1}{2})^2$. Alternatively, we may consider $(l+\frac{1}{2})^2$ as possessing a power series expansion in h^2 such that its zeroth-order approximation is ν^2. To zeroth order in h^2, (2.6) therefore becomes

$$D_\nu \varphi^{(0)} = 0, \tag{2.8}$$

where

$$D_\nu \equiv \frac{d^2}{d\omega^2} + \frac{1}{\omega}\frac{d}{d\omega} + \left\{1 - \frac{\nu^2}{\omega^2}\right\}. \tag{2.9}$$

But (2.8) is the well-known cylindrical equation; hence

$$\varphi^{(0)} = Z_\nu(\omega), \tag{2.10}$$

where Z_ν is a cylindrical function, e.g., J_ν, N_ν, $H_\nu^{(1)}$, $H_\nu^{(2)}$.

The zeroth-order approximation (2.10) leaves uncompensated on the right-hand side of (2.6) terms amounting to

$$R_\nu^{(0)} = 2h^2\left\{\frac{1}{\omega^2}Z_\nu + \frac{2}{\omega^2}\frac{d^2Z_\nu}{d\omega^2} + \frac{\Delta}{\omega^2}Z_\nu\right\}. \tag{2.11}$$

Using the recurrence relations for Bessel functions, i.e.,

$$\frac{\nu}{\omega}Z_\nu = \tfrac{1}{2}(Z_{\nu-1} + Z_{\nu+1}), \tag{2.12}$$

$$\frac{dZ_\nu}{d\omega} = -\frac{\nu}{\omega}Z_\nu + Z_{\nu-1} = \tfrac{1}{2}(Z_{\nu-1} - Z_{\nu+1}), \tag{2.13}$$

we may rewrite (2.11) as a linear combination of various Z_ν. However, it is very much more convenient to use these relations in order to rewrite (2.11) in terms of functions G_ν defined by

$$G_{\nu+\alpha} \equiv (\omega^2)^{-1}Z_{\nu+\alpha}. \tag{2.14}$$

The expression (2.11) is now particularly simple:

$$R_\nu^{(0)} = h^2(G_{\nu-2} + 2\Delta G_\nu + G_{\nu+2}). \tag{2.15}$$

Again for convenience it is now best to rewrite this expression as

$$R_\nu^{(0)} = h^2[(\nu,\nu-2)G_{\nu-2} + (\nu,\nu)G_\nu + (\nu,\nu+2)G_{\nu+2}] \tag{2.16}$$

where

$$(\nu,\nu\pm 2) = 1, \quad (\nu,\nu) = 2\Delta. \tag{2.17}$$

This apparent complication will pay rich dividends as will be seen later on.

We now observe that

$$D_\nu Z_\nu = 0, \quad D_{\nu+\alpha}Z_{\nu+\alpha} = 0,$$

but

$$D_{\nu+\alpha} = D_\nu - [\alpha(2\nu+\alpha)/\omega^2], \tag{2.18}$$

so that

$$D_\nu Z_{\nu+\alpha} = \frac{\alpha(2\nu+\alpha)}{\omega^2}Z_{\nu+\alpha} = \alpha(2\nu+\alpha)G_{\nu+\alpha}. \tag{2.19}$$

Thus a term $\mu G_{\nu+\alpha}$ on the right-hand side of (2.6) or—for instance—in (2.15) may be cancelled out by adding to $\varphi^{(0)}$ the new contribution $\mu Z_{\nu+\alpha}/\alpha(2\nu+\alpha)$ except, of course, when α or $2\nu+\alpha = 0$. We assume now (in the following) that $2\nu+\alpha \neq 0$; the case $2\nu+\alpha = 0$ will be considered separately at the end. The terms (2.15) therefore lead to first-order contribution

$$\varphi^{(1)} = h^2[(\nu,\nu-2)^*Z_{\nu-2} + (\nu,\nu+2)^*Z_{\nu+2}], \tag{2.20}$$

the starred coefficients being defined by

$$(\nu,\nu+\alpha)^* = (\nu,\nu+\alpha)/\alpha(2\nu+\alpha). \tag{2.21}$$

Now $\varphi^{(0)} = Z_\nu$ left uncompensated $R_\nu^{(0)}$; therefore, $\varphi^{(1)}$ leaves uncompensated

$$R_\nu^{(1)} = h^2[(\nu,\nu-2)^*R_{\nu-2}^{(0)} + (\nu,\nu+2)^*R_{\nu+2}^{(0)}]. \tag{2.22}$$

The next contribution therefore becomes

$$\begin{aligned}\varphi^{(2)} = h^4[&(\nu,\nu-2)^*(\nu-2,\nu-4)^*Z_{\nu-4}\\ &+ (\nu,\nu-2)^*(\nu-2,\nu-2)^*Z_{\nu-2}\\ &+ (\nu,\nu+2)^*(\nu+2,\nu+2)^*Z_{\nu+2}\\ &+ (\nu,\nu+2)^*(\nu+2,\nu+4)^*Z_{\nu+4}].\end{aligned} \tag{2.23}$$

Proceeding in this manner we obtain the solution (the terms in $R^{(0)}$, $R^{(1)}$, $\cdots$, left uncompensated so far will be considered below)

$$\begin{aligned}\varphi &= \varphi^{(0)} + \varphi^{(1)} + \varphi^{(2)} + \cdots\\ &= Z_\nu + \sum_{i=1}^{\infty} h^{2i} \sum_{\substack{j=-i\\ j\neq 0}}^{i} P_{2i}(2j)Z_{\nu+2j},\end{aligned} \tag{2.24}$$

where

$$\begin{aligned}&p_2(\pm 2) = (\nu,\nu\pm 2)^*,\\ &p_4(\pm 4) = (\nu,\nu\pm 2)^*(\nu\pm 2,\nu\pm 4)^*,\\ &p_4(\pm 2) = (\nu,\nu\pm 2)^*(\nu\pm\nu\pm 2)^*, \text{ etc.}\end{aligned} \tag{2.25}$$

These coefficients may also be obtained from the recurrence relation

$$\begin{aligned}p_{2i}(2j) = &\,p_{2i-2}(2j-2)\cdot(\nu+2j-2,\nu+2j)\\ &+ p_{2i-2}(2j)\cdot(\nu+2j,\nu+2j)\\ &+ p_{2i-2}(2j+2)\cdot(\nu+2j+2,\nu+2j),\end{aligned} \tag{2.26}$$

subject to the boundary conditions

$$\begin{aligned}&p_{2i}(2j) = 0 \quad \text{for } |j| > i, \quad p_0(0) = 1,\\ &p_0(2j\neq 0) = 0, \quad p_{2i\neq 0}(0) = 0.\end{aligned} \tag{2.27}$$

The relation (2.26) may be obtained either directly from (2.27), or by substituting (2.24) into (2.6).

Finally, we have to consider the terms in G_ν which were left unaccounted for in $R^{(0)}$, $R^{(1)}$, etc. Here we simply add all these terms and set the coefficient of $G_\nu = 0$. This gives the equation from which we can determine Δ and hence ν. Clearly,

$$\begin{aligned}0 = &\,h^2(\nu,\nu) + h^4[(\nu,\nu-2)^*(\nu-2,\nu) + (\nu,\nu+2)^*(\nu+2,\nu)]\\ &+ h^6[(\nu,\nu-2)^*(\nu-2,\nu-2)^*(\nu-2,\nu)\end{aligned}$$

$$+(\nu,\nu+2)^*(\nu+2,\nu+2)^*(\nu+2,\nu)]+\cdots. \tag{2.28}$$

Higher terms of this expansion may again be obtained in a manner analogous to that for the eigenvalues of the periodic Mathieu equation.[12] Evaluating the first five terms of (2.28), we obtain the expansion [cf. (2.7)]

$$(l+\tfrac{1}{2})^2=\nu^2+\frac{h^4}{2(\nu^2-1)}+\frac{(5\nu^2+7)h^8}{32(\nu^2-1)^3(\nu^2-4)}+\frac{(9\nu^4+58\nu^2+29)h^{12}}{64(\nu^2-1)^5(\nu^2-4)(\nu^2-9)}+O(h^{16}). \tag{2.29}$$

The expansion (2.29) is seen to be familiar from the theory of periodic Mathieu functions where $(l+\frac{1}{2})^2$ represents the eigenvalue. We now reverse (2.29) to calculate ν^2:

$$\nu^2=\alpha-\frac{h^4}{2(\alpha-1)}-\frac{(13\alpha-25)h^8}{32(\alpha-1)^3(\alpha-4)}-\frac{(45\alpha^3-455\alpha^2+1291\alpha-1169)h^{12}}{64(\alpha-1)^5(\alpha-4)^4(\alpha-9)}+O(h^{16}) \tag{2.30}$$

where

$$\alpha\equiv(l+\tfrac{1}{2})^2.$$

The solutions φ of the modified Mathieu equation are now completely determined—apart from a normalization factor which we have chosen (so far) such that the coefficient of $Z_{\nu+\alpha}$ in φ is 1 for $\alpha=0$.

We are still left with the question as to what will happen if [cf. (2.21)] $2\nu+\alpha=0$ or $\nu=\pm1,\pm2,\cdots$. We observe that the latter are precisely those values of for which successive terms of (2.29) become more and more divergent. On the other hand, we observe from (2.30) that—since h^2 is assumed to be moderately small—ν is approximately a half-integer (i.e., $l+\frac{1}{2}$ for l physical). Thus *physically* these conditions are unlikely. But *mathematically* they have a clear significance which we discuss later on.

For later purposes it is advantageous to derive yet another type of solutions. Substituting (2.7) into (2.4) we obtain

$$\frac{d^2\varphi}{dz^2}-\nu^2\varphi=2h^2(\Delta-\cosh2z)\varphi. \tag{2.31}$$

Thus to $O(0)$ in h we have

$$\varphi^{(0)}=\varphi_\nu=\cosh\nu z,\ \sinh\nu z,\quad\text{or } e^{\pm\nu z}, \tag{2.32}$$

so that

$$D_\nu\varphi_\nu=0,\quad D_\nu\equiv\frac{d^2}{dz^2}-\nu^2. \tag{2.33}$$

It follows that

$$D_{\nu+2n}\varphi_{\nu+2n}=0,\quad D_{\nu+2n}=D_\nu-4n(\nu+n), \tag{2.34}$$

so that

$$D_\nu\varphi_{\nu+2n}=4n(\nu+n)\varphi_{\nu+2n}. \tag{2.35}$$

Also since

$$\begin{aligned}2\cosh2z\cdot\cosh\nu z&=\cosh(\nu+2)z+\cosh(\nu-2)z,\\ 2\cosh2z\cdot\sinh\nu z&=\sinh(\nu+2)z+\sinh(\nu-2)z,\\ 2\cosh2z\cdot e^{\pm\nu z}&=\exp[\pm(\nu+2)z]+\exp[\pm(\nu-2)z],\end{aligned} \tag{2.36}$$

we may say that the first approximation $\varphi^{(0)}$ leaves uncompensated terms amounting to

$$\begin{aligned}R_\nu^{(0)}&=2h^2(\Delta-\cosh2z)\varphi_\nu\\ &=2h^2\Delta\varphi_\nu-h^2\{\varphi_{\nu+2}+\varphi_{\nu-2}\}\\ &=h^2[(\nu,\nu-2)\varphi_{\nu-2}+(\nu,\nu)\varphi_\nu+(\nu,\nu+2)\varphi_{\nu+2}],\end{aligned} \tag{2.37}$$

where

$$(\nu,\nu)=2\Delta,\quad(\nu,\nu\pm2)=-1. \tag{2.38}$$

The from of $R_\nu^{(0)}$ is seen to be almost identical with that of the corresponding expression for solutions in terms of Bessel functions. In fact, we could have got the same $R_\nu^{(0)}$ by starting with the modified Mathieu equation for h^2 replaced by $-h^2$. In order to avoid confusion arising from the use of different equations, we prefer to discuss one equation but different solutions. The use of the symbols $(\nu,\nu\pm2)$, etc. in the present context should not lead to confusion with the same symbols having a different meaning in the case of solutions in terms of Beseel functions since it is generally clear which type of solutions and hence coefficients is being discussed. Sometimes, however, we shall use subscripts B and h indicating that coefficients of solutions in terms of Bessel functions or hyperbolic functions are implied. Defining

$$(\nu,\nu+\alpha)^*=(\nu,\nu+\alpha)/\alpha(2\nu+\alpha), \tag{2.39}$$

we now obtain the solution

$$\varphi(z,h)=\varphi_\nu+\sum_{i=1}^{\infty}h^{2i}\sum_{\substack{j=-i\\ j\neq0}}^{i}\bar{p}_{2i}(2j)\varphi_{\nu+2j}, \tag{2.40}$$

where

$$\bar{p}_{2i}(\pm2)=(\nu,\nu\pm2)^*,\ \text{etc.}$$

We now compare this solution with our earlier solution (2.24) and examine the relationship between their coefficients $\bar{p}$, p. We have

$$\begin{aligned}\bar{p}_{2i}(2j)=&\bar{p}_{2i-2}(2j-2)\cdot(\nu+2j-2,\nu+2j)_h^*\\ &+\bar{p}_{2i-2}(2j)\cdot(\nu+2j,\nu+2j)_h^*\\ &+\bar{p}_{2i-2}(2j-2)\cdot(\nu+2j+2,\nu+2j)_h^*\\ =&-\bar{p}_{2i-2}(2j-2)\cdot(\nu+2j-2,\nu+2j)_B^*\\ &+\bar{p}_{2i-2}(2j)\cdot(\nu+2j,\nu+2j)_B^*\\ &-\bar{p}_{2i-2}(2j+2)\cdot(\nu+2j+2,\nu+2j)_B^*,\end{aligned}$$

so that

$$\begin{aligned}(-1)^j\bar{p}_{2i}(2j)=&(-1)^{j-1}\cdot\bar{p}_{2i-2}(2j-2)(\nu+2j-2,\nu+2j)_B^*\\ &+(-1)^j\bar{p}_{2i-2}(2j)\cdot(\nu+2j,\nu+2j)_B^*\\ &+(-1)^{j-1}\bar{p}_{2i-2}(2j+2)\cdot(\nu+2j+2,\nu+2j)_B^*.\end{aligned}$$

Thus

$$p_{2i}(2j)\equiv(-1)^j\bar{p}_{2i}(2j) \tag{2.41}$$

satisfies the equation

$$\begin{aligned}p_{2i}(2j)=&p_{2i-2}(2j-2)\cdot(\nu+2j-2,\nu+2j)_B^*\\ =&p_{2i-2}(2j)\cdot(\nu+2j,\nu+2j)_B^*\\ =&p_{2i-2}(2j+2)\cdot(\nu+2j+2,\nu+2j)_B^*,\end{aligned}$$

and the hyperbolic solution becomes

$$\varphi(z,h)=\varphi_\nu+\sum_{i=1}^{\infty}h^{2i}\sum_{\substack{j=-i\\ j\neq 0}}^{i}p_{2i}(2j)(-1)^j\varphi_{\nu+2j} \tag{2.42}$$

or

$$\varphi(z,h)=\bar{\varphi}_\nu+\sum_{i=1}^{\infty}h^{2i}\sum_{\substack{j=-i\\ j\neq 0}}^{i}p_{2i}(2j)\bar{\varphi}_{\nu+2j}, \tag{2.43}$$

where

$$\bar{\varphi}_{\nu+2j}\equiv(-1)^j\varphi_{\nu+2j}. \tag{2.44}$$

One can easily convince oneself [by looking at (2.28) and observing that $(\nu,\nu\pm 2)^*_B=-(\nu,\nu\pm 2)^*_h$] that the expansion (2.29) follows again from the necessary subsidiary condition. The solutions φ for $\varphi_\nu=\cosh\nu z$, $\sinh\nu z$ are generally[9] denoted by $Ce_\nu(z,h)$, $Se_\nu(z,h)$.

We now consider the following solutions (in the notation of MS)

$$\varphi(z,h)=\exp(\nu z)+\sum_{i=1}^{\infty}h^{2i}\sum_{\substack{j=-i\\ j\neq 0}}^{i}p_{2i}(2j)(-1)^j\exp[(\nu+2j)z]$$

$$\equiv Me_\nu(z,h) \tag{2.45}$$

$$[Me_{\pm\nu}=(Ce_\nu\pm Se_\nu)],$$

$$\varphi(z,h)=J_\nu(2h\cosh z)+\sum_{i=1}^{\infty}h^{2i}\sum_{\substack{j=-i\\ j\neq 0}}^{i}p_{2i}(2j)J_{\nu+2j}(2h\cosh z)$$

$$\equiv M_\nu^{(1)}(z,h) \tag{2.46}$$

Clearly,

$$Me_\nu(z+n\pi i,h)=\exp(\nu n\pi i)Me_\nu(z,h). \tag{2.47}$$

Also, since

$$J_\nu(2h\cosh(z+n\pi i))=J_\nu(2h\cosh z\cdot\exp(in\pi))$$

$$=\exp(in\nu\pi)J_\nu(2h\cosh z), \tag{2.48}$$

we have

$$M_\nu^{(1)}(z+n\pi i,h)=\exp(in\nu\pi)M_\nu^{(1)}(z,h). \tag{2.49}$$

$Me_\nu(z)$, $M_\nu^{(1)}(z)$ are therefore proportional to each other:

$$Me_\nu(z,h)=\alpha_\nu(h)M_\nu^{(1)}(z,k), \tag{2.50}$$

where clearly

$$\alpha_\nu(h^*)=Me_\nu(0,h)/M_\nu^{(1)}(0,h).$$

We define solutions $M_\nu(j)(z,h)$ for $j=2,3,4$ by $Z_\nu=N_\nu,H_\nu^{(1)},H_\nu^{(2)}$, respectively. Then, by using analogous properties of Bessel functions, we have

$$M_{-\nu}^{(3,4)}=\exp(\pm i\pi\nu)M_\nu^{(3,4)},\ M_\nu^{(3,4)}=M_\nu^{(1)}\pm iM_\nu^{(2)},$$

and thence (for ν nonintegral)

$$\pm i\sin\nu\pi\cdot M_\nu^{(3,4)}(z,h)=M_{-\nu}^{(1)}(z,h)-\exp(\mp i\nu\pi)M_\nu^{(1)}(z,h). \tag{2.51}$$

We still have to deal with the case $2\nu+\alpha=0$ or $\nu=\pm 1,\pm 2,\cdots$. As an example we discuss the case $\nu=+1$, choosing the zero-order solution $\varphi_\nu=\cosh\nu z$. Proceeding as before we have

$$R^{(0)}=2h^2(\Delta-\cosh 2z)\varphi_\nu=h^2[-\varphi_{-1}+2\Delta\varphi_1-\varphi_3]. \tag{2.52}$$

This is the part left uncompensated by the zero-order approximation in h^2. We observe immediately that—since $\varphi_{-1}=\varphi_1$—we now have a completely different situation. Thus

$$R^{(0)}=h^2[(2\Delta-1)\varphi_1-\varphi_3],$$

so that

$$\varphi^{(1)}=-\frac{h^2\varphi_3}{8}=-h^2\frac{\varphi_3}{8}=-h^2\frac{\varphi_{\nu+2n}}{4n(\nu+n)}\bigg|_{\nu,n=1}, \tag{2.53}$$

This contribution leaves uncompensated the terms

$$R^{(1)}=-\frac{h^2}{8}\cdot 2h^2(\Delta-\cosh 2z)\varphi_3=-\frac{h^4}{4}(\Delta\varphi_3-\tfrac{1}{2}\varphi_5-\tfrac{1}{2}\varphi_1), \tag{2.54}$$

so that

$$\varphi^{(2)}=-\frac{h^4}{4}\left[\frac{\Delta\varphi_3}{8}-\frac{\varphi_5}{48}\right]. \tag{2.55}$$

Proceeding in this manner we obtain the complete solution. Δ then follows by equating to zero the sum of coefficients of φ_1 in $R^{(0)},R^{(1)},\cdots$. It then follows that

$$(l+\tfrac{1}{2})^2=1+h^2-\frac{h^4}{8}-\frac{h^6}{64}-\cdots, \tag{2.56}$$

in agreement with formulas (36) of MS (p. 120).

If we choose instead of the above zero-order solution

$$\varphi_\nu=\sinh\nu z,\quad \nu=1,$$

we have

$$h^{(0)}=2h^2(\Delta-\cosh 2z)\sinh z=h^2[(2\Delta+1)\varphi_1-\varphi_3] \tag{2.57}$$

and again obtain the above eigenvalue expansion with h^2 replaced by $-h^2$. This applies to all odd-ν eigenvalue expansions and is a direct consequence of the relations

$$Ce_{2n+1}(z,-h^2)=(-1)^n(-i)Se_{2n+1}(z+i\pi/2,h^2),$$

$$Se_{2n+1}(z,-h^2)=(-1)^n(-i)Ce_{2n+1}(z+i\pi/2,h^2), \tag{2.58}$$

which are easily verified. For even values of ν the eigenvalues have to be recalculated separately in each case, since now

$$Ce_{2n}(z,-h^2)=(-1)^nCe_{2n}(z+i\pi/2,h^2)$$

$$Se_{2n+2}(z,-h^2)=-(-1)^nSe_{2n+2}(z+i\pi/2,h^2); \tag{2.59}$$

thus the symmetry between Ce, Se is destroyed. Explicit expansions for any of these cases may be found in the standard literature. Meixner and Schäfke also determine their regions of convergence.

Of course, we could also have started with a solution in terms of Bessel functions and used, for instance, the relation $J_{-n}=(-1)^nJ_n$ to derive corresponding eigenvalue expansions. In fact, one can show (cf. MS, pp. 200, 205) that for $m=0,1,2,\cdots$ $M_m^{(1)}(z,h)$ is proportional to $Ce_m(z,h^2)$ and similar relations hold for other functions. For rigorous convergence and validity discussions of any of the solutions discussed in this section we again refer to MS.

3. CALCULATION OF THE S MATRIX

We now proceed in the manner of Spector[3] to calculate the scattering matrix for the potential $1/r^4$. For this

purpose we seek first the regular solution of the radial Schrödinger equation at the origin, and then its analytic continuation to infinity.

We obtain the regular solution by choosing $Z_\nu(\omega) = H_\nu^{(1)}(\omega)$ for $\mathrm{Re}(z) < 0$. Then

$$Y_{\mathrm{reg}} = r^{1/2} M_\nu^{(3)}(z,h) = r^{1/2}\left(H_\nu^{(1)}(\omega) + \sum_{i=1}^{\infty} h^{2i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} \times p_{2i}(2j) H_{\nu+2j}^{(1)}(\omega)\right), \tag{3.1}$$

where by (2.5), (2.3)

$$\omega = 2h\cosh z = (kr + ig/r). \tag{3.2}$$

Thus $r \to 0$ implies $|\omega| \to \infty$. The asymptotic behavior of the Hankel functions $H^{(1,2)}(\omega)$ for $|\omega| \gg |\nu|$, $|\omega| \gg 1$, and $-\pi < \arg\omega < \pi$ is known to be given by

$$H_\nu^{(1,2)}(\omega) = \left(\frac{2}{\pi\omega}\right)^{1/2} \exp \pm i\left(\omega - \frac{\nu\pi}{2} - \frac{\pi}{4}\right) \left[1 + O\left(\frac{1}{\omega}\right)\right]. \tag{3.3}$$

The behavior of Y_{reg} near $r \approx 0$ is then found to be

$$Y_{\mathrm{reg}} \approx \left(\frac{2}{\pi g}\right)^{1/2} \exp(-g/r)\left(\exp[-i(\nu+1)\pi/2] + \sum_{i=1}^{\infty} h^{2i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} p_{2i}(2j) \exp[-(\pi/2)i(\nu+2j+1)]\right) \tag{3.4}$$

which tends to zero with r.

In a similar manner we may define solutions $Y^{(3,4)}$ by setting for $\mathrm{Re}(z) > 0$

$$Y^{(3,4)} = r^{1/2} M_\nu^{(3,4)}(z,h) = r^{1/2}\left(H_\nu^{(1,2)}(\omega) + \sum_{i=1}^{\infty} h^{2i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} p_{2i}(2j) H_{\nu+2j}^{(1,2)}(\omega)\right). \tag{3.5}$$

Using the above asymptotic expressions for the Hankel functions these solutions are found to have the required asymptotic behavior for $r \to \infty$:

$$Y^{(3,4)} \approx \left(\frac{2}{\pi k}\right)^{1/2} \exp(\pm ikr) \exp[\mp(i\pi/2)(\nu + \tfrac{1}{2})] \times \left[1 + \sum_{i=1}^{\infty} h^{2i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} p_{2i}(2j) \exp(\mp i\pi j)\right]. \tag{3.6}$$

In fact, we can derive $Y^{(4)}$ from $Y^{(3)}$ since one can show from the circuit relations of Hankel functions that

$$M_\nu^{(3)}(z + \pi i, h) = -\exp(-i\pi\nu) M_\nu^{(4)}(z,h).$$

We now require the analytic continuation of the regular solution to solutions behaving like $Y^{(3,4)}$ at infinity. From the relation $r = (ig/h)e^z$ we see that $r = 0$ corresponds to $\mathrm{Re}(z) \to -\infty$, and $r \to \infty$ to $\mathrm{Re}(z) \to +\infty$. We require, therefore, the continuation of $M_\nu^{(3)}$ through the whole range of $\mathrm{Re}(z)$.

Now the series $M_\nu^{(j)}$ can be shown (MS, p. 178) to be convergent for $|\cosh z| \geq 1$ but uniformly convergent only when $|\cosh z| > 1$ for otherwise complex values of z. Since $z = \ln\sqrt{k/g}\, r \mp i\pi/4$, the condition $|\cosh z| > 1$ implies

$$\sqrt{k/g}\, r > (2+\sqrt{3})^{1/2} > 1 \quad \text{and} \quad \sqrt{k/g}\, r < (2-\sqrt{3})^{1/2} < 1. \tag{3.7}$$

Thus there is a gap between the two regions of validity which has to be bridged by using another set of solutions. A suitable set is the pair of fundamental solutions $Me_{\pm\nu}$ defined by (2.45). These solutions converge uniformly for all finite complex values of z (MS, p. 130). Before we proceed with the actual matching we have to decide which Riemann sheet we want to choose, since $\sqrt{i}$ leads to a double-valuedness of the variable z. We shall choose the upper sign, i.e.,

$$Z = \ln\sqrt{k/g}\, r - i\pi/4. \tag{3.8}$$

We note that if we replace z by $-z$ in ω, kr is replaced by ig/r and vice versa. Thus if we let $\mathrm{Re}(z) \to -\infty$ in Y_{reg} (i.e., $r \to 0$) and then replace z by $-z$, the solution has the asymptotic behavior of $Y^{(3)}$, i.e., $\exp(ikr)$. To obtain the continuation of Y_{reg} to this solution, we consider the variables z, $-z$ and choose the sheet with $\mathrm{Re}(z) > 0$. Then by (3.7) we have to choose

$$z = -\ln\sqrt{k/g}\, r + i\pi/4 \quad \text{for } \sqrt{k/g}\, r < (2-\sqrt{3})^{1/2}$$

and

$$z = +\ln\sqrt{k/g}\, r - i\pi/4 \quad \text{for } \sqrt{k/g}\, r > (2+\sqrt{3})^{1/2}. \tag{3.9}$$

We may write therefore for $0 < \sqrt{k/g}\, r < (2-\sqrt{3})^{1/2}$

$$r^{1/2} M_\nu^{(3)}(r) = r^{1/2}(\alpha Me_\nu(r) + \beta Me_{-\nu}(r)),$$

$$\frac{d}{dr}[r^{1/2} M_\nu^{(3)}(r)] = \alpha\frac{d}{dr}[r^{1/2} Me_\nu(r)] + \beta\frac{d}{dr}[r^{1/2} Me_{-\nu}(r)], \tag{3.10}$$

and determine α and β. The right-hand side now represents the solution $M_\nu^{(3)}$ as continued to the right of $\sqrt{k/g}\, r = (2-\sqrt{3})^{1/2}$. In the region $(2+\sqrt{3})^{1/2} < \sqrt{k/g}\, r < \infty$ we require a solution of the form $r^{1/2}[AM_\nu^{(3)} + B_\nu^{(4)}]$, $A, B \neq 0$. This solution may be continued into the region below $\sqrt{k/g}\, r = (2+\sqrt{3})^{1/2}$ by writing

$$r^{1/2}[\alpha' Me_\nu(r) + \beta' Me_\nu(r)] = r^{1/2}[AM_\nu^{(3)}(r) + BM_\nu^{(4)}(r)],$$

$$\alpha'\frac{d}{dr} r^{1/2} Me_\nu(r) + \beta'\frac{d}{dr} r^{1/2} Me_{-\nu}(r) = A\frac{d}{dr} r^{1/2} M_\nu^{(3)}(r) + B\frac{d}{dr} r^{1/2} M_\nu^{(4)}(r). \tag{3.11}$$

We next have to join the branches

$$r^{1/2}[\alpha Me_\nu(r) + \beta Me_{-\nu}(r)] (z = -\ln\sqrt{k/g}\, r + i\pi/4),$$

$$r^{1/2}[\alpha' Me_\nu(r) + \beta' Me_{-\nu}(r)] (z = +\ln\sqrt{k/g}\, r - i\pi/4).$$

At $\mathrm{Re}(z) = 0$, $r = \sqrt{k/g}$. Then

$$r^{1/2}[\alpha Me_\nu(r) + \beta Me_{-\nu}(r)]_{z=i\pi/4} = r^{1/2}[\alpha' Me_\nu(r) + \beta' Me_{-\nu}(r)]_{z=-i\pi/4},$$

$$\left[\alpha\frac{d}{dr} r^{1/2} Me_\nu(r) + \beta\frac{d}{dr} r^{1/2} Me_{-\nu}(r)\right]_{z=i\pi/4} = \left[\alpha'\frac{d}{dr} r^{1/2} Me_\nu(r) + \beta'\frac{d}{dr} r^{1/2} Me_{-\nu}(r)\right]_{z=-i\pi/4}. \tag{3.12}$$

But since $Me_\nu(z) = Me_{-\nu}(-z)$ (MS, p. 131) these relations may be reexpressed for one and the same point $z = -i\pi/4$:

$$\alpha Me_{-\nu} + \beta Me_\nu = \alpha' Me_\nu + \beta' Me_\nu,$$

$$\alpha\frac{d}{dz} Me_{-\nu} + \beta\frac{d}{dz} Me_\nu = \alpha'\frac{d}{dz} Me_\nu + \beta'\frac{d}{dz} Me_{-\nu}, \tag{3.13}$$

where we have used the fact that for $r = \sqrt{g/k}$

$$\frac{d}{dr} = \mp\left(\frac{k}{g}\right)^{1/2}\frac{d}{dz} \quad \text{at } z = \pm i\pi/4.$$

One now derives readily

$$\alpha' = \beta, \quad \beta' = \alpha, \quad d \equiv W[Me_{-\nu}, Me_{\nu}]W(M_{\nu}^{(3)}, M_{\nu}^{(4)}],$$
$$dA = W[M_{\nu}^{(3)}, Me_{\nu}]W[Me_{\nu}, M_{\nu}^{(4)}] - W[M_{\nu}^{(3)}, Me_{-\nu}]\,W[Me_{-\nu}, M_{\nu}^{(4)}],$$
$$dB = W[M_{\nu}^{(3)}, Me_{-\nu}]W[Me_{-\nu}, M_{\nu}^{(3)}] = -\,W[M_{\nu}^{(3)}, Me_{\nu}]W[Me_{\nu}, M_{\nu}^{(3)}]. \tag{3.14}$$

Using the relation (2.50) the Wronskians (MS, p. 171)

$$[1,3] = -[1,4] = 2i/\pi, \quad [3,4] = -4i/\pi, \tag{3.15}$$

and the relations (2.51), we find [with $Me_{\nu}(0,h) = Me_{-\nu}(0,h)$],

$$A = \frac{R^2-1}{2iR\sin\nu\pi}, \quad B = \frac{R^2 - e^{-2i\nu\pi}}{2iR\sin\nu\pi}, \tag{3.16}$$

where

$$R = \alpha_{\nu}/\alpha_{-\nu} = M_{-\nu}^{(1)}(0,h)/M_{\nu}^{(1)}(0,h). \tag{3.17}$$

The asymptotic behavior of the regular solution is therefore given by

$$Y_{\text{reg}} = r^{1/2}[AM_{\nu}^{(3)}(r) + BM_{\nu}^{(4)}(r)]$$
$$\approx \left(\frac{2}{\pi k}\right)^{1/2}\left\{\frac{R^2-1}{2iR\sin\nu\pi}\exp[-i\pi/2(\nu+\tfrac{1}{2})]\exp(ikr)\right.$$
$$\left. + \frac{R^2 - \exp(-2i\nu\pi)}{2iR\sin\nu\pi}\exp\left[\left(\frac{i\pi}{2}\right)(\nu+\tfrac{1}{2}) - 2ikr\right]\right\}\cdot[1+O(h^2)]. \tag{3.18}$$

Defining "Jost function equivalents" $f(\pm k, l)$ by

$$+\frac{i}{\sqrt{k}}\,Y_{\text{reg}} \approx \frac{\exp(-i\pi\nu/2)}{2ik}[f(k,l)\exp(ikr) - f(-k,l)\exp(-ikr)] \tag{3.19}$$

(since Jost functions in the sense of regular potentials do not exist for singular potentials), we find by comparison

$$f(k,l) = \left(\frac{2}{\pi}\right)^{1/2}\frac{R^2-1}{R\sin\nu\pi}\exp[-i\pi/2(\nu-\tfrac{1}{2})]\exp[(i\pi/2)\nu],$$
$$f(-k,l) = \left(\frac{2}{\pi}\right)^{1/2}\frac{R^2-\exp(-2i\nu\pi)}{R\sin\nu\pi}\exp\,i\frac{\pi}{2}(\nu-\tfrac{1}{2})\;\exp\left(i\frac{\pi}{2}\right)\nu \tag{3.20}$$

The S matrix then becomes

$$S = \exp(2i\delta) = \exp(i\pi l)\frac{f(k,l)}{f(-k,l)} = \frac{R^2-1}{R^2-\exp(-2i\nu\pi)}$$
$$\times\exp[-i\pi(\nu-l-\tfrac{1}{2})]. \tag{3.21}$$

Of course, it would have sufficed to calculate just the ratio A/B, but for a discussion of Regge poles, it is essential to have the numerators and denominators separately.

We now note that the S matrix is unitary. To show this, we use the relation (Aly *et al.*[3])

$$R^* = R\exp(i\nu\pi), \tag{3.22}$$

where the asterisk on R as on S in $S^*S = 1$ indicates complex conjugation of the functional form of R or S together with the replacement $k \to -k$, the latter being equivalent to the interchange $h \to -ih$. Of course l is assumed to have real integral (i.e., physical) values, and ν is real by (2.30). Hence

$$f^*(k,l) = f(-k,l).$$

Next we observe that the S-matrix may be reexpressed in another important form first given by Bertocchi *et al.*[5] To derive this, we require the following relation between modified Mathieu functions and their derivatives:

$$\frac{M_{\nu}^{(1)\prime}(0)}{M_{-\nu}^{(1)\prime}(0)} = -\frac{M_{\nu}^{(1)}(0)}{M_{-\nu}^{(1)}(0)}. \tag{3.23}$$

To prove this relation, we recall the following relations:

$$M_{\nu}^{(1)}(z) = M_{\nu}^{(1)}(0)Me_{\nu}(z)/Me_{\nu}(0), \tag{2.50'}$$
$$\frac{Me_{\nu}'(0)}{Me_{-\nu}'(0)} = \frac{Ce_{\nu}'(0)+Se_{\nu}'(0)}{Ce_{\nu}'(0)-Se_{\nu}'(0)} = -1 (\sin Ce_{\nu}'(0) = 0) \tag{3.24}$$

by (2.45). Then (3.23) follows immediately. It is now a simple matter—again using the circuit relations for modified Mathieu functions, i.e., (2.51)—to derive the following formulas:

$$R - \exp(\mp i\nu\pi) = \pm i\sin\nu\pi M_{\nu}^{(3,4)}(0)/M_{\nu}^{(1)}(0),$$
$$R + \exp(\mp i\nu\pi) = \mp i\sin\nu\pi M_{\nu}^{(3,4)\prime}(0)/M_{\nu}^{(1)\prime}(0). \tag{3.25}$$

It then follows that

$$S = \left(\frac{d}{dz}[M_{\nu}^{(3)}(z)M_{\nu}^{(4)}(z)]_{z=0}\Big/\frac{d}{dz}[M_{\nu}^{(3)}(z)M_{\nu}^{(3)}(z)]_{z=0}\right)$$
$$\times\exp[-i\pi(\nu-l+\tfrac{1}{2})]. \tag{3.26}$$

To clear up the relation between the derivation of S as given above and another method used in the literature,[5] we now rederive this form of the S matrix by the latter method. This is *not* a triviality, since the plurality of modified Mathieu functions and their properties can easily lead to considerable confusion. Moreover, it is extremely instructive to understand this connection for dealing with potentials $1/r^m$, $3 < m \neq 0$.

Our regular solution is again $Y_{\text{reg}} = r^{1/2}M_{\nu}^{(3)}(z,h) \equiv r^{1/2}\varphi_{\text{reg}}(z,h)$. Further, since the modified Mathieu equation is invariant under the interchanges (a) $z \to -z$, $h \to -h$ (invariant point $z = 0$) and (b) $z \to -z - i\pi/2$, $h \to \pm ih$ (invariant point $z = -i\pi/4$), we may define—using (a)—two solutions $\varphi_{\pm}(z,h)$ by

$$\varphi_{\pm}(z,h) = M_{\nu}^{(3)}(-z, \pm h). \tag{3.27}$$

We note that (by the circuit relation for Hankel functions)

$$\varphi_{-}(z,h) = -\exp(-i\pi\nu)M_{\nu}^{(4)}(z,h). \tag{3.28}$$

$r^{1/2}\varphi_{\pm}$ are therefore solutions possessing the large $-r$ asymptotic behavior of Jost solutions, i.e., $\exp(\pm ikr)$. The S matrix then follows by setting

$$\varphi_{\text{reg}}(z,h) = A\varphi_{+}(z,h) + B\varphi_{-}(z,h) \tag{3.29}$$

and requiring continuity at the invariant point $z = 0$. One readily finds

$$\frac{A}{B} = \left(\frac{d}{dz}[M_{\nu}^{(3)}(z)M_{\nu}^{(4)}(z)]_{z=0}\Big/\frac{d}{dz}[M_{\nu}^{(3)}(z)M_{\nu}^{(3)}(z)]_{z=0}\right)\exp(-i\pi\nu). \tag{3.30}$$

The S matrix $S=\exp(2i\delta)$ being defined by the limiting behavior

$$Y_{\text{reg}} \approx C \sin(kr - l\pi/2 + \delta), \quad C \text{ const},$$

is then again found to be given by (3.26).

On the other hand, if we choose the interchange (b) (invariant point $z=-i\pi/4$), we define the solutions $\varphi_{\mp}(z,h)$ by

$$\varphi_{\mp}(z,h) = M_{\nu}^{(3)}(-z - \tfrac{1}{2}i\pi, \pm ih). \tag{3.31}$$

The asymptotic behavior of these solutions for large r is

$$\begin{aligned} Y_{\mp} &= r^{1/2}\varphi_{\mp} \\ &\approx \sqrt{2/\mp\pi k}\, \exp(\mp ikr)\exp[-i\pi/2(\nu+\tfrac{1}{2})] \\ &\quad \times\left[1+\sum_{i=1}^{\infty}(-h^2)^i \cdot \sum_{\substack{j=-i \\ j\neq 0}}^{i} p_{2i}(2j)\exp(i\pi j)\right]. \end{aligned} \tag{3.32}$$

Proceeding as before, and demanding continuity at the invariant point $z=-i\pi/4$, we now have

$$\begin{aligned} S &= \exp(2i\delta) \\ &= \left(\frac{d}{dz}[M_{\nu}^{(3)}(z,h)M_{\nu}^{(3)}(z,ih)]_{z=-i\pi/4} \Big/ \right. \\ &\quad \left. \frac{d}{dz}[M_{\nu}^{(3)}(z,h)M_{\nu}^{(3)}(z,-ih)]_{z=-i\pi/4}\right)\exp(i\pi/l - \tfrac{1}{2}), \end{aligned}$$

which is the expression we have used before.[5]

Here we have calculated S only in terms of small $-h$, i.e., low-energy expansions. The equivalent high-energy derivation has been discussed elsewhere.[6]

4. REGGE POLES

In order to determine the Regge poles and their behavior with varying energy, we next have to investigate the zeros of the Jost function equivalent $f(-k,1)$. These are given by

$$\begin{aligned} 0 &= \frac{R^2 - \exp(-2i\pi\nu)}{R\sin\nu\pi}\exp(i\pi\nu) \\ &= \exp(i\pi\nu)\frac{\sin\nu\pi \cdot M_{\nu}^{(3)}(0,h)M_{\nu}^{(3)\prime}(0,h)}{M_{\nu}^{(1)\prime}(0,h)M_{-\nu}^{(1)}(0,h)}. \end{aligned} \tag{4.1}$$

Clearly $\nu=n$, $n=0,\pm1,\pm2,\cdots$ are zeros of $f(-k,1)$. However, they are "phoney" zeros or indeterminacy points, being also zeros of $f(k,1)$ as a glance at (3.26) shows. We next determine the zeros of $M_{\nu}^{(3)}(0,h)$. The zeros of $M_{\nu}^{(3)\prime}(0,h)$ can be determined in a similar manner and will not be considered here. We also assume that the zeros of the functions in the numerator do not coincide with those of the denominator—which is plausible for small h^2 since J_{ν}, $H_{\nu}^{(1)}$, etc., have different zeros. Thus we consider

$$\begin{aligned} 0 &= M_{\nu}^{(3)}(0,h) \\ &= H_{\nu}^{(1)}(\omega) + \sum_{i=1}^{\infty} h^{2i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} p_{2i}(2j,\nu)H_{\nu+2j}^{(1)}(\omega), \end{aligned} \tag{4.2}$$

where $\omega = 2h\cosh z = 2h$. It is clear that as $h^2 \to 0$ the zeros of $M_{\nu}^{(3)}$ approach those of $H_{\nu}^{(1)}$. Let ω_n, $n=1,2,\cdots$ be the positive zeros of $H^{(1)}(\omega)$ or, alternatively, those values of ω which correspond to zeros $\nu=\nu_n$ of $H^{(1)}$ in the ν plane. Then these are also zeros of $M_{\nu}^{(3)}(z,0)$. In view of their analyticity in h^2, we may write for the nth zero

$$2h = \omega = \omega_n + \sum_{j=1}^{\infty}\alpha_j^{(n)}h^{2j}. \tag{4.3}$$

The coefficients $\alpha_j^{(n)}$ may be determined by substituting the expansion into (4.2), expanding around $\omega=\omega_h$, and equating coefficients of the same power of h^2. Particular care is necessary with our coefficients $p_{2i}(2j,\nu)$, since a factor $(\nu+2,\nu+2)$, for instance, contains Δ which is proportional to h^2. Since $H^{(1)}(\omega_i)=0$, we obtain

$$\begin{aligned} 0 &= \alpha_1^{(n)}\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n} + p_2(\nu,2)H_{\nu+2}^{(1)}(\omega_n) + p_2(\nu,-2)H_{\nu-2}^{(1)}(\omega_n), \\ 0 &= \alpha_2^{(n)}\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n} + \frac{\alpha_1^{(n)}}{2}\frac{d^2H_{\nu}^{(1)}}{d\omega^2}\bigg|_{\omega_n} + p_2(\nu,2)\alpha_1^{(n)}\frac{dH_{\nu+2}^{(1)}}{d\omega}\bigg|_{\omega_n} \\ &\quad + p_2(\nu,-2)\alpha_1^{(n)}\frac{dH_{\nu-2}^{(1)}}{d\omega}\bigg|_{\omega_n} + p_4(\nu,4)H_{\nu+4}^{(1)}(\omega_n) \\ &\quad + p_4(\nu,-4)H_{\nu-4}^{(1)}(\omega_n). \end{aligned} \tag{4.4}$$

[Note: Terms $p_4(\nu,\pm2)H_{\nu\pm2}^{(1)}$ contain by (2.25) a factor $(\nu\pm2,\nu\pm2)$ which is 2Δ by (2.17) and is therefore proportional to h^2; these terms therefore belong into the next equation.] With the help of the recurrence relations (2.12), (2.13) one can show that the following relations hold at the zero point $\omega_{i=n}$ of $H^{(1)}(\omega)$:

$$\begin{aligned} H_{\nu-1}^{(1)}(\omega_n) &= -H_{\nu+1}^{(1)}(\omega_n) = \frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n}, \\ H_{\nu+2}^{(1)}(\omega_n) &= -\frac{2(\nu+1)}{\omega_n}\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n}, \\ H_{\nu-2}^{(1)}(\omega_n) &= \frac{2(\nu-1)}{\omega_n}\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n}, \\ H_{\nu\pm4}^{(1)}(\omega_n) &= \pm\frac{4}{\omega_n}\left\{(\nu\pm2) - \frac{2(\nu\pm1)(\nu\pm2)(\nu\pm3)}{\omega_n^2}\right\}\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n}, \\ \frac{d^2H_{\nu}^{(1)}}{d\omega^2}\bigg|_{\omega_n} &= -\frac{1}{\omega_n}\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n}, \\ \frac{dH_{\nu\pm2}^{(1)}}{d\omega}\bigg|_{\omega_n} &= \left(-1 + \frac{2(\nu\pm1)(\nu\pm2)}{\omega_n^2}\right)\frac{dH_{\nu}^{(1)}}{d\omega}\bigg|_{\omega_n}. \end{aligned} \tag{4.5}$$

Substituting these expressions into (4.4), we see that all factors $(dH_{\nu}^{(1)}/d\omega)|_{\omega_n}$ cancel out, and we obtain

$$\begin{aligned} 0 &= \alpha_1^{(n)} - 1/\omega_n, \\ 0 &= \alpha_2^{(n)} - \frac{(\alpha_1^{(n)})^2}{2\omega_n} - \frac{1}{4\omega_n}\left(\frac{1}{\nu^2-1} + \frac{6}{\omega_n^2}\right) + \alpha_1^{(n)}\left(\frac{2}{\omega_n^2} + \frac{1}{2(\nu^2-1)}\right). \end{aligned}$$

We thus have for (4.3)

$$2h = \omega_n + \frac{h^2}{\omega_n} - \frac{h^4}{4(\nu^2-1)\omega_n} + O(h^6). \tag{4.6}$$

Hence

$$\omega_n = h \pm \frac{h^2}{2\sqrt{\nu^2-1}} + O(h^3). \tag{4.7}$$

The zeros $\omega=\omega_n$ of the Hankel function $H_{\nu}^{(1)}$ may be determined in the manner of Keller *et al.*[15] or Magnus and Kotin.[16] We start from the relation

$$i\sin\nu\pi H_{\nu}^{(1)}(\omega) = J_{-\nu}(\omega) - J_{\nu}(\omega)\exp(-i\nu\pi) \tag{4.8}$$

and substitute for the Bessel functions the power series

$$J_\nu(\omega)=\sum_{m=0}^{\infty}(-1)^m\left(\frac{\omega}{2}\right)^{\nu+2m}\frac{1}{m!\,\Gamma(\nu+m+1)}. \tag{4.9}$$

We then have for

$$0<|\omega|\ll 1 \quad (\text{or } |\nu|\gg 1+|\omega|^2),$$

$$\omega\equiv\omega_n,\quad H_\nu^{(1)}(\omega_n)=0,$$

$$\left(\frac{\omega}{2}\right)^{2\nu}\exp(-i\nu\pi)\left(1+\sum_{m=1}^{\infty}(-1)^m\left(\frac{\omega}{2}\right)^{2m}\frac{\Gamma(\nu+1)}{m!\,\Gamma(\nu+m+1)}\right)$$

$$=\frac{\Gamma(\nu+1)}{\Gamma(-\nu+1)}\left(1+\sum_{m=1}^{\infty}(-1)^m\left(\frac{\omega}{2}\right)^{2m}\frac{\Gamma(-\nu+1)}{m!\,\Gamma(-\nu+m+1)}\right). \tag{4.10}$$

Taking the logarithm of both sides, this becomes for $\omega/2=r\exp(i\varphi)$

$$2\nu\left(\ln\frac{\omega}{2}-i\frac{\pi}{2}\right)+2\pi in-\ln\frac{\Gamma(\nu+1)}{\Gamma(-\nu+1)}$$

$$=\frac{2(\omega/2)^2}{(1-\nu^2)}-\frac{2\nu(2\nu^2+1)(\omega/2)^4}{(1-\nu^2)^2(4-\nu^2)}+O(\omega^6). \tag{4.11}$$

Here n is an integer $\neq 0$. We now use the following series for the logarithm of gamma functions:

$$\ln\frac{\Gamma(\nu+1)}{\Gamma(-\nu+1)}=2\gamma_\nu-2\sum_{m=1}^{\infty}\frac{\zeta(2m+1)}{2m+1}\nu^{2m+1},\quad |\nu|\ll 1, \tag{4.12}$$

where γ is Euler's constant and ζ is the Riemann zeta function. Substituting this expansion in (4.11), we obtain

$$\ln\frac{\omega}{2}=-\frac{i\pi n}{\nu}+\frac{i\pi}{2}-\gamma-\sum_{m=1}^{\infty}\frac{\zeta(2m+1)}{2m+1}\nu^{2m}$$

$$+\frac{(\omega/2)^2}{\nu(1-\nu^2)}-\frac{(2\nu^2+1)(\omega/2)^4}{(1-\nu^2)^2(4-\nu^2)}+O(\omega^6). \tag{4.13}$$

Inserting $\omega/2=r\exp(i\varphi)$, we have

$$\ln r=-\frac{i\pi n}{\nu}+i\left(\frac{\pi}{2}-\varphi\right)-\gamma-\sum_{m=1}^{\infty}\frac{\zeta(2m+1)}{2m+1}\nu^{2m}$$

$$+\frac{r^2\exp(2i\varphi)}{\nu(1-\nu^2)}-\frac{(2\nu^2+1)r^4\exp(4i\varphi)}{(1-\nu^2)^2(4-\nu^2)}+O(r^6). \tag{4.14}$$

Reversing this series, we obtain for $n\neq 0$, $\nu\equiv\nu_n$,

$$\nu_n=-\frac{i\pi n}{\ln r}+\frac{\nu}{\ln r}\left[i\left(\frac{\pi}{2}-\varphi\right)-\gamma-\sum+\frac{r^2\exp(2i\varphi)}{\nu(1-\nu^2)}\right.$$

$$\left.-\frac{(2\nu^2+1)r^4\exp(4i\varphi)}{(1-\nu^2)^2(4-\nu^2)}+O(r^6)\right]$$

$$=-\frac{i\pi n}{\ln r}\left(1+\frac{[i(\pi/2-\varphi)-\gamma]}{\ln r}+\frac{[i(\pi/2-\varphi)-\gamma]^2}{(\ln r)^2}\right.$$

$$\left.+\frac{[i(\pi/2-\varphi)-\gamma]^3-\zeta(3)\pi^2n^2/3}{(\ln r)^3}+\cdots\right)$$

$$+\frac{r^2\exp(2i\varphi)}{\ln r}\left(1-\frac{\pi^2n^2}{(\ln r)^2}+\cdots\right)+\frac{i\pi n}{4}\frac{r^4\exp(4i\varphi)}{(\ln r)^2}+\cdots,$$

$$|z|<1,\quad |\nu|<1. \tag{4.15}$$

We now recall that $\omega_n\equiv\omega=2r\exp(i\varphi)$ is the position of the nth zero of the Hankel function of the first kind in the ω plane. Alternatively, if ω is given, (4.15) gives that value of ν for which $H^{(1)}(\omega)$ vanishes. Similarly, the Mathieu function $M_\nu^{(3)}$ vanishes for those values of ν, for which the zeros of the Hankel function are given by (4.7). Thus $M_\nu^{(3)}$ vanishes for those ν of (4.15) for which $\omega=\omega_n$ is replaced by (4.7). Hence

$$2r\exp(i\varphi)=h\pm\frac{h^2}{2\sqrt{\nu^2-1}}+O(h^3)$$

$$=\sqrt{kg}\,\exp(i\pi/4)\pm kg/2\sqrt{1-\nu^2}+O(h^3). \tag{4.16}$$

Substituting this expression into (4.15) and thence ν into (2.29), we find $l\equiv\alpha_n$, the Regge trajectories. By (2.29)

$$l+\tfrac{1}{2}=\nu-\frac{h^4}{4\nu(1-\nu^2)}+O(h^8), \tag{4.17}$$

or to lowest approximation

$$\alpha_n=-\frac{1}{2}+\frac{\pi n(\pi/2-\varphi)}{(\ln r)^2}$$

$$+i\left(-\frac{\pi n}{\ln r}+\frac{\ln r}{4\pi n}k^2g^2+\frac{k^2g^2\gamma}{4\pi n}\right), \tag{4.18}$$

where

$$r\approx\frac{kg}{4}\pm\frac{(kg)^{3/2}}{4\sqrt{2}}+\frac{(kg)^2}{16}$$

and

$$\varphi=\tan^{-1}[1\mp(kg/2)^{1/2}]\quad\text{for } |kg|\ll 1,\quad n\neq 0,\quad \gamma=0.577. \tag{4.19}$$

In Table I we give some values of α calculated from this formula in the region $0.08<kg<0.1$. The last column in the table gives α_1 for $kg=0.2$; we believe this value to be already too large to give a reliable estimate. We observe that in the region under consideration and for a fixed coupling constant, the real part of the trajectory rises[17] with the energy k^2. At $kg\sim 0.15$ (approximately) our formula presumably becomes meaningless—in agreement with the behavior of the zeros of the Hankel function observed by Keller *et al.*,[15] who found it necessary to use a completely different approximation scheme in the higher (though not infinite) region of kg. We shall not explore this here. The finding that Regge trajectories for a singular potential do definitely have a reasonable behavior in the low energy region is reassuring for models where such a property is assumed.

Keller *et al.*[15] have also derived zeros of derivatives of Hankel functions, which are seen to have similar characteristics as those of Hankel functions. Thus a similar analogy may be expected between zeros of Mathieu functions and those of their derivatives.

Finally, we remark for the sake of completeness that the high-energy behavior of the trajectories is considerably easier to study—in fact, one can use simply

TABLE I. Regge poles for $|kg|\ll 1$.

kg	0.08	0.09	0.1	(0.2)
Re α_1	−0.2	−0.15	0.73	(1.1)
Im α_1	0.75	0.9	1.5	(1.1)

the large-h expansion of the Mathieu eigenvalues as observed by various authors.[4,6-8]

5. THE PHASE SHIFT

We obtain the phase shift δ and hence the scattering amplitude by *componendo et dividendo* applied to the S matrix element (3.21). Then

$$\cot[\delta_l + \pi/2(\nu - l - \tfrac{1}{2})] - \cot\nu\pi = -\frac{R^2 \exp(i\nu\pi)}{\sin\nu\pi}, \tag{5.1}$$

where

$$R \equiv R_\nu(h) = [M_{-\nu}^{(1)}(0,h)/M_\nu^{(1)}(0,h)]$$
$$= \frac{J_{-\nu}(2h) + \sum_{i=1}^{\infty} h^{2i} \sum_{j=-i\neq 0}^{i} p_{2i}(-\nu, 2j) J_{-\nu+2j}(2h)}{J_\nu(2h) + \sum_{i=1}^{\infty} h^{2i} \sum_{j=-i\neq 0}^{i} p_{2i}(\nu, 2j) J_{\nu+2j}(2h)}. \tag{5.2}$$

Thus for energy $k^2 \to 0$

$$R_\nu(h) \to \frac{J_{-\nu}(2h)}{J_\nu(2h)} \frac{\delta(-\nu)}{\delta(\nu)} \to \frac{\Gamma(l+\frac{3}{2})\delta(-\nu)}{(ikg)^{l+1/2}\Gamma(-l+\frac{1}{2})\delta(\nu)},$$

where

$$\delta(\nu) = \sum_{i=0}^{\infty} \nu \frac{(-1)^i(\nu - i - 1)!}{4^i i!(\nu - 2i)!} \tag{5.3}$$

and hence (for integral l)

$$\cot\delta_l \to \frac{(-1)^{l+1}}{(kg)^{2l+1}} \left(\frac{\Gamma(l+\frac{3}{2})}{\Gamma(-l+\frac{1}{2})}\right)^2 \left(\frac{\delta(-l-\frac{1}{2})}{\delta(l+\frac{1}{2})}\right)^2 \quad \text{for } k^2 \to 0. \tag{5.4}$$

The scattering length $a(l)$ defined by[1,18]

$$\frac{1}{a(l)} = \lim_{k\to 0} k^{2l+1} \cot\delta_l \tag{5.5}$$

is therefore given by

$$\frac{1}{a(l)} = \frac{(-1)^l}{g^{2l+1}} \left\{\frac{\Gamma(l+\frac{3}{2})}{\Gamma(-l+\frac{1}{2})}\right\}^2 \cdot \left\{\frac{\delta(-l-\frac{1}{2})}{\delta(l+\frac{1}{2})}\right\}^2. \tag{5.6}$$

To minimize confusion we recall that some authors[19] define the scattering length as $A(l) = -a(l)$. The series (5.3) may be rewritten as

$$\delta(\nu) = \frac{\Gamma(1-\nu/2)\Gamma[(1-\nu)/2]}{\pi^{1/2}2^{\nu+1}\Gamma(-\nu)} \, {}_2F_1\left(1-\frac{\nu}{2}, 1-\frac{\nu+1}{2}; 1-\nu; 1\right). \tag{5.7}$$

By Raabe's test of convergence it may be shown that the hypergeometric function on the right is only conditionally convergent for the argument and coefficients given here—i.e., the series of moduli diverges. One finds, however, that the series here has in any case (i.e., for physical 1) all terms real and positive. Thus the series (5.7) diverges. In the special case $l = 0$ we find that the ratio $\delta(-\nu)/\delta(\nu)$ is finite. To see this, we recall the formulas

$$\cos az = \cos z F[\tfrac{1}{2}+\tfrac{1}{2}a, \tfrac{1}{2}-\tfrac{1}{2}a; \tfrac{1}{2}; (\sin z)^2],$$
$$\sin az = a \sin z \cos z F[1+\tfrac{1}{2}a, 1-\tfrac{1}{2}a; \tfrac{3}{2}; (\sin z)^2]. \tag{5.8}$$

Thus although the ratio $\cos a\frac{1}{2}\pi/\sin a\frac{1}{2}\pi$ does not exist, the limit of $(\cos az/\sin az)$ as $z \to \pi/2$ does; in fact, setting $a = \frac{1}{2}$, we have

$$\lim_{z\to\pi/2}\left(\frac{\cos z/2}{\sin z/2}\right) = 2\frac{F[\frac{3}{4},\frac{1}{4};\frac{1}{2};1]}{F[\frac{5}{4},\frac{3}{4};\frac{3}{2};1]} \tag{5.9}$$

On the other hand,

$$\frac{\delta(\frac{1}{2})}{\delta(-\frac{1}{2})} = -\frac{F[\frac{3}{4},\frac{1}{4};\frac{1}{2};1]}{F[\frac{5}{4},\frac{3}{4};\frac{3}{2};1]}. \tag{5.10}$$

Hence by (5.6)

$$a(0) = g\left(\frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{3}{2})}\right)^2 \left(\frac{\cot\pi/4}{2}\right)^2 = g. \tag{5.11}$$

This [or rather $A(0) = -g$] agrees with the value given in the literature.[19]

If we now tried to compute higher terms of the expansion (5.5), we would soon stumble into infinities. This is due to the fact that the effective range expansion is not ideally suited for phaseshift calculations in the case of singular potentials. In fact, the detailed study of O'Malley *et al.*[18] shows that even a scattering length, i.e., the first term of the low-energy expansion, can be defined only for $n > 2l+3$, where n is the integral power of the singular potential. Corresponding inequalities hold for the existence of higher terms. The source of these difficulties, of course, lies in the long-range character of these potentials which competes with a power falloff of the solutions. Thus new calculational techniques are generally required—such as approximation suggested by Calogero[20]—since the phase shift is otherwise well defined.

6. A NEW SOLUTION OF THE MODIFIED MATHIEU EQUATION

The modified Mathieu equation

$$\frac{d^2\varphi}{dz^2} + \{2h^2\cosh 2z - (l+\tfrac{1}{2})^2\}\varphi = 0 \tag{6.1}$$

may be transformed into yet another equation with solutions having interesting properties. Setting

$$z = \ln(r/\gamma), \quad r = a/R, \quad \gamma \text{ as before}, \quad a^2 = -g^2 \tag{6.2}$$

and

$$\varphi = R^{1/2}Y, \tag{6.3}$$

we find

$$\frac{d^2Y}{dR^2} + \frac{2}{R}\frac{dY}{dR} + \left\{1 + \frac{h^4}{R^4} - \frac{l(l+1)}{R^2}\right\} Y = 0 \tag{6.4}$$

or, writing $Y = \psi/R$, $h^2 = igk$,

$$\frac{d^2\psi}{dR^2} + \left(1 - \frac{l(l+1)}{R^2} - \frac{g^2k^2}{R^2}\right)\psi = 0. \tag{6.5}$$

It is important to note that Y satisfies the equation

$$\frac{d^2Y}{dr^2} + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{g^2}{r^4}\right)Y = 0 \tag{6.6}$$

or, since $Y = (r/a)\psi$,

$$\frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{g^2}{r^4}\right)\psi = 0. \tag{6.7}$$

The symmetry relating (6.4) to (6.7) may be seen by writing

$$\phi \equiv Y\sqrt{R} = \psi\sqrt{r/a}. \tag{6.8}$$

Then (6.4) becomes

$$\frac{d^2\phi}{dR^2} + \frac{1}{R}\frac{d\phi}{dR} + \left(1 - \frac{(l+\frac{1}{2})^2}{R^2} - \frac{g^2k^2}{R^4}\right)\phi = 0 \tag{6.9}$$

and (6.7)

$$\frac{d^2\phi}{d(kr)^2} + \frac{1}{kr}\frac{d\phi}{d(kr)} + \left(1 - \frac{(l+\frac{1}{2})^2}{(kr)^2} - \frac{g^2k^2}{(kr)^4}\right)\phi = 0. \tag{6.10}$$

Thus, if $\phi_l(gk, R)$ is a solution of (6.9), a solution of (6.10) is $\phi_l(gk, kr)$. This implies, of course, that both

$$\phi_l(gk, R) \quad \text{and} \quad \phi_l(gk, \pm igk/R) \tag{6.11}$$

are solutions of the same differential equation (6.9). We note again, that the solutions ϕ are modified Mathieu functions in terms of the variable R.

We now proceed to solve (6.9) by our perturbation method. Setting

$$(l+\tfrac{1}{2})^2 = \nu^2 + \Delta h^4, \tag{6.12}$$

we may rewrite (6.9) as

$$\frac{d^2\phi}{dR^2} + \frac{1}{R}\frac{d\phi}{dR} + \left(1 - \frac{\nu^2}{R^2}\right)\phi = \frac{h^4}{R^2}\left(\Delta - \frac{1}{R^2}\right)\phi. \tag{6.13}$$

Proceeding as before, we have the zeroth-order approximation

$$\phi^{(0)} = Z_\nu(R), \tag{6.14}$$

and the right-hand side of (6.13) leaves uncompensated the terms

$$R^{(0)} = \frac{R^4}{4}[(\nu, \nu-2)G_{\nu-2} + (\nu, \nu)G_\nu + (\nu, \nu+2)G_{\nu+2}], \tag{6.15}$$

where

$$G_\nu(R) = (R^2)^{-1}Z_\nu(R) \tag{6.16}$$

and

$$(\nu, \nu-2) = -1/\nu(\nu-1), \quad (\nu, \nu+2) = -1/\nu(\nu+1),$$
$$(\nu, \nu) = 4\Delta - 2/(\nu^2-1). \tag{6.17}$$

The calculations now proceed along exactly the same lines as in Sec. 2, the main difference being the power $h^4/4$ instead of h^2; the coefficients $(\nu, \nu+\alpha)$, of course, also differ and are now given by (6.17). Hence

$$\phi(R) = Z_\nu(R) + \sum_{i=1}^{\infty}\left(\frac{h^4}{4}\right)^i \sum_{\substack{j=-i \\ j\neq 0}}^{i} p_{2i}(2j)Z_{\nu+2j}(R), \tag{6.18}$$

and Δ again follows from the expansion

$$0 = \frac{h^4}{4}(\nu, \nu) + \left(\frac{h^4}{4}\right)^2\{(\nu, \nu-2)^*(\nu-2, \nu) + (\nu, \nu+2)^*(\nu+2, \nu)\} + \cdots. \tag{6.19}$$

Evaluating the first few terms we again obtain the expansion (2.29) for $(1+l/2)^2$—precisely as one would expect. Also, the solution $\phi_l(h^4, \pm h^2/R)$ remains unchanged under the simultaneous interchanges $R \to -R$, $h^2 \to -h^2$, a property which the solutions of Sec. 2 do not possess.

[1]For a review see the article by H.H. Aly, W. Güttinger, and H.J.W. Müller in *Lectures on Particle and Field*, edited by H.H. Aly (Gordon and Breach, New York 1969). For a list of references to earlier literature see also F. Calogero, Phys. Rev. **139**, B602 (1965).

[2]W. Güttinger, R. Penzl, and E. Pfaffelhuber, Ann. Phys. (N.Y.) **33**, 246 (1965); R. Rajaraman, Phys. Rev. **178**, 2211, 2221 (1969).

[3]R.M. Spector, J. Math. Phys. **5**, 1185 (1964); H.H. Aly and H.J.W. Müller, J. Math. Phys. **7**, 1 (1966).

[4]J. Challifour and R.J. Eden, J. Math. Phys. **4**, 359 (1963); N. Dombey and R.H. Jones, J. Math. Phys. **9**, 986 (1968); D. Yuan-Ben, Sci. Sinica (Peking) **13**, 1319 (1964).

[5]L. Bertocchi, S. Fubini, and G. Furlan, Nuovo Cimento **35**, 633 (1965); H.H. Aly and H.J.W. Müller, J. Math. Phys. **8**, 367 (1967).

[6]H.H. Aly, H.J.W. Müller and N. Vahedi-Faridi, Lett. Nuovo Cimento **2**, 485 (1969).

[7]D. Masson, Nuovo Cimento **35**, 125 (1965), Appendix.

[8]H.H. Aly and P. Narayanaswamy, Phys. Lett. **28B**, 603 (1969).

[9]J. Meixner and F.W. Schäfke, *Mathieusche Funktionen und Sphäroidfunktionen* (Springer, Berlin, 1953, 1954, 1956).

[10]The disadvantage of such trajectories for singular potentials is, of course, that they do not lead to narrow width Regge recurrences. From the point of view of application energy-dependent Yukawa-like potentials as discussed by (a) G. Tiktopoulos, Phys. Lett. **28 B**, 185 (1969), (b) U. Trivedi, Cal. I. Tech. preprint 68-199, 1969, (c) J.W. Johnson, Case Western Reserve University preprint, 1969 are therefore more realistic.

[11]For a review see H.J.W. Müller, "Perturbation Approach for Regular Interactions," in *Lectures in High Energy Theoretical Physics*, edited by H.H. Aly (Wiley-Interscience, New York, 1968).

[12]R.B. Dingle and H.J.W. Müller, J. Reine Angew. Math. **211**, 11 (1962).

[13]H.J.W. Müller and K. Schilcher, J. Math. Phys. **9**, 255 (1968).

[14]H.J.W. Müller, J. Math. Phys. **11**, 355 (1969).

[15]J.B. Keller, S.I. Rubinow, and M. Goldstein, J. Math. Phys. **4**, 829 (1963).

[16]W. Magnus and L. Kotin, Numerische Math. **2**, 228 (1960).

[17]This rise seems consistent with the general behaviour of the trajectories for the repulsive potential i/r^4 as discussed by N. Limic, Nuovo Cimento **26**, 581 (1962), who has shown that here all Regge poles (for physical k) are located in the sectors which, incidentally, also implies that there can be no narrow-width Regge recurrences.

[18]T.F. O'Malley, L. Spruch, and L. Rosenberg, J. Math. Phys. **2**, 491 (1961).

[19]F. Calogero, Nuovo Cimento **37**, 756 (1965); Phys. Rev. **139**, B 602 (1965).

[20]F. Calogero, Phys. Rev. **135**, B693 (1964).

Heat conduction model with finite signal speed*

B. DeFacio* †

Theoretical Physics Division, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87544

(Received 7 October 1974; revised manuscript received 15 November 1974)

A simple physical model is derived which has a finite signal speed for a heat pulse in a linear medium. The most general E^3 invariant constitutive equation for energy flux $\mathcal{E}$ which allows the finite signal speed is given. The assumptions which are required include continuum mechanics, thermodynamics of adiabatic processes, and a generalized Fourier heat law for the energy flux $\mathcal{E}$. Then we use singular perturbation theory with the finite signal speed u^{-1} as a parameter to reduce the hyperbolic heat equation to the usual parabolic heat conduction equation.

1. INTRODUCTION

One venerable question concerning the heat conduction equation, which Cattaneo[1] seems to have first raised, is that it implies an infinite signal speed for a thermal pulse. Cattaneo added a small "inertial term" of $\epsilon^2(\partial^2/\partial t^2)$ to the heat conduction equation based on long arguments from his previous papers using both thermodynamics and statistical mechanics.[2]

Since Cattaneo's original work there have been several other approaches to this problem. First, Gurtin and Pipkin[3] showed that the addition of a nonlinear memory to the medium that the heat pulse propagates through produces a finite signal speed for the pulse. This leaves open the question of obtaining heat propagation at a finite speed in linear media. Next, Müller[4] showed that special relativity restricted the heat pulse velocity u to values equal to or less than the speed of light c. Most recently, Meixner[5] has shown that certain modifications in continuum mechanics of the medium of propagation also produces the desired finite signal speed. Since the present writer believes continuum mechanics to have a far more sound foundation, both mathematically and physically, then most of physics, it seems desirable to seek some other mechanism to generate the finite signal speed.

In Sec. 2, we will present our notation and assumptions. In Sec. 3, it will be shown that replacement of the Fourier heat law for energy flux $\mathcal{E}$ in terms of temperature T as

$$\mathcal{E} = -\kappa\nabla T, \tag{1.1}$$

where κ is the heat conductivity function, by the generalized Fourier heat law[6,7]

$$\mathcal{E} = -\kappa\nabla T - h\nabla p - h'_{ij}\frac{\partial}{\partial x_i}\frac{\partial T}{\partial t}, \tag{1.2}$$

where h is a small, positive constant h_{ij} is a constant matrix and p is the mean stress of an elastic body (which reduces to the pressure of fluid) produces the desired result. We emphasize that Eq. (1.2) is the most general E^3-invariant generalization of Fourier's law which produces a finite signal speed. It includes Chapman and Cowling[6] and Roetman[7] as a special case when all $h_{ij}=0$ and Ruggeri[11,12] whenever $h=0$. That is, one gets the hyperbolic generalized heat conduction equation of the form

$$\frac{1}{u^2}\frac{\partial^2 T}{\partial t^2} + \beta\frac{\partial T}{\partial t} = -\nabla\cdot(\kappa\nabla T) + \text{terms}. \tag{1.3}$$

For comparison the ordinary heat conduction equation is of the form

$$\frac{\partial T}{\partial t} = -\nabla(\kappa\nabla T) + \text{terms}. \tag{1.4}$$

This raises the mathematical question of how Eq. (1.3) which is hyperbolic, approaches Eq. (1.4) which is parabolic.

In other words, Eq. (1.3) requires knowledge of both

$$T(\mathbf{x}, 0) = g_1(\mathbf{x}) \tag{1.5}$$

and

$$\frac{\partial T(\mathbf{x}, 0)}{\partial t} = g_2(\mathbf{x}) \tag{1.6}$$

whereas Eq. (1.4) only requires the first. Let $T_1(\mathbf{x}, t, \epsilon)$, with $\epsilon^2 \equiv 1/u^2$, denote a solution of Eq. (1.3) and let $T_2(\mathbf{x}, t)$ denote a solution of Eq. (1.4). In Sec. 4, we will study the singular perturbation theory[8,9] of the limit

$$\lim_{\epsilon\to 0}[T_1(\mathbf{x}, t, \epsilon)] = T(\mathbf{x}, t), \tag{1.7}$$

in the parameter ϵ, for the special case of a one-dimensional spatial coordinate x. Our arguments only hold for linear media. Then in Sec. 5, our conclusions will be presented.

2. NOTATION AND ASSUMPTIONS

Notation

Θ and Λ are the symmetric stress and strain tensors, respectively, $\mathbf{v}$ is the velocity field, u is the speed of the heat pulse, T is the temperature distribution function, $\mathbf{F}$ is the external force density, $\mathcal{E}$ is the energy flux vector, ξ is the internal energy density, q is the internal heat source density, κ is the heat conductivity function, $\mathbf{x}$ locates points in R^3, ∇ and ∇^2 are the gradient and Laplacian operators on R^3 functions, $\mathbf{I}$ is the identity tensor in R^3, α is the volume coefficient of thermal expansion, c_p and c_v are the constant pressure and constant volume specific heats, respectively, ρ is the volume density function, $w=1/\rho$ is the specific volume, ϵ^2 is defined as $1/u^2$, t is the instantaneous time and ":" denotes the contraction of a pair of tensors.

Assumptions

Our model is based upon three sets of assumptions:

(i) continuum mechanics,

(ii) the thermodynamics of adiabatic processes, and

(iii) the generalized Fourier heat law, i.e., Eq. (1.2).

From one of the classic sources of modern continuum mechanics[10] we take the equation of continuity,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{2.1}$$

the equation of motion,

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} X \mathbf{v}) = \nabla \cdot \Theta + \rho \mathbf{F}, \tag{2.2}$$

and the energy flow equation,

$$\rho \left(\frac{\partial \xi}{\partial t} + \mathbf{v} \cdot \nabla \xi \right) = \Theta : \Lambda - q - \nabla \cdot \mathcal{E}. \tag{2.3}$$

We restrict attention to linear media which are isotropic, homogeneous and free of shear stresses so that

$$\Theta = -\rho \mathbf{I}. \tag{2.4}$$

Also, the thermodynamics of adiabatic processes implies that the equation of state is given by

$$\xi = \xi(\omega, T) \tag{2.5}$$

and

$$d\xi = c_v \, dT + \left(\frac{\rho}{\alpha} (c_p - c_v) \right) d\omega \tag{2.6}$$

because

$$\rho = \rho(T) \quad \text{(only)} \tag{2.7}$$

for adiabatic processes. We shall also use the local relation

$$\rho(T) = \rho_0 (1 - \alpha T), \tag{2.8}$$

later but only to simplify our analysis. Although Eq. (2.8) is very much a special case of Eq. (2.7), it is still far more general than $\rho = \rho_0$ which follows from Meixner's second assumption that, "we shall neglect all notion of deformation."

Given the preceeding assumptions one now has

$$\mathbf{I} : \Lambda = \nabla \cdot \mathbf{u}. \tag{2.9}$$

Our other assumption is the generalized Fourier heat law

$$\mathcal{E} = -\kappa \nabla T - h \nabla \rho. \tag{2.10}$$

In the next section, these assumptions will be used to derive a hyperbolic heat conduction equation.

3. A HYPERBOLIC HEAT CONDUCTION EQUATION

Applying the assumptions in Eqs. (2.4)—(2.10) to Eqs. (2.1)—(2.3) produces the equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{3.1}$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} = -\nabla p + \rho \mathbf{F}, \tag{3.2}$$

and

$$\rho c_v \frac{\partial T}{\partial t} = \left(\frac{c_p - c_v}{\alpha} + \frac{p}{\rho} \right) \nabla \cdot (\rho \mathbf{v}) = -q - \nabla \cdot \mathcal{E}. \tag{3.3}$$

Next, take the gradient of Eq. (3.2) and interchange space and time partial derivatives to obtain that

$$\nabla^2 p = \nabla \cdot (\rho \mathbf{F}) - \frac{\partial}{\partial t} [\nabla \cdot (\rho \mathbf{v})]. \tag{3.4}$$

Using the continuity equation, Eq. (3.1) above, for the second term on the right-hand side of Eq. (3.4) yields

$$\nabla^2 p = \nabla \cdot (\rho \mathbf{F}) - \frac{\partial^2 \rho}{\partial t^2}, \tag{3.5}$$

which has the desired second derivative with respect to time. Now using the local behavior of ρ in Eq. (2.8), we find that

$$\frac{\partial^2 \rho}{\partial t^2} = -\rho_0 \alpha \frac{\partial^2 T}{\partial t^2}. \tag{3.6}$$

Define the function $g_3(\rho, p)$ as

$$g_3(\rho, p) \equiv \frac{(c_p - c_v)\rho - \alpha p}{\rho p}, \tag{3.7}$$

and define the speed u through the relation

$$1/u^2 \equiv \rho_0 h \alpha. \tag{3.8}$$

Putting Eqs. (3.5)—(3.8) into Eq. (3.3) yields the hyperbolic heat conduction equation

$$\frac{1}{u^2} \frac{\partial^2 T}{\partial t^2} + \rho c_v \frac{\partial T}{\partial t} = -\nabla \cdot (\kappa \nabla T) - q - \nabla \cdot (\rho \mathbf{F}) + g_3(p, \rho) \nabla \cdot (\rho \mathbf{v}). \tag{3.9}$$

One last simplification occurs if one uses the formula of Truesdell and Toupin[10] for heat conductivity, with s a constant,

$$\kappa = sT/p \tag{3.10}$$

in Eq. (3.9), one finds that

$$\frac{1}{u^2} \frac{\partial^2 T}{\partial t^2} + \rho c_v \frac{\partial T}{\partial t} = -\frac{s}{p} (\nabla^2 T) - \frac{s}{p} (\nabla T) \cdot (\nabla \cdot T) - q + g_3(\rho \mathbf{V}) - \nabla \cdot (\rho \mathbf{F}). \tag{3.11}$$

In Eq. (3.11) the temperature T is completely decoupled from the properties of the particular bulk medium under consideration.

Let us emphasize that Eq. (2.10) for $\mathcal{E}$ was the crucial ingredient in Eq. (3.3) which give the finite speed u in Eq. (3.9). Furthermore, since the physical validity of this model requires that both h and α be small the heat pulse must propagate at a relatively high speed compared to any local motions of the medium. The reader can easily verify that use of the ordinary Fourier heat law implies the ordinary heat conduction equation.

4. RELATION OF HYPERBOLIC HEAT EQUATION TO THE PARABOLIC HEAT EQUATION

In this section we will study the details of how our hyperbolic equation approaches the parabolic heat equation. A "physical treatment" would be to set $\epsilon = 0$ in Eq. (1.3) which implies Eq. (1.4) directly. Boillat and Ruggeri[11] have given a discussion of relativistic heat equations in which they simply add the $\epsilon^2(\partial^2/\partial t^2)$ term, but they gave no physical model beyond their mathemati-

cal observation that the more general equation cannot be obtained from the less general equation continuously. Also, Borghese, Denti, and Ruggeri[12] have treated the hyperbolic Klein—Gordon equation and Schrödinger equation by similar methods. They obtained the limiting equations by a "physical treatment" in both cases.[11,12] We shall show that Hadamard's study of the Cauchy problem together with the asymptotic expansions of the Bessel functions of the second kind of order n, l_n, imply this in a more mathematical manner.

For convenience let us specialize the 3-vector $\mathbf{x}$ to the one space dimension variable x, and rewrite Eq. (3.11) as

$$\epsilon^2\frac{\partial^2 T_1}{\partial t^2}+\frac{\partial T_1}{\partial t}=\frac{\partial^2 T_1}{\partial x^2}+G \tag{4.1}$$

with the initial conditions

$$T_1(x,0,\epsilon)=g_1(x) \tag{4.2}$$

and

$$\frac{\partial T_1(x,0,\epsilon)}{\partial t}=g_2(x). \tag{4.3}$$

Similarly, Eq. (1.4) reduces to

$$\frac{\partial T_2}{\partial t}=\frac{\partial^2 T_2}{\partial x^2}+G, \tag{4.4}$$

in this case. Physically, it seems quite reasonable that as the inertia of the wave in Eq. (4.1) is smoothly decreased to zero, i.e., $\epsilon \to 0$, it must reduce to Eq. (4.4). Using a method due to Hadamard,[13] this can be proven in the linear case. Gurtin and Pipkin[3] have treated the nonlinear case.

Let $l_n(x)$ denote the modified Bessel function of the first kind of order n, with argument x. These functions are given by

$$l_n(x)=\exp(-i\pi n)J_n[x\exp(i\pi/2)]=\sum_{m=0}^{\infty}(\tfrac{1}{2}x)^{2m+n}\frac{1}{m!\Gamma(m+v+1)}. \tag{4.5}$$

and let

$$y=y(x,t)=(1-\epsilon^2x^2/t^2)^{1/2}. \tag{4.6}$$

The formal solution to the initial value problem in Eq. (4.1)—(4.3) is

$$\begin{aligned}T(x,t,\epsilon)=&\frac{\partial}{\partial t}\left(\frac{\epsilon}{2}\int_{x_1}^{x_2}g_2(r)\exp(-t/2\epsilon^2)l_0[ty(x-r,t)/2\epsilon^2]\,dr\right)\\&+\frac{\epsilon}{2}\int_{x_1}^{x_2}g_1(r)\exp(-t/2\epsilon^2)l_0[ty(x-r,t)/2\epsilon^2]\,dr\\&-\frac{1}{2\epsilon}\int_0^t dt'\int_{x_1'}^{x_2'}G(r,t')\exp[-(t-2)/2\epsilon^2]l_0\\&\times[(t-t')y(x-r,t-t')/2\epsilon^2]\,dr,\end{aligned} \tag{4.7}$$

where integration limits are

$$x_1=x-t/\epsilon,$$

$$x_2=x+t/\epsilon,$$

$$x_1'=x+(t-t')/\epsilon,$$

and

$$x_2'=x-(t-t')/\epsilon. \tag{4.8}$$

Consider $t>0$ and define the three kernals K, K_1, K_2 as

$$K(x,t)=(4\pi t)^{-1/2}\exp[ct-x^2/4t], \tag{4.9}$$

$$K_1(x,t)=\begin{cases}\dfrac{1}{2\epsilon}\exp(-t/2\epsilon^2)l_0[ty(x-r,t)/2\epsilon^2] & (\epsilon^2x^2<t^2),\\ 0 & (\epsilon^2x^2\geq t^2),\end{cases} \tag{4.10}$$

and

$$K_2(x,t)=\begin{cases}\dfrac{1}{2\epsilon y(x,t)}\exp(-t/2\epsilon^2)l_0[ty(x,t)/2\epsilon^2] & (\epsilon^2x^2<t^2),\\ 0 & (\epsilon^2x^2\geq t^2).\end{cases} \tag{4.11}$$

Using Eqs. (4.9)—(4.11) the Riemann function for Eq. (4.7) from Hadamard,[13] implies that

$$\begin{aligned}T(x,t,\epsilon)=&\tfrac{1}{2}[g_1(x+t/\epsilon)+g_1(x-t/\epsilon)]\exp(-t/2\epsilon^2)\\&+\tfrac{1}{2}\int_{-\infty}^{\infty}[K_1(x-x',t,\epsilon)+K_2(x-x',t,\epsilon)]g_1(x')\,dx'\\&+\epsilon^2\int_{-\infty}^{\infty}K_1(x-x',t,\epsilon)g_2\,dx'\\&-\int_0^t dt'\int_{-\infty}^{\infty}K_1(x-x',t-t',\epsilon)G(x',t')\,dx'.\end{aligned} \tag{4.12}$$

Setting $\epsilon=0$ in Eq. (4.1) gives Eq. (4.4) whose solution only allows initial data of the form of Eq. (4.2). This solution is

$$\begin{aligned}T_2(x,t)=&\int_{-\infty}^{\infty}K(x-x',t)g_1(x')\,dx'\\&-\int_0^t dt'\int_{-\infty}^{\infty}K(x-x',t-t')G(x',t')\,dx'.\end{aligned} \tag{4.13}$$

Since for r real, small, and positive the Bessel functions I_0 in Eqs. (4.9)—(4.11) satisfy

$$0\leq I_0(r)\leq e^r \tag{4.14}$$

and for r real, large, and positive they satisfy

$$0\leq I_0(r)\leq e^r/\sqrt{r}, \tag{4.15}$$

we can bound K_1 and K_2 by

$$0\leq K_1(x,t,\epsilon)\leq D_1\exp(|c|t_1)K(x,t) \tag{4.16}$$

and

$$0\leq K_2(x,t,\epsilon)\leq D_2\exp(|c|t_1)K(x,t), \tag{4.17}$$

for real t_1, such that $0<t\leq t_1$, and for D_1 and D_2 real constants. Hence, the solution in Eq. (4.12) is bounded by the solution in Eq. (4.13), and must approach, as pointed out by Hadamard,[13] This is one more example of a singular perturbation in which the vanishing terms is one of the highest derivatives with respect to one of the variables so that a change of equation type occurs. This is reminiscent of Klauder's phenomenon[14] in which solutions are irretrivably lost due to an interaction which is too singular. However, this case differs from Klauder's case in that he has a function which is singular in a *variable* whereas we have a vanishing *parameter* which kills one initial condition function. Both ef-

fects, of course, share the feature that domain changes occur for the operators involved.

5. CONCLUSIONS

A specific model has been derived which gives a hyperbolic heat conduction equation by modifying the Fourier heat law, entirely without the draconian measures involving changes in continuum mechanics or thermodynamics. We emphasize that the generalized Fourier law used in this regard was suggested on physical grounds[6] and was not especially contrived for our purpose.

By changing a mere constitutive relation, a hyperbolic heat conduction equation was produced. This is a considerable improvement over present derivations of finite signal speed[3–5] for the following reasons:

(i) The modification of continuum mechanics[5] obscures an otherwise clear and fundamentally motivated physical theory. That such measures are *unnecessary* is the central point of the present work.

(ii) The addition of special relativity[4] produces a finite signal speed, but it is the *speed of light* and not the *heat pulse speed*. Again, the present model could be generalized to include special relativity but it is not necessary for heat propagation. Also, ordinary continuum mechanics together with Maxwell's electrodynamics are known[10] to imply the Lorentz transformation, providing the constitutive relations

$$D = \epsilon_0 E, \tag{5.1}$$

$$B = \mu_0 H, \tag{5.2}$$

retain this form in all inertial frames.

(iii) The addition of a nonlinear memory[3] also produces a finite signal speed, but Eq. (2.18) shows that even in a linear heat conduction theory finite signal speed occurs. Thus, memory is a sufficient condition but is not necessary for finite heat conduction speed.

The mapping of our hyperbolic equation back into a parabolic equation was studied, including the initial conditions. The asymptotic expressions and continuity of the I_n Bessel functions in the parameter $\epsilon = 1/u$ was found to imply this result.

In this work we have made some tacit assumptions about stability,[12] but neither stability nor entrophy production[13] has been studied. Both of these deserve study, but beyond Eq. (2.4), neither is required for the two effects exhibited here, (1) finite signal speed of heat conduction, and (2) the reduction of the hyperbolic heat equation to the usual heat equation as the parameter $\epsilon \downarrow 0$.

ACKNOWLEDGMENTS

I wish to thank Dr. Michael M. Nieto and Dr. P. Carruthers for their hospitality in the Theoretical Physics Division at the Los Alamos Scientific Laboratory, where most of this work was completed. I thank Professor E. L. Roetman of the University of Missouri-Columbia Applied Mathematics group, and Professor C. L. Hammer of the Iowa State University, and several other members of the LASL Theoretical Physics Division for useful conversations. Dr. Feigenbaum and Dr. Nieto, of LASL, are especially thanked for their comments on the manuscript. And the hospitality of the Ames Laboratory USAEC at Iowa State University, where the manuscript was revised, is acknowledged and appreciated.

*Work supported in part by the U.S. Atomic Energy Commission.

†Work partly performed at Ames Laboratory USAEC and Department of Physics, Iowa State University, Ames, Iowa 50010.

‡On sabbatical leave from the Department of Physics, University of Missouri-Columbia, Columbia, Mo. 65201.

[1] C. Cattaneo, C.R. Acad. Sci. Paris **247**, 431 (1958).

[2] In Ref. 1 Cattaneo refers to two of his earlier (long) papers which appeared in 1948 and 1949. These two papers are in Italian and are not readily available. However from his equations it is clear that his approach is different from the present work.

[3] M.E. Gurtin and A.C. Pipkin, Arch. Ratl. Mech. Anal. **31**, 113 (1968).

[4] I. Müller, Arch. Ration. Mech. Anal. **34**, 254 (1969).

[5] J. Meixner, Arch. Ration. Mech. Anal. **39**, 108 (1970).

[6] S. Chapman and T.G. Cowling, *The Mathematical Theory of Non-Uniform Gasses* (Cambridge U.P., London, 1970), 3rd ed.

[7] E. L. Roetman, private communication.

[8] A.H. Nayfeh, *Perturbation Methods* (Wiley, New York, 1974).

[9] P.A. Lagerstrom and R.G. Casten, SIAM Review **14**, 63 (1973).

[10] C. Truesdell and R. Toupin, *Handbuch der Physik* 111/1, edited by S. Flügge (Springer-Verlag, Berlin, 1960).

[11] F. Borghese, P. Denti, and T. Ruggeri, Int. J. Theor. Phys. **9**, 55 (1974).

[12] G. Bollat and T. Ruggeri, Rend. Accad. Nazion. Lincei L111, 208 (1972).

[13] J. Hadamard, *Lectures on Cauchy's Problem in Linear Partial Differential Equations* (Dover, New York, 1952).

[14] J.R. Klauder, Acta. Phys. Austr. Suppl. **XI**, 341 (1973).

Quantum mechanics on homogeneous spaces

H. D. Doebner* and J. Tolar†

International Centre for Theoretical Physics, Trieste, Italy
(Received 1 October 1974)

A complete description of quantum kinematics on a homogeneous G-space M is presented using imprimitivity systems for G based on M. The kinematics on M is considered (if possible and consistent with this quantization) as kinematics on a G-orbit equivalent to M in some Euclidean space R_n. This method gives a physically justified and mathematically well-defined method of connecting the free Hamiltonian of a quantum system in R_n with an operator proportional to the Laplace–Beltrami operator on M (with the Riemannian structure inherited from R_n) which is proposed to be the free Hamiltonian on M.

1. INTRODUCTION

(1) A quantum mechanical description of a nonrelativistic system moving on a C^∞-manifold is of physical importance and becomes mathematically feasible if a Lie group G acts with σ transitively on M. Then the triple (G, M, σ) is a differentiable G-transformation group and Mackey's theory of imprimitivity systems[1] yields all representations of (G, M, σ). This and his construction of representations of regular semidirect products with an Abelian invariant subgroup[2] provide a mathematical framework suited to formulate in a Hilbert space $\mathcal{H}$ quantum kinematics for a system bound on a homogeneous space M. The kinematical observables obtained in $\mathcal{H}$ are physically well justified and are connected with momentum, position, and generalized spin.

Dynamics has to be introduced on M consistently with its quantum kinematics via Hamiltonians being functions of the kinematical observables. The identification of such Hamiltonians with certain physical systems is difficult. Especially for the Hamiltonian $\mathbb{H}^0$ of a "free system on M" various procedures are known with different physical and mathematical background and with different results for $\mathbb{H}^0$.

(2) It is the purpose of this paper to present a complete description of quantum kinematics on M through representations of (G, M, σ) and to consider, if possible and consistent with this quantization, the kinematics on M as kinematics on a submanifold (G orbit) equivalent to M in some Euclidean space R_n. This method gives a physically justified and in many cases mathematically well-defined method to characterize and to connect observables on $M \subset R_n$ with corresponding observables on R_n, e.g., the free Hamiltonian on R_n and on M.

(3) Quantum systems on M correspond physically to systems with constraints. We quote two significant mechanisms which yields constraints: the bound state mechanism, e.g., the two-atom bound state (or molecule) which moves like a rigid body on a sphere, and the collective state mechanism present in certain many-body systems and interacting (quantum) fields, which produces substructures (collective states). They move, if the noncollective coordinates are frozen or decoupled, on a manifold, like string models, or on a homogeneous G space, as is the case for a meson field bound strongly to a fixed baryon source[3] with internal symmetry group G. Here a set of collective variables $\mathbb{Q}_\lambda = \int u(r)\varphi_\lambda(\mathbf{r})\, d^3r$ is constructed from the real meson fields φ_λ ($\lambda = 1, \ldots, n$; n is the dimension of the meson multiplet) such that for large values of the coupling constant their eigenvalues are bound to a certain G orbit M in R_n.

Quantization in space–time manifolds as used in gravitation theory[4] or in rotator models for particles[5] will not be discussed here. Our approach is not applicable to manifolds which are not homogeneous spaces.

(4) The material is organized as follows: Differentiable G-transformation groups are defined in Sec. 2A. There also their representation theory via imprimitivity systems and their physical interpretation are given. (G, M, σ) is embedded in a differentiable G-transformation group (G, R_n, τ) on R_n in Sec. 2B. We derive necessary and sufficient conditions such that the representations of (G, M, σ) can be constructed from (G, R_n, τ) in Lemma 2. Extrinsic methods, as the embedding in R_n, and intrinsic ones, as G-invariance, to characterize $\mathbb{H}^0$, are described in Sec. 3A. The most promising approach is a submersion of free Hamiltonian in R_n to $M \subset R_n$ consistent with quantum kinematics (Sec. 3B, Lemma 3). G-invariant operators on M are treated in 3C. The summary for the kinematical part is in Sec. 2D and for the part dealing with free systems in Sec. 3D. Section 4 gives a discussion of related results. Proofs and more technical definitions are collected in Appendix A and Appendix B.

2. QUANTUM KINEMATICS

We introduce differentiable G-transformation groups (G, M, σ) as geometrical structures for the kinematics of a system moving on M and develop along the lines of Mackey[1,2] and Varadarajan[6] a representation or quantization $\mathcal{G}(G, M, \sigma)$ of (G, M, σ) in some Hilbert space, which gives the quantum kinematics together with momentum operators and position projections. To utilize extrinsic properties of (G, M, σ) we define an equivariant embedding of (G, M, σ) in (G, R_n, τ) and derive necessary and sufficient conditions to derive $\mathcal{G}(G, M, \sigma)$ from $\mathcal{G}(G, R_n, \tau)$. The representation theory is given in Secs. 2A and 2B. Some examples can be found in Sec. 2C and a summary in 2D.

A. Representation theory for (G,M,σ)

(1) Let M be a (connected) C^∞-manifold[7,8] of dimension m, let G be a (connected) Lie group acting transitively on M, i.e., M is a homogeneous space of G; denote by σ_a the nonsingular differentiable action of $a \in G$ on M and assume in addition that the mapping $\sigma : G \ni a \to \sigma_a \in \mathrm{diff}M$

be a homomorphism [such that $\sum : G\times M \ni (a,p) \to \sigma_a(p) \in M$ is continuous]. Hence the triple (G,M,σ) is a *differentiable G-transformation group.*[9]

Take now the homogeneous G space M as classical configuration space of a quantum system. Let $\mathcal{H}$ be its separable complex Hilbert space[10] such that the states of the system are in one-to-one correspondence with rays[11] $\{f\}\subset\mathcal{H}$, given by the set of all vectors of the form λf with $f\in\mathcal{H}$ fixed and λ complex, $|\lambda|=1$.

(2) To define *momentum operators* the group structure in (G,M,σ) is utilized: An infinitesimal transformation σ_a shifts a representative point $p\in M$ of the system infinitesimally to $p'\in M$ and the elements X of the Lie algebra $\underline{G}$ of G acting on M should correspond to G-momenta on M. We assume that there exists for each $X\in\underline{G}$ an (in general unbounded) observable $\mathbb{D}(X)$ in $\mathcal{H}$, the (G-) momentum operators $\mathbb{D}(X)$ having the property that each $\mathbb{D}(X)$ is essentially self-adjoint on a common dense invariant domain $\mathcal{D}\subset\mathcal{H}$ and can be integrated to a unitary representation $\mathbf{U}(s)$ of the corresponding one-parameter subgroup $\exp(sX)$ of G. Bounded momentum observables can be constructed via the spectral measures of $\mathbb{D}(X)$.

From the physical point of view it is desirable that this set of unitary representations $\mathbf{U}(s)$ of one-parameter subgroups builds a representation $\mathbf{U}(G)$ of G which is unitary (faithful, continuous) and, because $\mathbf{U}(G)$ acts on rays $\{f\}$ in $\mathcal{H}$, furthermore projective. But even if all unitary projective representations of G are unitarily equivalent to vector representations, the one-parameter subgroups will in general not yield[12] a representation of G. So we strengthen the assumption and demand that there exists a unitary projective representation $\mathbf{U}(G)$ of G in $\mathcal{H}$ with generators being the G-momentum operators of the system. Under very mild restrictions[11] projective representations of G are unitarily equivalent to vector representations of the central extension $\tilde{G}$ of G.[13]

(3) To construct *position projectors* we require, as in Refs. 1, 6, 14, the localizability of the states of the system in M: A suitably chosen field $\mathcal{B}\equiv\mathcal{B}(M)$ of Borel sets S in M is represented in $\mathcal{H}$ by projection-valued measures[15] $\mathbb{E}(S)$. Then an observable $\mathbb{E}(S)$ corresponds to each S and its identification as a position projector to be applied to states $\{f\}$ is obvious.[14] Operators corresponding to local coordinates on M will not be introduced, except for $M=R_n$ (see Sec. 2C).

In (G,M,σ) the action of G on $\mathcal{B}$ is given by σ. So we have to connect $\mathbf{U}(G)$ and $\mathbb{E}(\mathcal{B})$ correspondingly and demand $\mathbf{U}(a)$ and $\mathbb{E}(S)$ to be such that

$$\mathbb{E}(\sigma_a(S))\,\mathbf{U}(a)=\mathbf{U}(a)\,\mathbb{E}(S) \tag{2.1}$$

holds for each $S\in\mathcal{B}$ and each $a\in G$. Hence in our physical interpretation (G,M,σ) contains the *covariance* of the system with respect to G: if $\{f\}\subset\mathcal{H}$ is a state localized in S, then $\{\mathbf{U}(a)f\}$ is localized in $\sigma_a(S)$.

(4) Mackey[1,2] considered the representation $\mathbf{U}(G)$ of G and the set of position projectors $\mathbb{E}(\mathcal{B})$ on $\mathcal{B}$ fulfilling (2.1) as a pair $(\mathbf{U},\mathbb{E})$ called *system of imprimitivity* (SI) for G based on M. The notation $(\mathbf{U},\mathbb{E})$ is shorthand for the triple $(\mathbf{U},\mathbb{E},\sigma)$. If G acts transitively on M, SI is called transitive. Each SI gives a natural realization of $\mathcal{H}$ as a linear space of equivalence classes of complex vector-valued functions f over M under the inner product

$$(f,g)=\int_M \langle f(p),g(p)\rangle\, d\mu(p),$$

where μ is a G-quasi-invariant measure on M.

There is a connection between the differentiable G-transformation group (G,M,σ) and the SI for G based on M in $\mathcal{H}$: Using $\mathcal{B}$ given above, we define from (G,M,σ) the triple $(G,\mathcal{B},\sigma)$. Then $(\mathbf{U}(a),\ \mathbb{E}(\mathcal{B}),\sigma)$ is a *representation of* $(G,\mathcal{B},\sigma)$ in $\mathcal{H}$, as there exists an isomorphism $\mathcal{J}$ mapping the pair $(a,S)\in(G,\mathcal{B})$ into a pair $(\mathbf{U}(a),\ \mathrm{E}(S))$ of bounded operators in $\mathcal{H}$,

$$\mathcal{J}:(G,\mathcal{B})\ni(a,S)\to(\mathbf{U}(a),\ \mathbb{E}(S))\in(\mathbf{U}(G),\ \mathbb{E}(\mathcal{B})),$$

such that

(i) $\mathcal{J}: G\to\mathbf{U}(G)$ is a G-isomorphism and $\mathbf{U}$ unitary,

(ii) $\mathcal{J}:\mathcal{B}\to\mathbb{E}(\mathcal{B})$ is a Borel isomorphism, and

(iii) G acts on $\mathcal{B}$ as $\mathbf{U}(G)$ on $\mathbb{E}(\mathcal{B})$ [Eq. (2.1)].

We call the geometrical object $(G,\mathcal{B}(M),\sigma)$ the *kinematical structure* of the quantum system and its representation $\mathcal{J}$ in $\mathcal{H}$, denoted by $\mathcal{J}(G,M,\sigma)$, a *quantization.*

(5) The question is (1) to construct all inequivalent representations of kinematical structures $(G,\mathcal{B},\sigma)$, and (2) to select the physical ones and to introduce Hamiltonians, i.e., quantum dynamics.

The answer to the first question was given by Mackey.[1] He constructed all (inequivalent) *canonical SI* (see Appendix A) and proved that each SI is unitarily equivalent to one canonical SI. However, Mackey's construction is not suited for all physical applications and for an attempt to answer the second question. This is mainly because a quantization of $(G,\mathcal{B},\sigma)$ relies on some of its not apparent geometrical properties which should have some impact on the physics of the system. For applications it is therefore useful to formulate $(G,\mathcal{B},\sigma)$ and $\mathcal{J}(G,M,\sigma)$ closer to geometrical concepts. A group structure is quite promising for this and is discussed in the next section.

B. Construction of quantum kinematics via embedding

(1) Let T_n be an n-dimensional real vector space and $\hat{T}_n$ its dual, respectively; consider T_n as an Abelian group and $\hat{T}_n$ as its character group, and let $G^\tau=T_n\otimes_\tau G$ be a semidirect product where $\tau: a\to\tau_a$ is a homomorphism from G into the *linear* group of automorphisms of T_n. The action of $a\in G$ on $\hat{T}_n$ induced by τ_a is denoted by $\hat{\tau}_a:\chi\to\hat{\tau}_a(\chi)$, $\chi\in\hat{T}_n$.

(2) Consider a representation $\mathcal{J}(G,\hat{T}_n,\hat{\tau})=(\mathbf{U}(G),\ \mathbb{E}(\mathcal{B}_n),\hat{\tau})$, $\mathcal{B}(\hat{T}_n)=\mathcal{B}_n$, with linear action τ in T_n and a unitary representation (UR) $\mathbf{U}(G^\tau)$ of G^τ. Both representations are intimately related. To indicate this, suppose $\mathbf{U}(G^\tau)$ is given. Then one can obtain $\mathbf{U}(G)$ from $\mathbf{U}(G^\tau)\downarrow G$ and $\mathbb{E}(\mathcal{B}_n)$ from harmonic analysis of $\mathbf{U}(G^\tau)\downarrow T_n$. The semidirect product ensures that $\mathbf{U}(G)$ acts via $\hat{\tau}$ covariantly on $\mathbb{E}(\mathcal{B}_n)$. Hence $\mathbf{U}(G)$ and $\mathbb{E}(\mathcal{B}_n)$ build a representation of $(G,\mathcal{B}_n,\hat{\tau})$. The reverse construction is also possible. The exact formulation is[16]

Lemma 1 (*Mackey*):

(a) Let $(\mathbb{U}, \mathbb{E})$ be a system of imprimitivity for G in $\mathcal{H}$ based on $\hat{T}_n$. Then there exists a unique unitary representation $\mathbb{U}(G^\tau)$ of $G^\tau = T_n \circledS_\tau G$ in $\mathcal{H}$ such that

1. $\mathbb{U}(G^\tau) \downarrow G = \mathbb{U}$,
2. $\mathbb{E}$ is a projection-valued measure on $\hat{T}_n$ corresponding[17] to $\mathbb{U}(G^\tau) \downarrow T_n$.

(b) Let $\mathbf{U}(G^\tau)$ be a unitary representation of G^τ. Then it determines uniquely a system of imprimitivity $(\mathbf{U}, \mathbb{E})$ for G based on $\hat{T}_n$ with

1. $\mathbb{U} = \mathbf{U}(G^\tau) \downarrow G$,
2. $\mathbb{E}$ being a projection-valued measure on $\hat{T}_n$ corresponding[17] to $\mathbb{U}(G^\tau) \downarrow T_n$.

(c) $(\mathbf{U}, \mathbb{E})$ is irreducible if and only if $\mathbf{U}(G^\tau)$ is; two systems of imprimitivity $(\mathbb{U}_i, \mathbb{E}_i)$, $i = 1, 2$, are unitarily equivalent, if and only if the corresponding $\mathbb{U}_i(G^\tau)$ are.

(3) Consider the sets

$$\mathcal{S}(G, M) = \{\mathrm{SI}(\mathbf{U}, \mathbb{E}, \sigma) \text{ of } G \text{ based on } M\},$$

$$\mathcal{U}(G^\tau) = \{\mathrm{UR} \text{ of } G^\tau\};$$

then[1,6]

$$\mathcal{S}(G, \hat{T}_n) \supset \mathcal{S}(G, M^0)$$

holds with M^0 being any G orbit in $\hat{T}_n$ and Mackey's lemma implies a one-to-one mapping ρ of $\mathcal{S}$ onto $\mathcal{U}$

$$\rho : \mathcal{S}(G, \hat{T}_n) \ni (\mathbf{U}, \mathbb{E}, \sigma) \longleftrightarrow \mathbf{U}(G^\tau) \in \mathcal{U}(G^\tau),$$

with restrictions

$$\rho^0 : \mathcal{S}(G, M^0) \to \mathcal{U}(G^\tau), \quad \rho^{\mathrm{irr}} : \mathcal{S}^{\mathrm{irr}}(G, \hat{T}_n) \longleftrightarrow \mathcal{U}^{\mathrm{irr}}(G^\tau).$$

Hence all (irreducible) representations of the kinematical structure (G, β, σ) together with a realization of $\mathcal{H}$ can be derived from (irreducible) UR of an inhomogenization of G, *if* M can be identified with a G orbit in $\hat{T}_n$.

However, this identification is not possible in general. Consider an embedding[18] $\iota : M \to \iota M \subset \hat{T}_n$; then the action σ of G on M and the action $\hat{\tau}$ of $G \subset G^\tau$ on ιM can be different. For an identification they must be compatible, i.e., ι is *equivariant* $\iota \sigma_a = \hat{\tau}_a \iota$; the diagram

$$\begin{array}{ccc} M & \xrightarrow{\sigma_a} & M \\ \iota \downarrow & & \downarrow \iota \\ \iota M & \xrightarrow{\hat{\tau}_a} & \iota M \end{array}$$

is commutative.

To formulate and to prove this, assume G^τ to be regular[19] and recall[1,6] that

(i) the irreducible UR (IUR) of G^τ in $\mathcal{H}$ are uniquely classified and each given by a G orbit $M^0 = G/K^0$ in $\hat{T}_n$ and an IUR $L(K^0)$ of K^0 in a Hilbert space $\mathcal{L}$ (K^0 is the corresponding isotropy subgroup); in short, irreducible $\mathbb{U}(G^\tau)$ are labelled by (M^0, L);

(ii) irreducible SI for G based on $M = G/K$ are uniquely classified and each given by an IUR $L(K)$ of K in $\mathcal{L}$; in short, irreducible $(\mathbb{U}, \mathbb{E}, \sigma)$ are labelled by (L);

(iii) the SI for G based on $\hat{T}_n$ determined from $\mathbf{U}(G^\tau)$ with (M^0, L) is unitarily equivalent to an SI based (only) on the G orbit M^0 and is labelled by (L).

Lemma 2: Consider $\mathbf{U}^0(G^\tau)$ with (M^0, L^0) and the SI $(\mathbf{U}^0(G), \mathbb{E}^0(\beta^0), \hat{\tau})$ determined from $\mathbf{U}^0(G^\tau)$. Let $(\mathbf{U}(G), \mathbb{E}(\beta), \sigma)$ be an SI based on $M = G/K$ with (L). Suppose K to be isomorphic to K^0 and L unitarily equivalent ($\cong$) to L^0. Then

$$(\mathbf{U}, \mathbb{E}, \sigma) \cong (\mathbf{U}, \mathbb{E}^0, \hat{\tau})$$

if and only if there exists an embedding $\iota : M \to \hat{T}_n$ with

(i) $\iota M = M^0$,

(ii) ι is equivariant with respect to σ and $\hat{\tau}$.

The proof is given in Appendix A.

(4) A mapping

$$\iota : (G, M, \sigma) \to (G, M', \sigma'), \quad \iota(G, M, \sigma) = (G, \iota M, \sigma')$$

for equivariant ι is called an embedding of (G, M, σ) in (G, M', σ').[20] We define accordingly an embedding ι_β for kinematical structures

$$\iota\beta : (G, \beta, \sigma) \to (G, \beta', \sigma'), \quad \iota_\beta(G, \beta, \sigma) = (G, \iota\beta, \sigma')$$

with equivariant ι.

With Υ connecting unitarily equivalent SI and the mappings $\mathcal{J}, \mathcal{J}^0, \rho^0$ defined before, we have the following *quantization diagram* ($M = G/K$, $M^0 = \iota M$):

$$\begin{array}{ccc} (G, \beta(M), \sigma) & \xrightarrow{\iota_\beta} & (G, \beta(\hat{T}_n), \hat{\tau}) \\ \mathcal{J} \downarrow & & \mathcal{J}^0 \downarrow \\ (\mathbf{U}(G), \mathbb{E}(\beta(M)), \sigma) & \xrightarrow{\Upsilon} & (\mathbf{U}(G), \mathbb{E}(\beta(M^0)), \hat{\tau}) \\ & & \rho^0 \downarrow \\ & & \mathbf{U}(G^\tau) \end{array}$$

geometrical level; quantum level

system moving on M — system moving in R_n bound on $M^0 \subset R_n$

Lemmas 1 and 2 imply that for given $\mathcal{J}$ and ι_β there exist $\mathcal{J}^0, \rho^0$, and Υ if and only if ι is equivariant. In this case the diagram is commutative. We formulate this as

Corollary: The representations of a kinematical structure (G, β, σ) can be determined uniquely (up to unitary equivalence) from $\mathbf{U}(G^\tau)$, if and only if there exist an integer $n > 0$ and $\hat{\tau}$ such that (G, β, σ) can be embedded in $(G, \beta_n, \hat{\tau})$.

It is known[21] that for compact G for each (G, M, σ) an embedding ι in a Euclidean G space $(G, R_n, \hat{\tau})$ exists.[22] A construction of ι for homogeneous M can be found in Ref. 20. For a useful necessary and sufficient condition, if a G orbit is contained in a linear representation of G in some Euclidean space, see Ref. 23.

C. Examples[24]

(1) Consider the kinematical structure $(T_n, \beta(R_n), \sigma)$ —R_n is the group space of T_n—with

$$\sigma : T_n \ni \mathsf{b} \to \sigma_{\mathsf{b}}, \quad \sigma_{\mathsf{b}}(\mathsf{q}) = \mathsf{q} + \mathsf{b}, \quad \mathsf{q} \in R_n.$$

Its quantization is given by $(\mathbf{U}(T_n), \mathbb{E}(\beta), \sigma)$ and is uni-

que (if irreducible). The position projections $\mathbb{E}(S)$ can be used to define self-adjoint operators $\mathbb{Q}_\kappa$, $\kappa = 1, \ldots, n$, on $\mathcal{D}$ dense in $\mathcal{H}$ by the spectral decomposition

$$\mathbb{Q}_\kappa = \int_{-\infty}^{+\infty} d\mathbb{E}(S_\lambda) \quad \text{where } S_\lambda = \{\mathbf{q} \mid q_\kappa \leq \lambda\}.$$

Because of the covariance condition (2.1) the $\mathbb{Q}_\kappa$ transform as

$$\mathbf{U}(\mathrm{b})\mathbb{Q}_\kappa \mathbf{U}(\mathrm{b})^{-1} = \mathbb{Q}_\kappa + \mathrm{b}_\kappa \mathbb{1} \text{ on } \mathcal{D},$$

and give infinitesimally an integrable representation of the Lie algebra $\underline{H}_n = (\underline{C} \oplus \underline{Q}_n) \dotplus \underline{T}_n$ of the Heisenberg group H_n; Q_n is Abelian and $\underline{C}$ is a central element.

(2) A slightly more general kinematical structure on R_n is $(G, \beta(R_n), \sigma)$ with $G = T_n \circledS \tilde{SO}_0(n)$, i.e., $R_n = G/\tilde{SO}_0(n)$ and with σ as standard linear action of the Euclidean group in R_n. Its quantization is characterized by $L(\tilde{SO}_0(n))$. Operators $\mathbb{Q}_\kappa$ can be defined as before and the covariance condition gives infinitesimally an integrable representation of the Lie algebra $\underline{G}_0 = (\underline{C} \oplus \underline{Q}_n) \dotplus (\underline{T}_n \dotplus \underline{so}(n))$ of the geometrical Galilei group G_0. The interpretation of $L(\tilde{SO}_0(n))$ as physical spin group is obvious.

(3) $\mathcal{G}(G, R_n, \sigma)$ has interesting properties:

(a) The spin of the system in R_n appears *after* quantization; it is part of the quantized kinematical structure, not present on the geometrical level, and its possible existence depends on the choice of the group G in (G, R_r, σ).

(b) G acts linearly on $M = R_n$. Hence (G, R_n, σ) can be considered as a Lie group: (T_n, R_n, σ) as H_n and $(T_n \circledS \tilde{SO}_0(n), R_n, \sigma)$ as G_0, and quantization yields representations of these Lie groups. Therefore, the construction of $\mathbb{Q}_\kappa$ is possible. For general (G, M, σ) global position operators defined intrinsically on M need not exist.

(c) The noncommutativity of $\mathbb{P}_\kappa$ and $\mathbb{Q}_\kappa$ is the result of the covariance condition and of the linear action of T_n or $T_n \circledS \tilde{SO}_0(n)$ in R_n. It is independent[25] of the fact that the states of the system have to be identified with rays in $\mathcal{H}$.

D. Summary

(1) A quantum system

(i) having a homogeneous space $M = G/K$ as configuration manifold,
(ii) being covariant with respect to G,
(iii) being localizable in M,
has on the geometrical level a kinematical structure (G, β, σ) constructed from a differentiable G-transformation group (G, M, σ) with β being a suitably chosen field of Borel sets S in M. The quantization of the kinematical structure is a representation in $\mathcal{H}$: $\mathcal{G}(G, \beta, \sigma) = (\mathbf{U}(G), \mathbb{E}(\beta), \sigma)$ with $\mathbf{U}(G)$ being a UR of G and $\mathbb{E}(\beta)$ being a set of projection-valued measures on M, both satisfying (2.1); they are systems of imprimitivity, completely classified by Mackey. The quantum kinematics[26] is independent of any coordinatization of the configuration space M.

(2) If (G, M, σ) can be embedded into a Euclidean G space $(G, \hat{T}_n, \hat{\tau})$, the kinematical structure can be quantized using a UR of the group $G^\tau = T_n \circledS_\tau G$, i.e., $\mathbf{U}(G)$ and $\mathrm{E}(\beta)$ are uniquely determined from $\mathbf{U}(G^\tau)$ and vice versa.

(3) The quantization of (G, β, σ) yielding an SI based on M can also be formulated in a more abstract (algebraic) way[27]: From (G, M, σ) one can construct a Banach $*$-algebra $L(G, M, \sigma)$ called the (G, M, σ)-*transformation group algebra*. Its nondegenerate $*$-representations can be constructed via a generalized inducing process, and are in natural one-to-one correspondence with $(\mathbf{U}(G), \mathbb{E}, (\beta), \sigma)$. $L(G, M, \sigma)$ is the completion of the convolution $*$-algebra of all continuous complex functions on $G \times M$ with compact support. Hence it contains (a) the group algebra $L(G)$, (b) the C^*-algebra $C_0(M)$ of all (continuous) complex functions on M with compact support, and the representations of $L(G)$ and $C_0(M)$ obtained from a representation of $L(G, M, \sigma)$ uniquely correspond to $\mathbf{U}(G)$ and $\mathbb{E}(\beta)$, respectively. So there is a formulation in which M is determined by $C_0(M)$ which is more reasonable than Borel sets. However, the quantization on M with $L(G, M, \sigma)$ is more complicated than the approach used here and will lead to the same results.

3. FREE QUANTUM SYSTEMS

A Hamiltonian for a system with $\mathcal{G}(G, M, \sigma)$ is an essentially self-adjoint (e.s.a.) operator and a function of the momentum operators and position projections of $\mathcal{G}(G, M, \sigma)$. To define a free Hamiltonian $\mathbb{H}^0$ on M consistently with $\mathcal{G}(G, M, \sigma)$ we discuss different methods on the geometrical and on the quantum level: *Extrinsic* ones which try to project properties of systems in R_n to an embedding ιM of M in R_n, and *intrinsic* ones which rely only on properties of $\mathcal{G}(G, M, \sigma)$.

A general outline of the different methods is given in Sec. 3A, for an extrinsic and an intrinsic method see Secs. 3B and 3C, respectively. Examples are treated in Sec. 3D and a summary is given in 3E.

A. The Hamiltonian

(1) We propose first an *extrinsic* method on the quantum level to define the free Hamiltonian $\mathbb{H}^0$ on M. Consider a quantum system moving on R_n with $\mathcal{G}(G, R_n, \tau)$, $G = T_n \circledS \tilde{SO}_0(n)$. Its free Hamiltonian is $\mathbb{H}_n^0 = q\,\mathbb{\Delta}_n$ with $\mathbb{\Delta}_n$ being the Laplacian and $q = (2m_0)^{-1}$ being a factor of dimension $[m^{-1}]$; m_0 is the mass of the system in R_n. Following Sec. 2B, (G, β, σ) can be quantized in two steps: An embedding $\iota : M \to R_n$ in $(G, \beta(R_n), \tau)$ and a restriction of $\mathcal{G}(G, R_n, \tau)$ to ιM. An application of this result (Lemma 2) to a calculation of $\mathbb{H}^0$ is reasonable: Take $\mathbb{H}_n^0$ defined in $\mathcal{G}(G, R_n, \tau)$ and restrict $\mathbb{H}_n^0$ to M with a submersion π: $R_n \to M$. The unique result is an operator on M which, if e.s.a. may be identified with $\mathbb{H}^0$.

(2) An intrinsic method on the quantum level uses an *invariance* argument. For a given $\mathcal{G}(G, M, \sigma)$ a differential operator $\mathbb{D}$ e.s.a. on $\mathcal{D}$ may be identified with $\mathbb{H}^0$ if

(i) $\mathbb{D}$ is G-invariant: $\mathbf{U}(G)\mathbb{D}\mathbf{U}(G)^{-1} = \mathbb{D}$ on $\mathcal{D}$,
(ii) $\mathbb{D}$ is a differential operator of minimal order.

If momentum and energy conservation for "free system

on M" is enforced, assumption (i) is necessary. Assumption (ii) is motivated only by the poor analogy to the free system in R_n. If there is no G-invariant differential operator on M, the conservation laws fail for free systems on M.

(3) In both methods discussed so far the Hamiltonian was introduced on the quantum level (see the quantization diagram), so an additional quantization of the Hamiltonian was not necessary. However, it is possible also to introduce dynamics on the *geometrical level* and to quantize it in a second step, using, e.g., a procedure similar to the correspondence principle. The difficulty is that one has to justify *both* the classical Hamiltonian *and* its quantization. It is well known that the quantization of a classical observable is in general not unique and need not be compatible with the quantized kinematical structure. However, there are also unique and compatible quantizations.

To indicate this we sketch shortly a method starting on the *kinematical* level. Consider M, (R_n, g_n) and $\iota: M \to R_n$. Then the Riemannian structure g on M [and its associated (2,0)-tensor field g'] are uniquely given by

$$g = \iota^* g_n, \quad \iota_*: T(M) \to T(R_n),$$
$$\iota^* g_n(X, Y) = g_n(\iota_* X, \iota_* Y), \quad X, Y \in T(M).$$

The classical free Hamiltonian on R_n is given by qg_n', so as a first step we define $q \cdot (\iota^* g_n)'$ as classical free Hamiltonian.

To reach the quantum level in a second step, we give two quantization procedures:

(a) $\mathcal{G}(G, M, \sigma)$ contains a natural mapping $d\mathcal{G}$ of vector fields X_i on M at p into $d\mathbb{U}(\underline{G})$ considered as an r-dimensional vector space

$$d\mathcal{G}: T_p(M) \ni X_i \to \mathbf{X}_i = d\mathbb{U}(X_i) \in d\mathbb{U}(\underline{G}), \quad i = 1, \ldots, r.$$

Hence $d\mathcal{G}$ applied to $T_p(M) \times T_p(M)$ sends $\sum_{i} g(X_i, X_i)_p$ to an operator $\mathbf{g}_p$ in $\mathcal{H}$, and gives a "Riemann operator" $\mathbf{g}$ which is a second-order polynomial in the generators of $\mathbb{U}(G)$ with p-dependent coefficients. $q\mathbf{g}$ can be used as quantized free Hamiltonian. However, $\mathbf{g}$ is not symmetric in general; it has to be symmetrized, and this can be done in various ways with quite different results.

(b) The Laplace–Beltrami operator Δ_M on (M, g) is unique. $\mathbf{H}_n^0$ is proportional to Δ_n on (R_n, g_n), i.e., the quantization of g_n' is Δ_n. The corresponding procedure applied to $(\iota^* g_n)'$ gives uniquely

$$\mathbf{H}^0 = q\Delta_M \quad \text{on } (M, \iota^* g_n) \text{ in } C^\infty(M) \subset L^2(M, \mu_g),$$
$$d\mu_g = \sqrt{\det(g_{ba})}\, d^m x.$$

Δ_M is a second-order differential operator. For (M, g) being a complete Riemannian manifold, e.g., a Riemannian homogeneous space, Δ_M is e.s.a. in $L^2(M, \mu_g)$ of vector-valued functions.[28] Note that Δ_M is not necessarily G-invariant. The justification of the procedure is weak [see Sec. 3B(6)]; however, the result is reasonable.

B. Hamiltonians via submersion

(1) R_n is a Euclidean Riemannian space (R_n, g_n) if the Euclidean Riemannian structure g_n is imposed on R_n. Because the Laplacian Δ_n on (R_n, g_n) and hence $\mathbf{H}_n^0$ are directly related with properties of (R_n, g_n), we introduce a Riemannian structure g on M. If g is G-invariant, (M, g) is a Riemannian homogeneous space. Note that a G-invariant g determines a G-invariant Riemannian measure μ_g on M which can be used as quasi-invariant measure on $M = G/K$ for the inner product in $\mathcal{H}$ (see Appendix A).

(2) We explain the submersion in a simple example. Consider (R_2, g_2) and the circle S^1. Map S^1 with ι onto the unit circle in (R_2, g_2). Take the manifold $W = R_2 \setminus \{0\}$ with 0 as origin of R_2. Define a mapping $\pi: W \to S^1$ such that all points r of a fixed ray N_p in W starting from 0 are mapped into its intersection p with S^1, i.e., $\pi(r) = p$. It is easily checked that π is a submersion (see below) of W onto S^1 along totally geodesic fibers $\pi^{-1}(p)$. The tangent spaces $T_r(W)$ can be decomposed in (here one-dimensional) orthogonal subspaces $T_r^{\parallel}$ and $T_r^{\perp}$ such that π induces a mapping π_{*r} on $T_r(W)$ sending $T_r^{\parallel}$ onto $T_{\pi(r)}(S^1)$ and $T_r^{\perp}$ to the null vector $0_{\pi(r)}$ of $T_{\pi(r)}(S^1)$; π is even a Riemannian submersion (see below).

Take now the Laplacian Δ_2 on R_2, i.e., in Cartesian coordinates, $\Delta_2 \tilde{f} = (\partial^2/\partial q_{\parallel}^2)\tilde{f} + (\partial^2/\partial q_{\perp}^2)\tilde{f}$ with $\tilde{f}(\mathbf{q}) \in C^\infty(R_2)$ and $\mathbf{q} \in R_2$. Then $\Delta_2(f \circ \pi)(\mathbf{q}) = (\partial^2/\partial q_{\parallel}^2)(f \circ \pi)(\mathbf{q}) + (\partial^2/\partial q_{\perp}^2)(f \circ \pi)(\mathbf{q})$ is a "restriction" of Δ_2 in R_2 to S^1 and because of π (Riemannian submersion along totally geodesic fibers) the second term vanishes. With $c(t)$ an R_2-geodesic perpendicular to N_p and parametrized by t, the first term is $(\Delta_2 f)(r) = (d^2/dt^2)(f \circ \pi)(c(t))|_{t=0}$ and the introduction of the polar angle φ leads to the known result.

(3) In a general setting, let W and M be C^∞-manifolds. A mapping $\pi: W \to M$ is called a *submersion at point* $r \in W$, if there exist charts (V, ξ) at r and (U, x) at $\pi(r)$ such that ξ determines an isomorphism of the set V on a product $V_1 \times V_2$ where V_1, V_2 are open subsets of some model Euclidean spaces and the mapping

$$f_{U;V} = X \circ \pi \circ \xi^{-1}: V_1 \times V_2 \to xU$$

is a projection.[29] A submersion π at r can also be characterized by its differential π_{*r} being surjective and its kernel decomposing $T_r(W)$.

If $\pi: W \to M$ is a submersion, and if (W, g_n) is a Riemannian manifold, then $T_r(W)$ has a canonical decomposition

$$T_r(W) = (\pi_{*r})^{-1}(0_{\pi(r)}) \oplus M_r,$$

where M_r is the subspace of $T_r(W)$ which is orthogonal to the kernel of π_{*r}, $0_{\pi(r)}$ is the null vector in $T_{\pi(r)}(M)$, and π_{*r} induces an isomorphism of M_r onto $T_{\pi(r)}(M)$.

A submersion π is called *Riemannian submersion*, if π_{*r} induces an isomorphism of Euclidean spaces from M_r on $T_{\pi(r)}(M)$.

A connected submanifold S of a Riemannian manifold W is *geodesic at* $p \in S$, if each W geodesic tangent to S at p is a curve in S; S is *totally* geodesic if it is geodesic at each of its points.

(4) The following theorem is essential for a restriction of the Laplace operator Δ_n to $M \subset R_n$.

Theorem 1[30,31,32]: Let M be a homogeneous space and W a submanifold of dimension n in R_n; Δ_n and Δ_M the Laplace–Beltrami operators on (R_n, g_n) and on (M, g), resp.; π: $(W, g_n) \to (M, g)$ a Riemannian submersion; $\pi^{-1}(p)$ totally geodesic in W for each $p \in M$; $f(p) \in C^\infty(M) \subset L^2(M, \mu_g)$.

Then

$$\Delta_n(f \circ \pi) = (\Delta f) \circ \pi. \tag{3.1}$$

(5) To apply this to a quantized kinematical structure $\mathcal{G}(G, M, \sigma)$ note that the above Riemannian submersion π (along totally geodesic fibers) determines an associated isometric embedding ι: $(M, g) \to (W, g_n)$ defining the same submanifold M in R_n as π. However, the quantization of $(G, \mathcal{B}(M), \sigma)$ via an embedding in $(G, \mathcal{B}(R_n), \tau)$ already determines an (equivariant) mapping of M onto a given G orbit (or an orbit of the same type) and one must ensure that π yields an associated embedding which maps M onto an orbit of a given type. Insofar as the existence of π is known, this is the case. Consider the set of G orbits of one type. Suppose that they build a submanifold, (called "orbit manifold") W in R_n with $\dim W = n$. Then π: $(W, g_n) \to (M, g)$ exists[33] with $\pi^{-1}(p)$ totally geodesic in W for each $p \in M$ and the associated embedding ι is equivariant. G orbits with orbit manifold of dimension n exist, e.g., for $G = SO(2)$ and R_2, where the circles centered at 0 are $SO(2)$ orbits of one type and dense in R_2. More generally, for compact G the principal G orbits build an orbit manifold with dimension n dense in R_n, and all nonprincipal G orbits build a topological submanifold in R_n.[20,21] There are no results for noncompact groups.

For the application of Theorem 1 we formulate:

Lemma 3: Let ι be an equivariant embedding of (G, M, σ) in (G, R_n, τ). Consider $\mathcal{G}(G, R_n, \tau)$ labelled by a trivial $L(K)$ and by a G orbit ιM with an orbit manifold of dimension n; $\mathcal{G}(G, R_n, \tau)$ is unitarily equivalent to some $\mathcal{G}(G, M, \sigma)$.

Then a Riemannian submersion along totally geodesic fibers restricts $\mathbb{H}_n^0$ on $C^\infty(R_n)$ to a free Hamiltonian $\mathbb{H}^0$ on $C^\infty(M)$ with $\mathcal{G}(G, M, \sigma)$ as quantized kinematical structure. $\mathbb{H}^0$ is up to a constant multiple the Laplace–Beltrami operator Δ_M on $(M, \iota^* g_n)$ and ι is associated with π.

(6) The submersion π is (up to now) applicable to (G, M, σ) with compact G, with quantization on principal G orbits and with a Hilbert space spanned by scalar functions. For the self-adjointness of $\not\Delta_M$ see Sec. 3A(3). Generalizations to vector-valued functions and hence to $\mathcal{G}(G, M, \sigma)$ with nontrivial $L(K)$ are possible.

(7) We add a remark concerning *quantization by embedding and submersion*. The calculation of $\mathbb{H}^0$ is a special case of a more general (extrinsic) procedure[34] to describe quantum mechanics on M: Embed M in R_n. Then the physical observables on ιM are restrictions of the corresponding observables in R_n which are known from $\mathcal{G}(T_n, R_n, \tau)$. There are examples in which this procedure fails.

We give the momentum and the position operators $\mathbb{P}_\kappa^\iota$, $\mathbb{Q}_\kappa^\iota$, $\kappa = 1, \ldots, n$, on $\iota M \subset R_n$ which refer to Cartesian coordinates q_κ of the ambient space R_n, not to local coordinates on M, as, e.g., x^a in $U \subset M$. The $\mathbb{Q}_\kappa^\iota$ are easily calculated from ι: $M \ni p \to \iota(p) \in R_n$,

$$\mathbb{Q}_\kappa^\iota f(\iota(p)) = q_\kappa(\iota(p)) f(\iota(p)) \quad \text{on } C^\infty(\iota M),$$

and can be constructed also from $\mathbb{U}(G^\tau) \downarrow T_n = \mathbb{U}(T_n)$ if $\mathcal{G}(G, M, \sigma)$ is determined from $\mathbb{U}(G^\tau)$ with $(\iota M, L)$, L being trivial. One can check that $d\mathbb{U}(T_n)$ acts as $\mathbb{Q}_\kappa^\iota$ on $C^\infty(\iota M)$.

To derive $\mathbb{P}_\kappa^\iota$, express π and ι in local coordinates[35] (x^a), $a = 1, \ldots, m$, at $p \in M$ and (ξ^κ), $\kappa = 1, \ldots, n$, at $r \in W$ as

$$\iota_{*p}: \; T_p(M) \to T_r(W) : \partial_b \mapsto B_b^\lambda \partial_\lambda, \quad r = \iota(p),$$

$$\pi_{*r}: \; T_r(W) \to T_p(M) : \partial_\kappa \mapsto B_\kappa^a \partial_a, \quad p = \pi(r),$$

where $B_\kappa^a = \partial_\kappa x^a$, $B_a^\lambda = \partial_a \xi^\lambda$, $\partial_a = \partial/\partial x^a$, $\partial_\lambda = \partial/\partial \xi^\lambda$. Assuming that ι and π determine the same submanifold M of W, we can define the product mapping

$$\iota_{*\pi(r)} \circ \pi_{*r} : T_r(W) \to T_{\iota \circ \pi(r)}(W) : \partial_\kappa \mapsto B_\kappa^\lambda \partial_\lambda,$$

where $B_\kappa^\lambda = B_\kappa^a B_a^\lambda$ is a perpendicular projection of rank $m < n$.

With this projection we have (in symmetrized form)

$$\mathbb{P}_\lambda^\iota = \tfrac{1}{2}(B_\lambda^\kappa \mathbb{P}_\kappa + \mathbb{P}_\kappa B_\lambda^\kappa) \quad \text{on } C^\infty(\iota M), \quad \mathbb{P}_\kappa = -i \frac{\partial}{\partial q_\kappa}.$$

The free Hamiltonian was given above for special cases only. The result is generalized to

$$\mathbb{H}^0 = q \, \Delta_M^\iota \quad \text{on } (\iota M, \iota^* g_n) \text{ on } C^\infty(\iota M).$$

Δ_M^ι can be expressed in Cartesian coordinates q_κ as (for a proof see Appendix B)

$$\not\Delta_M^\iota = \delta^{\lambda\kappa} \partial_\mu B_\lambda^\mu \partial_\kappa \quad \text{on } C^\infty(\iota M). \tag{3.2}$$

Because $\mathbb{P}_\kappa$, $\mathbb{Q}_\kappa$ and $\mathbb{H}_n^0$ are related for the free particle as $\mathbb{P}_\kappa = -im_0[\mathbb{Q}_{\kappa 1}, \mathbb{H}_n^0]$ on $C^\infty(R_n)$, our ansatz for $\mathbb{H}^0$ should be consistent with $\mathbb{P}_\kappa^\iota = -im_0[\mathbb{Q}_\kappa^\iota, \mathbb{H}^0]$ on $C^\infty(\iota M)$ and this is in fact the case as can easily be checked using (3.2).

C. G-invariant operators

(1) We discuss systems with $\mathcal{G}(G, M, \sigma)$ with trivial $L(K)$ and with Hilbert space $L^2(M, \mu_g)$. The application of the mapping d to $\mathbb{U}(G)$ in $\mathcal{G}(G, M, \sigma)$ gives (first-order differential) operators $\mathbf{X}_i$, $i = 1, \ldots, r$ on $C^\infty(M)$ representing the generators of G. In our case there are no invariant linear differential operators of first order on $C^\infty(M)$.[36] So we start with second-order ones denoted by $\mathbb{J}$.

(2) For some classes of homogeneous spaces we give now a list for $\mathbb{J}$ on $C^\infty(M)$.

(A) M being a *group manifold* of a connected *semisimple* Lie group G,

$$\mathbb{J} = q^{ij} \mathbf{X}_i \mathbf{X}_j \quad \text{on } C^\infty(M), \tag{3.3}$$

where q^{ij} is any Ad(G)-invariant symmetric tensor on $\underline{G}$. If G is *simple*, q^{ij} is proportional to the Cartan–Killing metric tensor and

$$\mathbb{J} = q \, \Delta_M \quad \text{on } C^\infty(M); \tag{3.4}$$

Δ_M is the Laplace–Beltrami operator on $M=G$ for the canonical Riemannian structure. For G semisimple with $G=G_1\otimes\cdots\otimes G_k$ and G_j simple, $\mathfrak{J}$ can be written as a real linear combination of the Laplace–Beltrami operators on $M_j=G_j$.[37]

(B) M being a *reductive homogeneous space*[38] G/K [i.e., in the Lie algebra $\underline{G}$ there exists a subspace $\underline{M}$ such that $\underline{G}=\underline{K}\oplus\underline{M}$ and $\mathrm{Ad}_G(k)\underline{M}\subset\underline{M}$ for all $k\in K$], $\mathfrak{J}$ has the form (3.3) where q^{ij} is an $\mathrm{Ad}_G(K)$-invariant tensor on $T_0(M)=\underline{M}$. The simpler form (3.4) is obtained if the Riemannian homogeneous space $(M=G/K,g)$ is *isotropy irreducible*,[39] i.e., if $G=I_0(M)=$component of identity in the group of isometries of M, and the connected component of $\mathrm{Ad}_G(K)$ acts irreducibly on $\underline{M}$. For a classification of such manifolds see Ref. 40.

(C) M being a Riemannian globally *symmetric space*,[8] $\mathfrak{J}$ has the same properties as in (B); there exist l algebraically independent (l is the rank of M) invariant symmetric differential operators which commute.

(D) M being of rank 1 (or Euclidean space), Is it uniquely given by (3.4).

(3) The list shows that $\mathfrak{J}$ is unique and proportional to the Laplace–Beltrami operator on (M,g) for $M=G$ and G simple and for M being an isotropy irreducible Riemannian homogeneous space. For the self-adjointness see Sec. 3A(3).

D. Summary

(1) The problem was the following: Consider a quantized kinematical structure $\mathcal{J}(G,M,\sigma)$, $M=G/K$. It is possible to define a Hamiltonian $\mathbb{H}^0$ of a free system on M, i.e., of a free particle, moving on M, consistently with the $\mathcal{J}(G,M,\sigma)$?

The answer is not affirmative. The best one can say is: For a larger class of M and G, depending on the method used to select $\mathbb{H}^0$ and for $\mathcal{J}(G,M,\sigma)$ obtained from $\mathfrak{U}(T_n\otimes_\tau G)$ with trivial $L(K)$ and a labelling G-orbit $\iota M\subset R_n$, e.g., for a spinless particle moving on M, $\mathbb{H}^0$ is uniquely given as the real multiple of the Laplace–Beltrami operator on (M,ι^*g_n), e.s.a. on $C^\infty(M)\subset L^2(M,\mu_g)$.

Because different methods, if applicable and if the solution is unique, give the same result, the ansatz

$$\mathbb{H}^0=q\,\Delta_M \quad \text{on } (M,\iota^*g_n) \text{ in } C^\infty(M) \tag{3.5}$$

is well justified.

(2) We discussed three methods:

(I) An intrinsic method on the quantum level was based on transformation properties of $\mathcal{J}(G,M,\sigma)$. We assumed $\mathbb{H}^0$ to be G-invariant and of minimal order. Result: For $M=G$ and for M being an isotropy irreducible Riemannian homogeneous space, $\mathbb{H}^0$ is uniquely given by (3.5).

(II) An extrinsic method on the quantum level is based on a submersion $\pi: R_n\to M$. The idea was to restrict consistently with $\mathcal{J}(G,M,\sigma)$ the free Hamiltonian $\mathbb{H}_n^0$ in R_n via a submersion to an operator $\mathbb{H}^0$ on M. Result: For compact G and $\mathcal{J}(G,M,\sigma)$ induced from principal orbits $\mathbb{H}^0$ is uniquely given by (3.5).

(III) An extrinsic method on the geometrical level is based on an embedding $\iota: M\to R_n$. The Riemannian structure ι^*g_n is imposed on M. The classical Hamiltonian on M is $q\cdot(\iota^*g_n)'$ and for its quantization the same procedure is applied as for the classical Hamiltonian on R_n. Result: For all Riemannian homogeneous spaces and for all G, $\mathbb{H}^0$ is uniquely given by (3.5).

4. DISCUSSION

(1). We give a short (and not complete) account of previous attempts to quantize systems on manifolds.

(A) One of the first was *formal quantization* of classical generalized coordinates x^b and canonical momenta p_a done in close analogy with the canonical quantization in R_n.[41] For given (M,g) the result is

$$\mathbb{Q}^b=x^b,\quad \mathbb{P}_a=-i\hbar\partial_a-\tfrac{1}{4}i\hbar\,\partial_a(\ln g),\quad g=\det(g_{ba}),$$

and the operators are symmetric in $L^2(M,\mu_g)$.

In nonrelativistic quantum mechanics this "quantization in curvilinear coordinates" has been applied to special systems with constraints like the rigid body, the rigid rotator and the symmetric top,[42] and further, in the strong coupling theory[3] and the rotator models of elementary particles.[5]

Another, more recent, generalization of canonical quantization when the system satisfies supplementary conditions has been proposed by Dirac[43] and applied to the quantization of gauge fields.[44] A more rigorous approach to the quantization on a Riemannian manifold (M,g) was indicated in Ref. 45.

The main difficulty of formal quantization of generalized coordinates and momenta is connected with the fact (mentioned in Sec. 2A) that on M the coordinates can, in most of the cases, be defined only locally. In the usual curvilinear coordinates the operators corresponding to them may not be well defined as can be exhibited in the simplest case of the unit circle $M=S^1$, where the multiplication by the angle $x=\varphi$ is not an operator in the Hilbert space $L^2(S^1,d\varphi)$ of periodic functions[46] $f(\varphi)=f(\varphi+2\pi)$.

(B) A second and promising approach generalizes *Feynman's path integral method*[47] to manifolds[48] and was applied to define the free Hamiltonian on M. The results obtained are different from ours: The Hamiltonian $\mathbb{H}^0$ on M has an additional term depending on the (intrinsic) scalar curvature R of (M,g),

$$\mathbb{H}^0=-\frac{1}{2m_0}(\Delta_M-\tfrac{1}{6}R).$$

However, the path integral method has mathematical problems; it was originally formulated as a set of rules which define the measure on the space of classical paths by means of a special procedure.[49] The connection to the proposed method is not yet clarified.

(C) Two further methods are to be mentioned:

The *dynamical group approach*,[50] in which the kinematics and, if possible, also the dynamics are given by a unitary representation of a Lie group such that momentum, position operators, and the Hamiltonian are among its generators. If (G,M,σ) can be replaced by a

Lie group, it is the kinematical subgroup of a dynamical group.

The *"Kostantification,"*[51] i.e., the construction of certain representations of Lie groups using a method developed by Kostant and Souriau based on properties of the phase space considered as symplectic manifold.

(2) The results of our attempt to tie up the group-theoretical approach to quantum kinematics with the differential-geometrical approach[52] to free particle dynamics are collected in Secs. 2D and 3D.

A generalization to locally compact separable group G is possible[1] because the SI exist in this case but the mapping $\alpha: G/K \to M$ is only a homeomorphism. So this is excluded by physics where we need a differential structure on M. According to Arens' theorem,[53] in order that α be a diffeomorphism we have to assume that G is a transitive differentiable transformation group of M, i.e., G is a Lie group.

ACKNOWLEDGMENTS

The authors would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality extended to them at the International Center for Theoretical Physics, Trieste, where the work was completed. One of the authors (J. T.) is greatly indebted to the Alexander von Humboldt Stiftung and to the University of Clausthal for financial support. Discussions with Drs. J. Hennig and J. Niederle are gratefully acknowledged.

APPENDIX A

(1) With the definitions of Sec. 2 the *canonical SI*[1,2] $(\mathbb{U}(G), \mathbb{E}(\mathcal{B}), \sigma)$ based on $M = G/K$ and given by $L(K)$ in $\mathcal{L}$ with inner product $\langle \cdot, \cdot \rangle$ is defined in $\mathcal{H}$ spanned by vector-valued functions $f: M \to \mathcal{L}$ with finite norm given by the inner product

$$(f,g) = \int_M \langle f,g\rangle(p)\, d\mu(p) \qquad (p \in M),$$

where μ denotes a G-quasi-invariant measure on M, as as follows: $\mathbb{U}(G)$ is given by $[\rho_a = d\mu_a/d\mu,\ \mu_a(S) = \mu(\sigma_a(S))]$

$$[\mathbb{U}(a)f](p) = \sqrt{\rho_{a^{-1}}(p)}\ f(\sigma_{a^{-1}}(p)) \begin{cases} 1 & (a \in G,\ a \notin K) \\ \overline{L}(a) & (a \in K) \end{cases}.$$

$\mathbb{E}(\mathcal{B})$ is given by

$$[\mathbb{E}(S)f](p) = (\chi_S f)(p),$$

where the characteristic function

$$\chi_S(p) = \begin{cases} 1 & (p \in S) \\ 0 & (p \notin S) \end{cases}.$$

An SI $(\mathbb{U}, \mathrm{E})$ is called *irreducible*, if there are no non-trivial subspaces in $\mathcal{H}$ which are invariant with respect to both $\mathbb{U}(a)$ and $\mathbb{E}(S)$ for all $a \in G$ and all $S \in \mathcal{B}$. Two SI $(\mathbb{U}_i, \mathbb{E}_i)$, $i = 1,2$, are *unitarily equivalent*, if there exists a unitary operator $\mathbb{Y}$ on $\mathcal{H}$ such that

$$\mathbb{U}_2(a) = \mathbb{Y}\,\mathbb{U}_1(a)\mathbb{Y}^{-1} \quad \text{and} \quad \mathbb{E}_2(S) = \mathbb{Y}\,\mathbb{E}_1(S)\,\mathbb{Y}^{-1}$$

for all $a \in G$ and all $S \in \mathcal{B}$.

(2) The IUR $\mathbb{U}(G^\tau)$ induced by $\chi \in M^0 = G/K^0$ and $L^0(K^0)$ in $\mathcal{L}^0$ with inner product $\langle \cdot, \cdot \rangle_0$ is defined in $\mathcal{H}^0$ spanned by vector-valued function $f: M^0 \to \mathcal{L}^0$ with finite norm given[1,2,6] by the inner product

$$(f,g) = \int_{M^0} \langle f,g\rangle_0(p)\, d\mu^0(p) \qquad (p \in M^0),$$

where μ^0 denotes a G-quasi-invariant measure on M^0, as follows $[a^\tau = (t,a) \in G^\tau]$:

$$[\mathbb{U}(a^\tau)f](p) = \sqrt{\rho^0_{a^{-1}}(p)}\ f(\hat{\tau}_{a^{-1}}(p)) \begin{cases} 1 & (a^\tau \notin T_n \otimes_\tau K) \\ \overline{L}(a)\,\overline{\chi}(t) & (a^\tau \in T_n \otimes_\tau K) \end{cases}.$$

(3) *Proof of Lemma* 2: Define an isometric mapping $\mathbb{Y}$ of $\mathcal{H}$ onto $\mathcal{H}^0$ [see (1) and (2)] $\mathbb{Y}: f(p) \to f^0(\iota p) = f^0(p^0)$ $[= f(p)]$. The projections $\mathbb{E}^0$ constructed from $\mathbb{U}^0(G^\tau)$ are unitarily equivalent to $[\mathbb{E}^0(S^0)f^0](p^0) = (\chi_{S^0} f^0)(p^0)$, $p^0 \in M^0$, $f^0 \in \mathcal{H}^0$ and coincide with the canonical $\mathbb{E}$ in $(\mathbb{U}, \mathbb{E}, \sigma)$ if the same Borel field is used for M^0 and M, which is possible.

For representations of G we find

$$\mathbb{U}^0(G^\tau) \downarrow G: \ [\mathbb{U}^0(a)f^0](p^0) = \sqrt{\rho^0_{a^{-1}}(p^0)}\ f^0(\hat{\tau}_{a^{-1}}(p^0)) \begin{cases} 1 & (a \in G,\ a \notin K^0) \\ \overline{L}^0(a) & (a \in K^0) \end{cases},$$

$$\mathbb{U}(G): \ [\mathbb{U}(a)f](p) = \sqrt{\rho_{a^{-1}}(p)}\ f(\sigma_{a^{-1}}(p)) \begin{cases} 1 & (a \in G, a \notin K) \\ L(a) & (a \notin K) \end{cases},$$

where ρ^0_a and ρ_a denote the appropriate Radon—Nikodym derivatives.

Suppose now ι to be equivariant, then $f^0(\hat{\tau}_{a^{-1}}\iota(p)) = f^0(\iota\sigma_{a^{-1}}(p)) = f(\sigma_{a^{-1}}(p))$, and the G-quasi-invariant measures μ^0, μ on $\mathcal{B}^0$, $\mathcal{B}$ are equivalent, which, because of $\mathbb{Y}$ and $L^0 \overset{\sim}{\subset} L$, implies unitary equivalence of $\mathcal{H}^0$ and $\mathcal{H}$, and of $\mathbb{U}^0(G)$ with $\mathbb{U}(G)$. If $\iota\sigma_a \neq \hat{\tau}_a\iota$ for at least one $a \in G$, then there are $f(p) \in \mathcal{H}$ such that $[\mathbb{U}^0(a)f^0](p^0) \neq [\mathbb{U}(a)f](p)$ and the representations cannot be unitarily equivalent.

APPENDIX B

Proof of $\Delta^L_M \tilde{f} = \delta^{\lambda\kappa}\partial_\mu B^\mu_\lambda \partial_\kappa \tilde{f}$, $\tilde{f} \in C^\infty(\iota M)$: The Laplace—Beltrami operator on (M,g) is

$$[\Delta_M f](p) = g^{ba}\nabla_b \nabla_a f(p) = g^{ba}(\partial_b\partial_a - \{{}^c_{ba}\}\partial_c) f(p),$$

where ∇_a is the covariant derivative on (M,g), $f \in C^\infty(M)$. Using relations (van der Waerden—Bortolotti formalism[35]) as, e.g.,

$$g_{ba} = B^\lambda_b B^\kappa_a (g_n)_{\lambda\kappa}, \quad \{{}^c_{ba}\} = B^\lambda_b B^\kappa_a B^c_\mu \{{}^\mu_{\lambda\kappa}\}_n - B^\mu_a \partial_b B^c_\mu,$$

we get $(\tilde{f} = f \circ \pi)$

$$\Delta^L_M \tilde{f} = g_n^{\lambda\kappa} B^\nu_\lambda [\partial_\nu B^\mu_\kappa \partial_\mu - B^\mu_\kappa \{{}^\rho_{\nu\mu}\}_n B^\sigma_\rho \partial_\sigma]\tilde{f} - g_n^{\lambda\kappa} B^\nu_\lambda (\delta^\mu_\kappa - B^\mu_\kappa)(\partial_\nu B^\sigma_\mu) B^\sigma_a \partial_\sigma \tilde{f}.$$

The last term is zero because of the idempotence of the projection B^ν_λ, hence

$$\Delta_M^L \tilde{f} = g_n^{\lambda\kappa} B_\lambda^\nu \partial_\nu B_\kappa^\mu \partial_\mu \tilde{f} - B_\kappa^\mu \left\{ {\rho \atop \nu\mu} \right\}_n B_\rho^\sigma \partial_\sigma \tilde{f},$$

and in Cartesian coordinates q^λ in R_n

$$\Delta_M^L \tilde{f} = \delta^{\lambda\kappa} \partial_\mu B_\lambda^\mu \partial_\kappa \tilde{f}$$

because $g_n^{\lambda\kappa} = \delta^{\lambda\kappa}$ and $\partial_\nu B_\lambda^\nu = m\eta_\lambda$ is perpendicular to B_κ^μ [$\eta_\lambda = \frac{1}{m} H_a{}^a{}_\lambda$ is the mean curvature normal of (M, g) in (R_n, g_n) expressed in terms of the second fundamental tensor $H_b{}^a{}_\lambda = \nabla_b B_\lambda^a$, $m = \dim M$].

*On leave of absence from Universität Osnabrück, Federal Republic of Germany. Permanent address: Technische Universität Clausthal, Federal Republic of Germany.

†On leave of absence from the Faculty of Nuclear Science and Physical Engineering, Czech Technical University, Prague, Czechoslovakia.

[1]G. W. Mackey, Bull. Amer. Math. Soc. 69, 628 (1963); *Induced Representations and Quantum Mechanics* (Benjamin, New York 1968); "Induced representations of locally compact groups and applications," in *Functional Analysis and Related Fields*, edited by F. E. Browder (Springer-Verlag, Berlin, 1970).

[2]G. W. Mackey, Proc. Natl. Acad. Sci. (USA) 35, 537 (1949); *The Theory of Induced Representations*, mimeographed lecture notes (University of Chicago Press, Chicago, 1955); Acta Math. (Uppsala) 99, 265 (1958).

[3]G. Wentzel, Helv. Phys. Acta 13, 269 (1940); 14, 633 (1941); H. Jahn, Nucl. Phys. 26, 353 (1961); M. Bednar and J. Tolar, Nucl. Phys. B 5, 255 (1968); H. D. Doebner and H. Jahn, quoted in H. Jahn, Topical Conf. on Dynamical Groups and Infinite Multiplets, ICTP, Trieste, Preprint IC/69/54; J. Tolar, Czech, J. Phys. B 20, 1093 (1970); Acta Phys. Austr., Suppl. VII, 610 (1970).

[4]See, e.g., C. Fronsdal, Rev. Mod. Phys. 37, 221 (1965); ICTP, Trieste, Preprint IC/73/7.

[5]See, e.g., F. Bopp and R. Haag, Z. Naturforsch. 5A, 644 (1950); D. Finkelstein, Phys. Rev. 100, 924 (1955); D. Bohm, P. Hillion, and J. P. Vigier, Prog. Theor. Phys. 24, 761 (1960).

[6]V. S. Varadarajan, *Geometry of Quantum Theory*, *Quantum Theory of Covariant Systems* (Van Nostrand Reinhold, New York, 1970), Vol. 2.

[7]All manifolds, transformations, vector fields, etc., will be assumed C^∞-differentiable.

[8]S. Helgason, *Differential Geometry and Symmetric Spaces* (Academic, New York, 1962).

[9]See Secs. II.3 and II.4 of Ref. 8.

[10]It is assumed that the system corresponds to a single "particle" on M; systems of many such particles should be treated by usual methods of quantum mechanics.

[11]V. Bargmann, Ann. Math. (2) 59, 1 (1954); K. R. Parthasarathy, *Multipliers on Locally Compact Groups*, *Lecture Notes in Mathematics* (Springer-Verlag, Berlin, 1969), Vol. 93.

[12]H. D. Doebner and J. Werth, Research report Deutsche Forschungsgemeinschaft DO 155/3 (1973).

[13]In the following we shall omit the twiddle, denoting by $\mathbb{U}(G)$ a vector representation corresponding to a given projective representation.

[14]A. S. Wightman, Rev. Mod. Phys. 34, 845 (1962).

[15]$\mathbb{E}(S)$ is a projection operator in $\mathcal{H}$ such that $\mathbb{E}(S_1 \cap S_2) = \mathbb{E}(S_1) \cdot \mathbb{E}(S_2)$, $\mathbb{E}(S_1 \cup S_2) = \mathbb{E}(S_1) + \mathbb{E}(S_2) - \mathbb{E}(S_1 \cap S_2)$, $\mathbb{E}(\cup_i S_i) = \Sigma_i \mathbb{E}(S_i)$ for disjoint subsets $S_i \subset M$, $\mathbb{E}(M) = \mathbb{1}$.

[16]See, e.g., Ref. 6, p. 92.

[17]The correspondence between $\mathbb{W} = \mathbb{U}(G^\tau) \dotplus T_n$ and the projection-valued measures $\mathbb{E}(S)$, $S \subset \hat{T}_n$, is given by $(f, \mathbb{W}(t)g) = \int_{\hat{T}_n} \chi(t)\, d\nu_{fg}(\chi)$, $t \in T_n$, $\chi \in \hat{T}_n$, $\nu_{fg}(S) = (f, \mathbb{E}(S)g)$.

[18]A mapping $\iota : M \to W$ is called an *immersion at point* $p \in M$ if there exists a submanifold S of W, an open neighborhood U of p and an open neighborhood V of $\iota(p)$ such that $\iota(U) \subset V \cap S$ and the induced mapping $\iota_S : U \to V \cap S$ is isomorphism. Mapping ι is called *immersion* if it is immersion at each point. Immersion which determines an isomorphism on a submanifold is called *embedding*. The immersion ι at p can be characterized by its differential: ι is an immersion at $p \in M$ if an only if ι_{*p} is injective and decomposes $T_{\iota(p)}(W)$. Every manifold of dimension m embeds in R_{2m}, H. Whitney, Ann. Math. (2) 45, 220, 247 (1944).

[19]One criterion of regularity of G^τ is the existence of a Borel subset in $\hat{T}_n$ which meets each G orbit just once; see Ref. 2.

[20]R. S. Palais, Mem. Amer. Math. Soc. Nr. 36 (1960).

[21]G. D. Mostow, Ann. Math. (2) 65, 432 (1957); R. S. Palais, J. Math. Mech. 6, 673 (1957); see also Ref. 20 and G. E. Bredon, *Introduction to Compact Transformation Groups* (Academic, New York, 1972).

[22]Euclidean G-space is a space (G, R_n, τ) with τ_a linear and with an inner product. In the following we shall use the notation (G, R_n, τ) also for $(G, \hat{T}_n, \hat{\tau})$.

[23]J. Mickelsson and J. Niederle, Commun. Math. Phys. 16, 191 (1970).

[24]Corresponding treatments can be found in Refs. 1 and 6.

[25]If one describes the kinematics in R_n via Galilei transformations (dynamical group approach), a ray representation is necessary to have the canonical commutation relations.

[26]Quantum kinematics of $(SU(2) \otimes SU(2),\ SO(3), \sigma)$ is treated in J. D. Smith, Nuovo Cimento 22B, 337 (1974).

[27]J. Glimm, Pacific J. Math. 12, 885 (1962); J. M. G. Fell, in *Conference on Harmonic Analysis*, *Lecture Notes in Mathematics* (Springer-Verlag, Berlin, 1972), Vol. 266, p. 43.

[28]M. P. Gaffney, Proc. Natl. Acad. Sci. (USA) 37, 48 (1951); W. Roelcke, Math. Nachr. 21, 132 (1960); P. R. Chernoff, J. Funct. Anal. 12, 401 (1973).

[29]S. Lang, *Introduction to Differentiable Manifolds* (Interscience, New York, 1962).

[30]M. Berger, P. Gauduchon and E. Mazet, *Le Spectre d'une Variété Riemannienne*, *Lecture Notes in Mathematics* (Springer-Verlag, Berlin, 1971), Vol. 194.

[31]See Proposition 7.1 of N. R. Wallach, in *Symmetric Spaces: Short Courses Presented at Washington University*, edited by W. M. Boothby and G. L. Weiss (Dekker, New York, 1972), p. 1.

[32]Proof is based on the formula (Ref. 30, p. 129)

$$\Delta_n(f \circ \pi) = \sum_{\lambda=1}^{n} \frac{d^2}{dt^2} (f \circ \pi \circ c_\lambda(t))\Big|_{t=0} = \sum_{b=1}^{m} \frac{d^2}{dt^2} (f \circ \pi \circ c_b(t))\Big|_{t=0} + \sum_{y=m+1}^{n} \frac{d^2}{dt^2} (f \circ \pi \circ c_y(t))\Big|_{t=0},$$

where $\{c_y(t)\}$ are n geodesics in W through $r \in W$ defined by n orthonormal vectors $e_\lambda \in T_r(W)$ such that $e_b \in T_{\pi(r)}(M)$, $e_y \in T_{\pi(r)}(M)^\perp$; now $\pi \circ c_b(t)$ is the geodesic in M corresponding to e_b, whereas $f \circ \pi \circ c_y(t) = \text{const}$. Then for any $f \in C^\infty(M)$ (3.1) is valid.

[33]S. Helgason, J. Diff. Geom. 6, 411 (1972).

[34]A discussion of this quantization will be given elsewhere. The method is not connected with the construction and motivation of $\mathcal{J}(G, M, \sigma)$ but it is partly related.

[35]J. A. Schouten, *Ricci Calculus: An Introduction to Tensor Analysis and Its Geometrical Applications* (Springer-Verlag, Berlin, 1954), 2nd edition.

[36]There are linear invariant differential operators in Hilbert spaces for $\mathcal{J}(G, M, \sigma)$ with nontrivial $L(K)$.

[37]F. A. Berezin, Trudy Mosk. Matem. Obshchestva 6, 371 (1957) [English transl., Amer. Math. Soc. Translations (2) 21, 239 (1962), p. 273].

[38]S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Interscience, New York, 1963, 1969), Vols. I and II.

[39]J. A. Wolf, *Spaces of Constant Curvature* (McGraw-Hill, New York, 1967).

[40]J. A. Wolf, Acta Math. (Uppsala) 120, 59 (1968).

[41]E. Schrödinger, Ann. Physik 79, 734 (1926), Eq. (31), p. 748; B. Podolsky, Phys. Rev. 32, 812 (1928); W. Pauli, "Wellenmechanik," *Handbuch der Physik*, Bd. 24, I (Springer-Verlag, Berlin, 1933), p. 120; "Die allgemeinen Prinzipien der Wellenmechanik," *Handbuch der Physik*, Bd. V, Teil 1 (Springer-Verlag, Berlin 1958), Sec. A. 5; H. Welker, Z. Physik 101, 95 (1936); Math. Ann. 113, 304 (1937); L. Brillouin, *Les Tenseurs en Mécanique et en*

Elasticité (Masson, Paris, 1938), Sec. IX.6; A. Sommerfeld, *Atombau und Spektrallinien*, Bd. 2 (Vieweg, Braunschweig, 1939), Appendix 10; B.S. DeWitt, Phys. Rev. 85, 653 (1952); H.A. Kramers, *Quantum Mechanics* (North-Holland, Amsterdam, 1957), Sec. IV.A.34; K. Simon, Amer. J. Phys. 33, 60 (1965); J.M. Charap, J. Phys. A 6, 393 (1973).

[42]F. Reiche and H. Rademacher, Z. Physik 39, 444 (1926); 41, 453 (1927); R. de L. Kronig and I.I. Rabi, Phys. Rev. 29, 262 (1927); F. Hund, Z. Physik 51, 11 (1928); S.C. Wang, Phys. Rev. 34, 243 (1929); H.B.G. Casimir, "Rotation of a rigid body in quantum mechanics," thesis (1931); D.M. Dennison, Rev. Mod. Phys. 3, 310 (1931); W. Pauli, Helv. Phys. Acta 12, 147 (1939); A.R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, N.J., 1957); S. Flügge and A. Weiguny, Z. Physik 171, 171 (1963); and others.

[43]P.A.M. Dirac, Can. J. Math. 2, 129 (1950).

[44]See, e.g., L.D. Faddeyev, Theor. Math. Phys. 1, 3 (1969) (in Russian); *Actes du Congrès Intern. des Mathématiciens, Nice*, 1970 (Gauthier-Villars, Paris, 1971), Vol. 3, p. 35.

[45]G.W. Mackey, *The Mathematical Foundations of Quantum Mechanics* (Benjamin, New York, 1963); K.R. Parthasarathy, Commun. Math. Phys. 9, 303 (1968); F.J. Bloore and J. Underhill, J. Phys. A 6, L 79 (1973).

[46]H.D. Doebner and O. Melsheimer, Nuovo Cimento 49, 73 (1967); P. Carruthers and M.M. Nieto, Rev. Mod. Phys. 40, 411 (1968); K.B. Wolf, Communicaciones Técnicas CIMAS, Vol. 4B, No. 50 (1973), to appear in *Group Theory and Its Applications*, edited by E.M. Loebl (Academic, New York), Vol. 3.

[47]R.P. Feynman, Rev. Mod. Phys. 20, 367 (1948); R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[48]B.S. DeWitt, Rev. Mod. Phys. 29, 377 (1957); L. Schulman, Phys. Rev. 176, 1558 (1968); J.S. Dowker, Ann. Phys. 62, 361 (1971); 71, 577 (1972); J. Phys. A 5, 936 (1972); J.S. Dowker and I.W. Mayes, Nucl. Phys. B 29, 259 (1971); Proc. Roy. Soc. (London) A 327, 131 (1972); K.S. Cheng, J. Math. Phys. 13, 1723 (1972); S.I. Ben Abraham and A. Lonke, J. Math. Phys. 14, 1935 (1973).

[49]For a rigorous formulation see E. Nelson, J. Math. Phys. 5, 332 (1964); C. Morette DeWitt, Commun. Math. Phys. 28, 47 (1972).

[50]H.D. Doebner and O. Melsheimer, J. Math. Phys. 9, 1638 (1968); 11, 1463 (1970); H.D. Doebner and J. Hennig, J. Math. Phys. 15, 602 (1974).

[51]Its present state is shown, e.g., by R.J. Blattner, in *Harmonic Analysis on Homogeneous Spaces* (Proceedings Symposia in Pure Mathematics, Vol. 26, Amer. Math. Soc., Providence, R.I., 1973), p. 147. For further references see, e.g., E. Onofri and M. Pauri, J. Math. Phys. 13, 533 (1972).

[52]Similar methods were applied to chiral dynamics, C.J. Isham, Nuovo Cimento 61 A, 188, 729 (1969).

[53]See, e.g., Ref. 8, Sec. II.4, Proposition 4.3.

On the duality condition for a Hermitian scalar field

Joseph J. Bisognano*†

Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720

Eyvind H. Wichmann‡

Department of Physics, University of California, Berkeley, California 94720
(Received 13 November 1974)

A general Hermitian scalar field, assumed to be an operator-valued tempered distribution, is considered. A theorem which relates certain complex Lorentz transformations to the TCP transformation is stated and proved. With reference to this theorem, duality conditions are considered, and it is shown that such conditions hold under various physically reasonable assumptions about the field. A theorem analogous to Borchers' theorem on relatively local fields is stated and proved. Local internal symmetries are discussed, and it is shown that any such symmetry commutes with the Poincaré group and with the TCP transformation.

I. INTRODUCTION AND OUTLINE

The so-called duality condition in quantum field theory and in the theory of algebras of local observables has been discussed by many authors.[1–8] From these studies it appears that it would be a desirable, if not essential, feature of a local theory that such a condition holds. *Very* roughly stated the duality condition for a region R in spacetime says that the set of all operators which commute with all operators locally associated with R is equal to the set of all operators locally associated with the causal complement of R. It was first shown by Araki[2] that conditions of this nature do hold for a class of suitably restricted regions R in the case of a free Hermitian scalar field. It is the purpose of this paper to discuss the duality condition in quantum field theory in the general case, i.e., without making the assumption that the field is free.

Our considerations are within the framework of conventional quantum field theory, as formulated by Wightman and others.[9–11] We shall restrict our discussion to the case of a single local Hermitian scalar field, assumed to be an operator-valued tempered distribution. We will state the assumptions in some detail in Sec. II, in which we also explain the notation to be followed. Our discussion can readily be extended to more general cases, but, in order to avoid complications which might obscure the main line of argument, we present our ideas in what appears to us to be the simplest possible setting.

In Sec. III we consider some implications of the "spectral condition", i.e., the assumption that the spectrum of the 4-momentum operator P associated with the translation subgroup of the Poincaré group is contained in the closed forward light cone. We here review some facts, by and large well known, which will be of interest in the subsequent discussion, and we consider a slightly modified version of a well-known theorem of Reeh and Schlieder.[12]

In Sec. IV we consider complex Lorentz transformations, and a connection between these and the antiunitary inversion transformation (TCP-operation). Since the Hilbert space of physical states carries a strongly continuous unitary representation of the Poincaré group, it follows that there exist dense sets of analytic vectors of the associated Lie algebra and of sub-Lie algebras of this Lie algebra. It is a characteristic feature of quantum field theory that such sets of analytic vectors can be constructed "naturally" in terms of suitable multilinear expressions in the fields and the vacuum state vector Ω. We shall in particular consider the following issue. Let W_R be the wedge-shaped region $W_R = \{x \mid x^3 > |x^4|\}$ in Minkowski space, and let $\mathcal{P}_0(W_R)$ be the polynomial algebra generated by field operators averaged with test functions with support in W_R. Let $V(\mathbf{e}_3, t)$, t real, denote the velocity transformation in the Poincaré group whose action on Minkowski space is described by the four×four matrix

$$V(\mathbf{e}_3, t) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cosh(t) & \sinh(t) \\ 0 & 0 & \sinh(t) & \cosh(t) \end{bmatrix} . \tag{1}$$

The set of all $V(\mathbf{e}_3, t)$ is thus a one-parameter Abelian group of velocity transformations in the 3-direction which maps the wedge region W_R onto itself. To the element $V(\mathbf{e}_3, t)$ corresponds the unitary operator $U(V(\mathbf{e}_3, t), 0) = \exp(-itK_3)$ on the Hilbert space, where K_3 is an (unbounded) self-adjoint operator. We shall show that every vector $X\Omega$, with $X \in \mathcal{P}_0(W_R)$, is in the domain of the normal operators $\exp(-izK_3)$ for the complex variable z in the closed strip $\pi \geq \mathrm{Im}(z) \geq 0$. The vector-valued function $\exp(-izK_3)X\Omega$ is a strongly continuous function of z on the above closed strip, and an analytic function of z on the (open) interior of the strip. We shall furthermore show that for any such vector

$$\exp(\pi K_3) X\Omega = JX^*\Omega \tag{2}$$

where J is the antiunitary involution defined by

$$J = U(R(\mathbf{e}_3, \pi), 0)\Theta_0 \tag{3}$$

where $R(\mathbf{e}_3, \pi)$ is the rotation by angle π about the 3-axis [and $U(R(\mathbf{e}_3, \pi), 0)$ the corresponding unitary operator on the Hilbert space], and where Θ_0 is the TCP-operator.

The relation (2) is the main result of Sec. IV. It holds, in fact, for a somewhat larger class of field operators, as stated precisely in Theorem 1.

Section V is devoted to a discussion of some mathematical questions relating to (2). We consider families of operators which satisfy the relation (2), and, in particular, we discuss the properties of any von Neumann algebra $\mathcal{A}_R$ of bounded operators X which satisfy (2), and such that furthermore $J\mathcal{A}_R J = \mathcal{A}_R'$, where $\mathcal{A}_R'$ denotes the commutant of $\mathcal{A}_R$. The main results, relative to the subsequent discussion in Secs. VI and VII, are stated in Theorem 2 and Lemma 15. Our discussion is closely related to a theory of Tomita[13] on the structure of von Neumann algebras (and of modular Hilbert algebras), and we discuss the connection.

In Sec. VI we discuss a *particular* duality condition, for the wedge region W_R. Let W_L be the causal complement of $\overline{W}_R$, i. e., the wedge region $W_L = \{x \mid x^3 < -|x^4|\}$, and let $\mathcal{P}_0(W_L)$ be the polynomial algebra generated by field operators averaged with test functions with support in W_L. We consider four particular conditions on the quantum field under which the polynomial algebras $\mathcal{P}_0(W_R)$, respectively $\mathcal{P}_0(W_L)$, of *unbounded* operators define von Neumann algebras $\mathcal{A}(W_R)$, respectively $\mathcal{A}(W_L)$, of *bounded* operators which can be regarded as locally associated with the wedge regions W_R and W_L, and we prove that these von Neumann algebras satisfy the *duality condition* $\mathcal{A}(W_R)' = \mathcal{A}(W_L)$. We also show that the TCP-symmetry of the field carries over to the system of bounded local operators in the sense that $J\mathcal{A}(W_R)J = \mathcal{A}(W_L)$. These results are formulated in Theorems 3 and 4.

Theorem 3 includes in particular the following result, which holds *generally*, i. e., without any additional assumption about the quantum field beyond the minimum assumptions discussed in Sec. II. If X is a bounded operator which commutes with all (linear) field operators averaged with test functions with support in W_L, and if Y is a bounded operator which commutes with all field operators averaged with test functions with support in W_R, then X commutes with Y. This statement is analogous to a well-known theorem of Borchers on the local nature of fields which are local relative to a local irreducible field.[14]

We have not solved the problem of whether the von Neumann algebras (of bounded operators) associated with wedge regions, or other regions, always exist, and we are thus forced to make additional assumptions, which, however, are not unreasonable physically. This question appears to be intimately related to the hitherto unsolved problem of whether a sufficiently large set of quantum field operators have *local* self-adjoint extensions (within the framework of the customary minimal assumptions of quantum field theory). We discuss the notion of a local self-adjoint extension of the field, and we show that it implies the existence of a system of local von Neumann algebras which satisfies the duality condition. We also show that the existence of such a system follows from other conditions which appear to be less restrictive than the condition that the field has a local self-adjoint extension.

In Sec. VII we discuss the duality condition for a particular set of bounded regions, namely the set of all so-called double cones. The von Neumann algebras associated with the bounded regions are constructed from the von Neumann algebras associated with the wedge regions. We describe the properties of these algebras in Theorems 5 and 6, and we show that the duality condition for the algebras associated with the wedge regions implies an appropriate duality condition for the algebras associated with double cones.

Finally, we consider the notion of a local internal symmetry, and we prove (Theorem 7) that if the duality condition holds for the wedge algebras, then every local internal symmetry commutes with the Poincaré group, and with the TCP-transformation.

II. BASIC ASSUMPTIONS; DISCUSSION OF NOTATION

Minkowski space $\mathcal{M}$ is parametrized by the customary Cartesian coordinates $x = (x^1, x^2, x^3, x^4)$. The Lorentz "metric" is so defined that $x \cdot y = x^4y^4 - x^1y^1 - x^2y^2 - x^3y^3$. The elements $\Lambda = \Lambda(M, y)$ of the *proper* Poincaré group $\overline{L}_0$ are parametrized by a four-by-four Lorentz matrix M, and a real 4-vector y, such that the image Λx of a point $x \in \mathcal{M}$ under any $\Lambda \in \overline{L}_0$ is given by $\Lambda x = \Lambda(M, y)x = Mx + y$.

The Hilbert space $\mathcal{H}$ of physical states is assumed to be *separable*. It is assumed to carry a strongly continuous unitary representation $\Lambda \to U(\Lambda)$ of the Poincaré group $\overline{L}_0$. We write $U(\Lambda(M, x)) = U(M, x)$, and we employ the special notation $T(x) = U(I, x)$ for the representatives of the translation subgroup. The translations have the common spectral resolution

$$T(x) = U(I, x) = \int \exp(ix \circ p)\, \mu(d^4p) \tag{4}$$

and it is assumed that the support of the spectral measure μ is contained in the closed forward light cone $\overline{V}_+$ (in momentum space). This assumption about the support of μ will be referred to as the "spectral condition" in what follows.

We assume the existence of a vacuum state, represented by the unit vector Ω, *uniquely* characterized by its invariance under all Poincaré translations: thus $U(\Lambda)\,\Omega = \Omega$.

We denote by $\mathcal{D}(R^n)$ the set of all complex-valued infinitely differentiable function of compact support on n-dimensional Euclidean space R^n, and we denote by $\mathcal{S}(R^n)$ the space of test functions on R^n in terms of which tempered distributions are defined. The space $\mathcal{S}(R^n)$ is regarded as endowed with the particular topology appropriate to the definition of tempered distributions,[15] and we employ the notation

$$\mathcal{S}\text{-}\lim_{\alpha \to \infty} f_\alpha = 0 \tag{5}$$

to state that a sequence of test functions f_α converges to zero relative to this topology. We shall be concerned with test functions on R^{4n}, where R^{4n} is regarded as the direct sum of an ordered n-tuplet of replicas of Minkowski space, and the points of R^{4n} are accordingly parametrized by an ordered n-tuplet $(x_1, x_2, \ldots, x_n)$ of 4-vectors x_k. A *specific* interpretation of R^{4n} in this manner is always understood, as reflected in the above parametrization of the space. In accordance with the above we define an action of $\overline{L}_0$ on $\mathcal{S}(R^{4n})$ by

$$f(x_1, \ldots, x_n) \to \Lambda f(x_1, \ldots, x_n) = f(\Lambda^{-1}x_1, \ldots, \Lambda^{-1}x_n). \tag{6}$$

This mapping is continuous relative to the test function space topology, and

$$\mathcal{S}\text{-}\lim_{\Lambda\to I} \Lambda f = f. \tag{7}$$

Throughout this paper it will be important to keep track of the domains of unbounded operators. To deal effectively with such issues we shall frequently employ the unorthodox notation (X, D) for an operator X defined on a domain D. The adjoint of (X, D) is denoted $(X, D)^*$ and if $D(X^*)$ is the domain of the adjoint we can write $(X, D)^* = (X^*, D(X^*))$. If (X, D) is closable we write $(X, D)^{**} = (X^{**}, D(X^{**}))$ for the closure. This notation is never employed for manifestly bounded operators, which are regarded as defined on the entire Hilbert space.

We shall consider a theory of a single local Hermitian scalar field $\varphi(x)$, assumed to be an operator-valued tempered distribution.[9-11,16] Such a theory is characterized by the following features:

(a) There exists a linear manifold D_1, *dense* in the Hilbert space $\mathcal{H}$, and an algebra $\mathcal{P}(\mathcal{H})$ of operators (X, D_1) defined on D_1. The domain D_1 contains the vacuum state vector Ω. For each $n \geq 1$ there exists a linear mapping of $\mathcal{S}(R^{4n})$ into $\mathcal{P}(\mathcal{H})$. The image of any $f \in \mathcal{S}(R^{4n})$ under this mapping is denoted $\varphi\{f\}$. We note here that $\varphi\{f\}$ is the operator which is customarily defined symbolically by the integral at right in

$$\varphi\{f\} = \int_{(\infty)} d^4(x_1) \cdots d^4(x_n) f(x_1, \ldots, x_n)\, \varphi(x_1) \cdots \varphi(x_n). \tag{8}$$

The domain D_1 is *precisely* equal to $\mathcal{P}(\mathcal{H})\Omega$, and the algebra $\mathcal{P}(\mathcal{H})$ is *precisely* equal to the linear span of the identity operator I and the set of all operators $\varphi\{f\}$. If $f \in \mathcal{S}(R^{4n})$ and $g \in \mathcal{S}(R^{4m})$, and if $h \in \mathcal{S}(R^{4n+4m})$ is given by

$$h(x_1, \ldots, x_n, x_{n+1}, \ldots, x_{n+m}) = f(x_1, \ldots, x_n)\, g(x_{n+1}, \ldots, x_{n+m}), \tag{9}$$

then

$$\varphi\{f\}\,\varphi\{g\} = \varphi\{h\} \quad \text{on } D_1. \tag{10}$$

We note that this is consistent with the symbolic definition in (8).

(b) Let $(X, D_1) \to (X^\dagger, D_1)$ denote the *antilinear* involutory mapping of $\mathcal{P}(\mathcal{H})$ onto itself uniquely determined by

$$\mathrm{I}^\dagger = \mathrm{I}, \quad \varphi\{f\}^\dagger = \varphi\{f^\dagger\}, \tag{11}$$

where

$$f^\dagger(x_1, x_2, \ldots, x_n) = f^*(x_n, \ldots, x_2, x_1) \tag{12}$$

for any $f \in \mathcal{S}(R^{4n})$.

The domain D_1 is contained in the domain of the adjoint $(X, D_1)^*$ of every $(X, D_1) \in \mathcal{P}(\mathcal{H})$, and

$$(X^\dagger, D_1) = (X^*, D_1) \subset (X, D_1)^*. \tag{13a}$$

In particular,

$$(\varphi\{f^\dagger\}, D_1) \subset (\varphi\{f\}, D_1)^*. \tag{13b}$$

Every operator $(X, D_1) \in \mathcal{P}(\mathcal{H})$ is thus closable, and $(X^\dagger, D_1)$ is the Hermitian conjugate of (X, D_1).

(c) The domain D_1 is invariant under the Poincaré group: $U(\Lambda) D_1 = D_1$ for all $\Lambda \in \overline{L}_0$. The action of $\overline{L}_0$ by conjugation on $\mathcal{P}(\mathcal{H})$ (and hence the action of $\overline{L}_0$ of the Hilbert space $\mathcal{H}$) is uniquely determined by the condition

$$U(\Lambda)(\varphi\{f\}, D_1)\, U(\Lambda)^{-1} = (\varphi\{\Lambda f\}, D_1) \tag{14}$$

(d) The mapping $f \to \varphi\{f\}$ is such that if $\{f_\alpha \mid f_\alpha \in \mathcal{S}(R^{4n}), \alpha = 1, \ldots, \infty\}$ is any sequence of test functions which tends to zero in the sense of the test function space topology, i. e., such that (5) holds, then

$$\text{s-}\lim_{\alpha\to\infty} X\varphi\{f_\alpha\}\psi = 0 \tag{15}$$

for any $(X, D_1) \in \mathcal{P}(\mathcal{H})$ and any $\psi \in D_1$.

(e) Let R be any open subset of Minkowski space. Let $\mathcal{P}(R)$ denote the linear span of the identity operator I and all operators $(\varphi\{f\}, D_1)$, where $f \in \mathcal{S}(R^{4n})$ for some $n \geq 1$ and such that $\mathrm{supp}(f) \subset \{(x_1, \ldots, x_n) \mid x_k \in R, k = 1, \ldots, n\}$.

Then, if R_1 and R_2 are any two open subsets of Minkowski space which are spacelike separated [i. e., $(x - y) \circ (x - y) < 0$ for any $x \in R_1$, $y \in R_2$], we have

$$[X, Y]\psi = 0, \quad \text{all } \psi \in D_1, \tag{16}$$

for all $X \in \mathcal{P}(R_1)$ and all $Y \in \mathcal{P}(R_2)$.

Our purpose with the preceding account was to state precisely what we assume, and not to formulate a minimal set of postulates for field theory. It will be noted that the conditions which we have stated are in fact not all logically independent of each other. It should also be noted that we do not assume anything beyond what is implied by the usual *minimal* assumptions for quantum field theory.

Since operators linear in the field will be of particular interest, we employ a special notation for the case $f \in \mathcal{S}(R^4)$, namely,

$$\varphi[f] = \varphi\{f\} = \int_{(\infty)} d^4(x) f(x)\, \varphi(x). \tag{17}$$

For any open subset R of Minkowski space we denote by $\mathcal{P}_0(R)$ the polynomial algebra generated by the identity I, and all operators $(\varphi[f], D_1)$ such that $\mathrm{supp}(f) \subset R$. With reference to the definition of the algebra $\mathcal{P}(R)$ in (e) above, we then have $\mathcal{P}_0(R) \subset \mathcal{P}(R) \subset \mathcal{P}(\mathcal{H})$. We state some well-known properties of these algebras as follows.

Lemma 1: (a) (Theorem of Reeh and Schlieder[12]) Let R be any open, nonempty subset of Minkowski space $\mathcal{M}$. Then $\mathcal{P}_0(R)\Omega$ is dense in the Hilbert space $\mathcal{H}$.

(b) Let $(X, D_1) \in \mathcal{P}(R)$. Then there exists a sequence of operators $\{(X_\alpha, D_1) \mid (X_\alpha, D_1) \in \mathcal{P}_0(R), \alpha = 1, \ldots, \infty\}$ such that

$$\text{s-}\lim_{\alpha\to\infty} YX_\alpha\psi = YX\psi \tag{18}$$

for every $Y \in \mathcal{P}(\mathcal{H})$ and every $\psi \in D_1$.

(c) The linear manifold $D_0 \subset D_1$ defined as $D_0 = \mathcal{P}_0(\mathcal{H})\Omega$ is dense in the Hilbert space, and

$$(X, D_0)^* = (X, D_1)^*, \quad (X, D_0)^{**} = (X, D_1)^{**} \tag{19}$$

for every $(X, D_1) \in \mathcal{P}(\mathcal{H})$.

The above is of interest with reference to other approaches to field theory, in which the initial object of

interest is $\varphi[f]$, defined on D_0, and where the commutation relation (16) is at first assumed only for operators X and Y of this special form. After the appropriate extensions and constructions one arrives at the equivalent of our formulation. We preferred to introduce the domain D_1 immediately, and to regard all field operators as defined on precisely D_1. The symbols X^*, X^{**}, and $X^\dagger$, for $(X, D_1) \in \rho(\mathcal{H})$, thus refer to the adjoint, closure and Hermitian conjugate defined relative to this domain.

Whereas the domains D_0 and D_1 are Poincaré invariant, this is, of course, in general not the case for the domain $D(X^*)$ of $(X, D_1)^*$ and the domain $D(X^{**})$ of $(X, D_1)^{**}$. We have the relations

$$(U(\Lambda)XU(\Lambda)^{-1}, D_1)^* = (U(\Lambda)X^*U(\Lambda)^{-1},\ U(\Lambda)D(X^*)) \tag{20a}$$

$$(U(\Lambda)XU(\Lambda)^{-1}, D_1)^{**} = (U(\Lambda)X^{**}U(\Lambda)^{-1}, U(\Lambda)D(X^{**})). \tag{20b}$$

We finally note that it trivially follows from (13a) that

$$(X^\dagger, D_1)^{**} = (X^{\dagger **}, D(X^{\dagger **})) \subset (X, D_1)^* = (X^*, D(X^*)). \tag{21}$$

For a particular operator (X, D_1) equality obtains in (21) above if and only if D_1 is a core for $(X, D_1)^*$. [For a Hermitian operator this means that (X, D_1) is essentially self-adjoint.] In general discussions of field theory no assumption is made about the possible existence of a set of field operators for which (21) might hold as an equality.

III. ABOUT SOME CONSEQUENCES OF THE SPECTRAL CONDITION

It is well-known that the unitary representation $x \to T(x)$ of the translation group can be extended to a representation of the semigroup of all complex translations $z = x + iy$, with x and y real, $y \in \overline{V}_+$, by

$$T(z) = \int \exp(iz \cdot p)\mu(d^4p) = \exp(iz \cdot P) \tag{22}$$

where the operator-valued function $T(z)$ satisfies $\|T(z)\| = 1$ and is a strongly continuous function of z on the closed forward imaginary tube $\overline{V}_{+i} = \{z \mid \mathrm{Im}(z) \in \overline{V}_+\}$. Furthermore, the function $T(z)$ is analytic in the sense of the uniform topology on the open forward imaginary tube V_{+i}, which implies in particular that the vector-valued function $T(z)\psi$ of z is strongly analytic on V_{+i} for any $\psi \in \mathcal{H}$.

Let $f \in \mathcal{S}(R^{4n})$. We define a Fourier transform $\tilde{f}$ of f by

$$\tilde{f}(p_1, \ldots, p_n) = \int_{(\infty)} d^4(x_1) \cdots d^4(x_n) f(x_1, \ldots, x_n) \exp\left(i \sum_{r=1}^{n} x_r \cdot p_r\right). \tag{23}$$

We consider the following:

Lemma 2: Let $z \in \overline{V}_{+i}$, i.e., z is any complex 4-vector in the closed forward imaginary tube. Then

$$T(z)D_1 \subset D_1. \tag{24}$$

If $f \in \mathcal{S}(R^{4n})$ there exists an $f_z \in \mathcal{S}(R^{4n})$ such that

$$\tilde{f}_z(p_1, \ldots, p_n) = \tilde{f}(p_1, \ldots, p_n) \exp\left(iz \cdot \sum_{r=1}^{n} p_r\right) \tag{25a}$$

for $(p_1, \ldots, p_n) \in V_n$, where V_n is the subset of R^{4n} defined by

$$V_n = \left\{(p_1, \ldots, p_n) \,\middle|\, \sum_{r=k}^{n} p_r \in \overline{V}_+,\ k = 1, \ldots, n\right\} \tag{25b}$$

and for every such f_z we have

$$T(z)\varphi\{f\}\Omega = \varphi\{f_z\}\Omega. \tag{25c}$$

The above facts are well known, and we refer to the monograph by Jost[17] for a discussion of these and related issues. Here we only note the following. It is a consequence of the spectral condition that any vector $\varphi\{f\}\Omega$ only depends on the restriction of $\tilde{f}$ to the set V_n defined in (25b), i.e., if $\tilde{f} = 0$ on V_n, then the vector vanishes. It is of interest to exhibit a particular function f_z which satisfies (25a), and hence (25c). Let $u_0(t)$ be an infinitely differentiable function of t on R^1 such that $u_0(t) = 1$ for $t \geq 0$ and $u_0(t) = 0$ for $t \leq -1$. We define a function $E(p; z)$ of the real 4-vector p and the complex 4-vector z by

$$E(p; z) = u_0(p \cdot p)u_0(p^4)\exp(iz \cdot p). \tag{26}$$

This function satisfies $E(p; z) = \exp(iz \cdot p)$ for $p \in \overline{V}_+$. It is easily seen that for any $z \in V_{+i}$ the function $E(p; z)$, as a function of p, is included in $\mathcal{S}(R^4)$. Furthermore, if $f \in \mathcal{S}(R^{4n})$, then the function f_z with the Fourier transform

$$\tilde{f}_z(p_1, \ldots, p_n) = E(p; z)\tilde{f}(p_1, \ldots, p_n), \quad p = \sum_{r=1}^{n} p_r, \tag{27}$$

is, as a function of $(x_1, \ldots, x_n)$, included in $\mathcal{S}(R^{4n})$ for any $z \in \overline{V}_{+i}$. Now (25a) holds trivially, and it follows that (25c) holds.

The next lemma can be regarded as a generalization of the preceding lemma.

Lemma 3: Let T_n be the open tube region in $4n$-dimensional complex space C^{4n}, regarded as the direct sum of n replicas of complex Minkowski space, which is defined by

$$T_n = \{(z_1, \ldots, z_n) \mid z_k \in V_{+i},\ k = 1, \ldots, n\}. \tag{28}$$

Let $\{f_k \mid f_k \in \mathcal{S}(R^4),\ k = 1, \ldots, n\}$ be any n-tuplet of test functions. Then we have the following:

(a) The vector

$$\beta(z_1, \ldots, z_n) = T(z_1)\varphi[f_1]T(z_2)\varphi[f_2] \cdots T(z_n)\varphi[f_n]\Omega \tag{29}$$

is well defined (through successive left multiplications) for all $(z_1, \ldots, z_n) \in \overline{T}_n$, and

$$\beta(z_1, \ldots, z_n) = \varphi\{f\}\Omega, \tag{30a}$$

where $f = f(x_1, \ldots, x_n; z_1, \ldots, z_n)$ is the function whose Fourier transform with respect to the variables $(x_1, \ldots, x_n)$ is given by

$$\tilde{f}(p_1, \ldots, p_n; z_1, \ldots, z_n) = \prod_{k=1}^{n} \tilde{f}_k(p_k) E\left(\sum_{r=k}^{n} p_r; z_k\right) \tag{30b}$$

and where $E(p; z)$ is the function defined in (26).

(b) The vector-valued function $\beta(z_1, \ldots, z_n)$ of $(z_1, \ldots, z_n)$ is strongly continuous on the closed tube $\overline{T}_n$, and analytic on the open tube T_n.

Proof: (1) The assertions in part (a) follow trivially from Lemma 2, by induction on n.

(2) The proof that β is strongly continuous on $\overline{T}_n$ requires an examination of the function $\tilde{f}$ given by (30b). We regard this function as a vector-valued function on $\overline{T}_n$, i. e., as a function of $(z_1, \ldots, z_n)$ with range in $\mathcal{S}(R^{4n})$. In view of the simple nature of the function $E(p;z)$, as given by (26), it is now easily shown that $\tilde{f}$ is continuous on $\overline{T}_n$ in the sense of the test function space topology; since this topology is invariant under the Fourier transform, the same holds for f, regarded as an $\mathcal{S}(R^{4n})$-valued function on $\overline{T}_n$. It follows, in view of the assumption expressed in (15), that β is strongly continuous as asserted.

(3) Since β is strongly continuous on $\overline{T}_n$ it follows that β is bounded on any closed polydisc contained in $\overline{T}_n$. To show that β is analytic on T_n it therefore suffices to show that the function $\langle \eta | \beta(z_1, \ldots, z_n) \rangle$ is analytic in each complex 4-vector z_k separately for each η in a dense set of vectors in the Hilbert space. We select D_1 as the dense set and we then have, for $k = 1, \ldots, n$, $\langle \eta | \beta(z_1, \ldots, z_n) \rangle = \langle \xi_k | T(z_k) \zeta_k \rangle$, with ζ_k, ξ_k independent of z_k. This scalar product is trivially analytic for $z_k \in V_{+i}$, which establishes the second assertion in part (b).

We are specifically interested in vectors of the form shown in (29), but it is worth noting that the lemma has an obvious generalization, in which the operators $\varphi[f_k]$ in (29) are replaced by arbitrary operators $X_k \in \mathcal{P}(\mathcal{H})$.

We next consider an almost trivial extension of the theorem of Reeh and Schlieder, [12] which will be needed later.

Lemma 4: Let $\{R_n | n = 1, \ldots, \infty\}$ be any set of open, nonempty subsets of Minkowski space. For such a set, and for any $n \geq 1$, let S_n denote the linear span of all vectors of the form

$$\psi = \varphi[f_1]\varphi[f_2] \cdots \varphi[f_n]\Omega \tag{31}$$

with $f_k \in \mathcal{S}(R^4)$, $\operatorname{supp}(f_k) \subset R_k$, for $k = 1, \ldots, n$.

Then the linear span of the vacuum vector Ω and the union of all the linear manifolds S_n is dense in the Hilbert space $\mathcal{H}$.

This version differs from the original formulation only in the circumstance that the regions R_k need not all be the same. We feel justified in omitting the proof since it requires only a very minor modification of the proof in the case of equal regions, as presented in the monograph of Streater and Wightman. [18] The lemma can also easily be proved on the basis of Lemma 3.

We next consider an interesting family of vector-valued functions on T_n discussed by Jost. [19]

Lemma 5: (a) For each $n \geq 1$, let E_n be the set of all functions $f(x_1, \ldots, x_n; z_1, \ldots, z_n)$ defined for $(x_1, \ldots, x_n) \in R^{4n}$ and $(z_1, \ldots, z_n) \in T_n$, and such that $f \in \mathcal{S}(R^{4n})$ and such that the Fourier transform $\tilde{f}$ of f relative to the variables $(x_1, \ldots, x_n)$ satisfies the condition

$$\tilde{f}(p_1, \ldots, p_n; z_1, \ldots, z_n) = \exp\left(i \sum_{k=1}^{n} \sum_{r=k}^{n} z_k \cdot p_r\right) \tag{32a}$$

for all $(p_1, \ldots, p_n) \in V_n$, with V_n defined as in (25b). The set E_n is nonempty, and it contains in particular the function f_0 defined in terms of its Fourier transform by

$$\tilde{f}_0(p_1, \ldots, p_n; z_1, \ldots, z_n) = \prod_{k=1}^{n} E\left(\sum_{r=k}^{n} p_r; z_k\right) \tag{32b}$$

where the function $E(p;z)$ is defined as in (26).

To the set E_n corresponds a *unique* vector-valued function $\phi(z_1, \ldots, z_n)$ on T_n, defined by

$$\phi(z_1, \ldots, z_n) = \varphi\{f\}\Omega \tag{32c}$$

where f is any element of E_n.

(b) The vector-valued function $\phi(z_1, \ldots, z_n)$ is strongly continuous on T_n.

(c) Let $\{f_k | f_k \in \mathcal{D}(R^4),\ k = 1, \ldots, n\}$ be any n-tuplet of test functions of compact support. Then, for any $(z_1, \ldots, z_n) \in T_n$,

$$\begin{aligned} &\int_{(\infty)} d^4(x_1) \cdots d^4(x_n) f_1(x_1) f_2(x_2) \cdots f_n(x_n) \\ &\quad \times \phi(z_1 + x_1, z_2 + x_2 - x_1, z_3 + x_3 - x_2, \ldots, z_n + x_n - x_{n-1}) \\ &\qquad = T(z_1)\varphi[f_1]T(z_2)\varphi[f_2] \cdots T(z_n)\varphi[f_n]\Omega \end{aligned} \tag{33}$$

where the integral at left exists as a vector-valued Riemann integral relative to the strong topology for $\mathcal{H}$.

Proof: (1) The function f_0 trivially satisfies (32a). That it is included in $\mathcal{S}(R^{4n})$, as a function of $(x_1, \ldots, x_n)$, for any $(z_1, \ldots, z_n) \in T_n$, follows readily from the fact that $E(p;z) \in \mathcal{S}(R^4)$, for any $z \in V_{+i}$. That the vector at right in (32c) is the same for all $f \in E_n$ follows from the fact that this vector depends only on the restriction of $\tilde{f}$ to V_n.

(2) That the function ϕ is strongly continuous on T_n is easily established through an examination of the properties of the function f_0, as defined in (32b). The considerations are the same as in the proof of the strong continuity of the vector β in Lemma 3, and in fact somewhat simpler since $(z_1, \ldots, z_n)$ is now restricted to the open tube T_n.

(3) The assertion about the integral in (33) is now trivial, and the identity follows from a well-known convolution theorem for tempered distributions. [20] We note that the restriction that the functions f_k be of compact support is in fact unnecessary, but since we shall only require the lemma as stated, we selected this version in order to make the matter completely trivial.

We conclude this section by a statement of some well-known facts about the vector-valued functions ϕ, which will be of crucial importance in our subsequent discussion.

Lemma 6: (a) The vector-valued function $\phi(z_1, \ldots, z_n)$, defined as in Lemma 5, is an analytic function of $(z_1, \ldots, z_n)$ on T_n.

(b) For any element $\Lambda = \Lambda(M, x)$ of the Poincaré group $\overline{L}_0$,

$$U(\Lambda)\phi(z_1, \ldots, z_n) = \phi(Mz_1 + x, Mz_2, Mz_3, \ldots, Mz_n). \tag{34}$$

(c) For any $(z_1, \ldots, z_n) \in T_n$ the vector $\phi(z_1, \ldots, z_n)$ is an analytic vector for the Lie algebra of the group $U(\overline{L}_0)$.

About the proof: A detailed proof of the assertion (a) based on an examination of the properties of the func-

tion f_0 defined in (32b) is straightforward but somewhat cumbersome. For this reason it might be worthwhile to note that there is a simple proof based on Lemmas 3 and 5, as follows. Let $g(x) \in \mathcal{D}(R^4)$ be such that $\tilde{g}(0) = 1$. Let $\lambda > 1$. We construct the vector $\beta(z_1, \ldots, z_n; \lambda)$ as in (29), with $f_k(x) = \lambda^4 g(\lambda x)$, for $k = 1, \ldots, n$. This vector-valued function of $(z_1, \ldots, z_n)$ is an analytic function of these variables on T_n, by Lemma 3. It is easily seen, in view of (33), and in view of the strong continuity of ϕ on T_n, that $\beta(z_1, \ldots, z_n; \lambda)$ tends to $\phi(z_1, \ldots, z_n)$ as λ tends to infinity, *uniformly* on any closed polydisc contained in T_n, and hence ϕ is analytic on T_n.

The assertion (b) of the lemma is trivial, and the assertion (c) follows trivially from (a) and (b).

We finally note that the vector ϕ might be written as

$$\phi(z_1, \ldots, z_n) = \varphi(z_1)\varphi(z_1 + z_2) \cdots \varphi(z_1 + z_2 + \cdots + z_n)\Omega. \quad (35)$$

This formula has a proper interpretation within distribution theory, but it is here offered for heuristic purposes only.

IV. COMPLEX LORENTZ TRANSFORMATIONS AND THE INVERSION TRANSFORMATION

We define a "right wedge" W_R, and a "left wedge" W_L, as the following open subsets of Minkowski space:

$$W_R = \{x \mid x^3 > |x^4|\}, \quad W_L = \{x \mid x^3 < -|x^4|\}. \quad (36)$$

These two regions are bounded by two characteristic planes whose intersection is the 2-plane $\{x \mid x^3 = x^4 = 0\}$.

For *any* subset R of Minkowski space $\mathcal{M}$ we define the *causal complement* R^c of R by

$$R^c = \{x \mid (x - y) \cdot (x - y) < 0, \text{ all } y \in R\}. \quad (37)$$

We note that with this definition $W_R{}^c = \overline{W}_L$ and $W_L{}^c = \overline{W}_R$, where the bar denotes the closure. We shall say that W_R and W_L form a complementary pair of wedges, despite the fact that W_R is not precisely the causal complement of W_L within our definition of this notion.[21]

To the pair of wedges W_R and W_L corresponds a four-dimensional subgroup $\bar{L}_0(W_R) = \bar{L}_0(W_L)$ of the group $\bar{L}_0$, namely, the group of all Poincaré transformations which map W_R *onto* W_R, and W_L *onto* W_L. It is easily seen that this subgroup contains, and is generated by, all translations in the 1- and 2-directions, all rotations about the 3-axis, and all velocity transformations $V(\mathbf{e}_3, t)$ in the 3-direction. We consider the one-parameter Abelian subgroup $\{V(\mathbf{e}_3, t) \mid t \in R^1\}$ of these velocity transformations, where $V(\mathbf{e}_3, t)$ is the four-by-four Lorentz matrix given in (1) in Sec. I. To $V(\mathbf{e}_3, t)$ corresponds the unitary operator $U(V(\mathbf{e}_3, t), 0)$, which we shall also denote by the shorter symbol $V(t)$, since it will play an important role in our discussion. By Stone's theorem there exists a unique self-adjoint operator (K_3, D_K) such that

$$V(t) = U(V(\mathbf{e}_3, t), 0) = \exp(-itK_3), \quad \text{all real } t. \quad (38)$$

We shall consider the analytic continuation of the function $V(t)$ to the complex plane. It is well known that to any self-adjoint operator (K_3, D_K) corresponds a representation $\tau \to \exp(-i\tau K_3) = V(\tau)$ of the additive group of all complex numbers τ by (in general unbounded) operators. These operators have the common spectral resolution

$$V(\tau) = \exp(-i\tau K_3) = \int \exp(-i\tau s)\mu_K(ds) \quad (39)$$

where μ_K is the spectral measure in the spectral resolution of the operator (K_3, D_K). The domain of the closed operators $V(\tau)$ depends only on $\mathrm{Im}(\tau)$. Hence, for any $\tau = \rho + i\lambda$, with ρ, λ real, let $D_V(\lambda)$ be the linear manifold such that the operator $(V(\tau), D_V(\lambda))$ is *closed* and *normal*. The domain $D_V(\lambda)$ is given by

$$D_V(\lambda) = (1 + V(i\lambda))^{-1}\mathcal{H} \quad (40)$$

for any real λ.

Let $\lambda \neq 0$ be real. Then $D_V(\lambda)$ is a core for all operators $(V(\tau), D_V(\mathrm{Im}(\tau)))$ such that $0 \leq \mathrm{Im}(\tau)/\lambda \leq 1$. If $\psi \in D_V(\lambda)$, then the vector-valued function $V(\tau)\psi$ of τ is well defined, strongly continuous and bounded on the closed strip $0 \leq \mathrm{Im}(\tau)/\lambda \leq 1$, and an analytic function of τ on the interior of this strip.

Common cores exist for the operators $V(\tau)$. For later reference we state as a lemma some well-known facts about a particular family of such cores.

Lemma 7: (a) Let $c(s) \in \mathcal{D}(R^1)$, and let the bounded operator $c(K_3)$ be defined by

$$c(K_3) = \int c(s)\mu_K(ds). \quad (41)$$

Then $c(K_3)\mathcal{H} \subset D_V(\lambda)$ for all real λ. The function $\exp(-i\tau s)c(s)$ is also in $\mathcal{D}(R^1)$ for any complex τ, and

$$V(\tau)c(K_3) = \int \exp(-i\tau s)c(s)\mu_K(ds). \quad (42)$$

The operator-valued function $V(\tau)c(K_3)$ is a bounded operator for every complex τ, and it is an entire analytic function of τ in the sense of the uniform topology.

(b) Let D be any dense linear manifold, and let the linear manifold D_c be defined by

$$D_c = \mathrm{span}\{c(K_3)D \mid c(s) \in \mathcal{D}(R^1)\}. \quad (43a)$$

Then D_c is dense, and a core for every operator $(V(\tau), D_V(\mathrm{Im}(\tau)))$, i.e., $D_c \subset D_V(\mathrm{Im}(\tau))$ and

$$(V(\tau), D_c)^{**} = (V(\tau), D_V(\mathrm{Im}(\tau))). \quad (43b)$$

(c) If $c(s) \in \mathcal{D}(R^1)$, then $c(K_3)$ is also given by

$$c(K_3) = \int_{-\infty}^{\infty} dt\hat{c}(t)V(t) \quad (44a)$$

where $\hat{c}(t)$ is the Fourier transform of $c(s)$ defined by

$$\hat{c}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} ds \exp(its)c(s). \quad (44b)$$

We shall next consider the action of the complex velocity transformation $V(\tau)$ on the vectors $\phi(z_1, \ldots, z_n)$ introduced in Lemma 5. We first note that the matrix-valued function $V(\mathbf{e}_3, t)$, defined in (1) in Sec. I, is an entire analytic function of t. Let $z = x + iy$, x and y real, be any complex 4-vector, and let τ be any complex number. We shall write

$$z(\tau) = V(\mathbf{e}_3, \tau)z \quad (45a)$$

and we then have, for $\tau = i\lambda$,

$$z^1(i\lambda) = x^1 + iy^1, \quad z^2(i\lambda) = x^2 + iy^2,$$

$$z^3(i\lambda) = (x^3\cos(\lambda) - y^4\sin(\lambda)) + i(y^3\cos(\lambda) + x^4\sin(\lambda)),$$

$$z^4(i\lambda) = (x^4\cos(\lambda) - y^3\sin(\lambda)) + i(y^4\cos(\lambda) + x^3\sin(\lambda)). \tag{45b}$$

We have written the explicit transformation formulas in the above form because we are particularly interested in the case of a real λ, i. e., the case of a pure imaginary velocity transformation. We can now state the following:

Lemma 8: Let $(z_1, \ldots, z_n)$ be an n-tuplet of complex 4-vectors $z_k = x_k + iy_k$, where x_k, y_k, real, $y_k{}^1 = y_k{}^2 = 0$, $y_k{}^4 > |y_k{}^3|$, for $k = 1, \ldots, n$.

(a) If $x_k \in W_R$ (i. e., $x_k{}^3 > |x_k{}^4|$), for $k = 1, \ldots, n$, then $(z_1(i\lambda), \ldots, z_n(i\lambda)) \in T_n$ for all $\lambda \in [0, \pi/2]$. The vector $\phi(z_1, \ldots, z_n)$ is in the domain $D_V(\pi/2)$, and

$$V(i\lambda)\phi(z_1, \ldots, z_n) = \phi(z_1(i\lambda), \ldots, z_n(i\lambda)) \tag{46}$$

for all $\lambda \in [0, \pi/2]$.

(b) If $x_k \in W_L$ (i. e., $x_k{}^3 < -|x_k{}^4|$), for $k = 1, \ldots, n$, then $(z_1(i\lambda), \ldots, z_n(i\lambda)) \in T_n$ for all $\lambda \in [-\pi/2, 0]$. The vector $\phi(z_1, \ldots, z_n)$ is in the domain $D_V(-\pi/2)$, and the relation (46) holds for all $\lambda \in [-\pi/2, 0]$.

Proof: (1) We consider the assertions in part (a). By inspection of the explicit formulas (45b), it is easily seen that if $z = x + iy$ is a complex four-vector such that $y^1 = y^2 = 0$, $y^4 > |y^3|$, and $x^3 > |x^4|$, then $\mathrm{Im}(z(i\lambda)) \in V_+$ for all $\lambda \in [0, \pi/2]$. Hence, in view of the stated conditions on $(z_1, \ldots, z_n)$, we have $(z_1(i\lambda), \ldots, z_n(i\lambda)) \in T_n$ for all λ on the closed interval, with T_n defined as in Lemma 3. Since T_n is open there exists a connected open neighborhood N (in the complex λ-plane) of the closed segment $[0, \pi/2]$ such that $(z_1(i\lambda), \ldots, z_n(i\lambda)) \in T_n$ for $\lambda \in N$, and hence the vector $\phi(z_1(i\lambda), \ldots, z_n(i\lambda))$ is well defined for $\lambda \in N$. By Lemma 6 this vector, regarded as a function of λ, is an analytic function on N.

(2) Let D_c be defined as in (43a), with $D = \mathcal{H}$. For any $\eta \in D_c$ the function $f_1(\lambda) = \langle V(i\lambda)^*\eta \,|\, \phi(z_1, \ldots, z_n)\rangle$ is an entire analytic function of λ, by Lemma 7. We define the function $f_2(\lambda)$ on N by $f_2(\lambda) = \langle \eta \,|\, \phi(z_1(i\lambda), \ldots, z_n(i\lambda))\rangle$. By Lemma 6 we have $f_1(\lambda) = f_2(\lambda)$ for $i\lambda$ in some *real* neighborhood of $\lambda = 0$, and it follows that $f_1(\lambda) = f_2(\lambda)$ on N. Since this holds for any $\eta \in D_c$, and since D_c is a core for every $(V(\tau), D_V(\mathrm{Im}(\tau)))$, it follows that $\phi(z_1, \ldots, z_n) \in D_V(\mathrm{Im}(i\lambda))$ for $\lambda \in N$, and that (46) holds for all $\lambda \in N$. This proves the assertions in part (a).

(3) The assertions in part (b) are proved in an entirely analogous fashion.

We next consider an *involutory* mapping $x \to \mathcal{J}x$ of Minkowski space onto itself, defined by

$$\mathcal{J}x = -R(\mathbf{e}_3, \pi)x \quad \text{or} \quad \mathcal{J}(x^1, x^2, x^3, x^4) = (x^1, x^2, -x^3, -x^4) \tag{47}$$

where $R(\mathbf{e}_3, \pi)$ denotes the rotation by angle π about the 3-axis. We see that $\mathcal{J}$ maps W_R onto W_L, and the mapping can be described as a reflection in the common "edge" $\{x \,|\, x^3 = x^4 = 0\}$ of the pair of wedges W_R and W_L.

By inspection of (45b) we see that

$$\mathcal{J} = V(\mathbf{e}_3, i\pi) \tag{48}$$

and this circumstance suggests the heuristic idea that something akin to $V(i\pi)\varphi(x)V(i\pi)^{-1} = \varphi(\mathcal{J}x)$ might hold. This formula is, of course, pure nonsense as it stands, but in the following we shall establish some facts which in a sense reflect the above heuristic idea.

Lemma 9: Let $(x_1, \ldots, x_n)$ be such that $x_k \in W_R$ for $k = 1, \ldots, n$. Let v be the real forward timelike 4-vector with components $v = (0, 0, 0, 1)$, and let t be a real variable. Then

$$\begin{aligned} &\text{s-lim}_{t \to 0+} V(i\pi/2)\phi(x_1 + itv, x_2 + itv, \ldots, x_n + itv) \\ &\quad = \text{s-lim}_{t \to 0+} V(-i\pi/2)\phi(\mathcal{J}x_1 + itv, \mathcal{J}x_2 + itv, \ldots, \mathcal{J}x_n + itv) \\ &\quad = \phi(z_1, \ldots, z_n) \end{aligned} \tag{49}$$

where $z_k = (x_k{}^1, x_k{}^2, ix_k{}^4, ix_k{}^3)$, for $k = 1, \ldots, n$.

Proof: By Lemma 8, part (a), we have, for $t > 0$,

$$V(i\pi/2)\phi(x_1 + itv, \ldots, x_n + itv) = \phi(z_1', \ldots, z_n') \tag{50a}$$

where

$$z_k' = z_k'(t) = z_k - (0, 0, t, 0), \quad \text{for } k = 1, \ldots, n. \tag{50b}$$

Since $\mathcal{J}x_k \in W_L$ if $x_k \in W_R$, we similarly have, by part (b) of Lemma 8, for any $t > 0$,

$$V(-i\pi/2)\phi(\mathcal{J}x_1 + itv, \ldots, \mathcal{J}x_n + itv) = \phi(z_1'', \ldots, z_n'') \tag{50c}$$

with

$$z_k'' = z_k''(t) = z_k + (0, 0, t, 0), \quad \text{for } k = 1, \ldots, n. \tag{50d}$$

We note that $(z_1', \ldots, z_n') \in T_n$, and $(z_1'', \ldots, z_n'') \in T_n$, for all real t, and it follows from Lemma 5 that the vectors at right in (50a) and (50c) have well-defined strong limits as t tends to zero. The equalities in (49) then follow from (50b) and (50d).

Lemma 10: Let R_1 be a bounded, open, nonempty subset of W_R, and let $x_0 \in W_R$ be such that $(x - x_0) \in W_L$ for all $x \in \bar{R}_1$. For any integer $n > 1$ we define the set R_n by

$$R_n = \{x + (n-1)x_0 \,|\, x \in R_1\}. \tag{51}$$

(a) Then $R_n \subset W_R$ for all n, and if $n > k$, then $(x' - x'') \in W_R$ for all $x' \in R_n$, $x'' \in R_k$. In particular, R_n is spacelike separated from R_k (i. e., $R_n \subset R_k{}^c$) if $n \neq k$.

(b) Let $\{f_k \,|\, k = 1, \ldots, n\}$ be an n-tuplet of test functions such that $f_k \in \mathcal{S}(R^4)$ and $\mathrm{supp}(f_k) \subset R_k$, for $k = 1, \ldots, n$. Let $f_k{}^j$ denote the test function defined by $f_k{}^j(x) = f_k(\mathcal{J}x)$. Let $c(s) \in \mathcal{D}(R^1)$. Then

$$\begin{aligned} &V(i\pi)c(K_3)\varphi[f_1]\varphi[f_2]\cdots\varphi[f_n]\Omega \\ &\quad = c(K_3)\varphi[f_1{}^j]\varphi[f_2{}^j]\cdots\varphi[f_n{}^j]\Omega. \end{aligned} \tag{52}$$

Proof: (1) The assertions in part (a) are trivial, and need not be proved here.

(2) Let $v = (0, 0, 0, 1)$. We consider the string of equalities:

$$\begin{aligned} &V(i\pi/2)c(K_3)\varphi[f_1]\varphi[f_2]\cdots\varphi[f_n]\Omega \\ &= \text{s-lim}_{t \to 0+} V(i\pi/2)c(K_3)T(itv)\varphi[f_1]T(itv)\varphi[f_2]\cdots T(itv) \\ &\quad \times \varphi[f_n]\Omega \end{aligned}$$

$$= \text{s-}\lim_{t\to 0+} V(i\pi/2)c(K_3)\int_{(\infty)} d^4(x_1)\cdots d^4(x_n) f_1(x_1)f_2(x_2)\cdots f_n(x_n)$$
$$\times \phi(itv + x_1, itv + x_2 - x_1, itv + x_3 - x_2, \ldots, itv + x_n - x_{n-1})$$
$$= \int_{(\infty)} d^4(x_1)\cdots d^4(x_n) f_1(x_1)f_2(x_2)\cdots f_n(x_n)$$
$$\times \text{s-}\lim_{t\to 0+} V(i\pi/2)c(K_3)$$
$$\times \phi(itv + x_1, itv + x_2 - x_1, itv + x_3 - x_2, \ldots, itv + x_n - x_{n-1})$$
$$= \int_{(\infty)} d^4(x_1)\cdots d^4(x_n) f_1{}^j(x_1)f_2{}^j(x_2)\cdots f_n{}^j(x_n)$$
$$\times \text{s-}\lim_{t\to 0+} V(-i\pi/2)c(K_3)$$
$$\times \phi(itv + x_1, itv + x_2 - x_1, itv + x_3 - x_2, \ldots, itv + x_n - x_{n-1})$$
$$= \text{s-}\lim_{t\to 0+} V(-i\pi/2)c(K_3)T(itv)$$
$$\times \varphi[f_1{}^j]T(itv)\varphi[f_2{}^j]\cdots T(itv)\varphi[f_n{}^j]\Omega$$
$$= V(-i\pi/2)c(K_3)\varphi[f_1{}^j]\varphi[f_2{}^j]\cdots\varphi[f_n{}^j]\Omega. \tag{53}$$

That the first member in (53) is equal to the second member, and that the last member is equal to the next to the last member, follows from Lemma 3 (i. e., from the strong continuity of the function there denoted β), and from the fact that the operators $V(i\pi/2)c(K_3)$ and $V(-i\pi/2)c(K_3)$ are bounded. That the second member is equal to the third member follows from the formula (33) in Lemma 5. In view of the properties of the integrand in the third member which follow from the facts stated in Lemma 9, and from the nature of the functions f_k, it is permissible to let the bounded operator $V(i\pi/2)c(K_3)$ act on the integrand, and to take the strong limit before integration. We note that the relationships between the supports of the function f_k, as expressed in the assertions (a) of the present lemma, are essential at this step. Because of these relationships the arguments of the function ϕ appearing in the integrand satisfy the premises of Lemma 9, which is thus applicable. The third and the fourth members are thus equal. In a similar fashion we conclude that the fifth and the sixth members are equal. The equality of the fourth and the fifth members follows from Lemma 9. (Note the trivial change in integration variables).

(3) We finally note that the vector in (53) is in the domain of $(V(i\pi/2), D_V(\pi/2))$, and if we multiply the first and the last members in the string by this operator we obtain (52).

It should be noted that the condition that the field be *local* has played no role in our discussion so far, and in particular the formula (52) does not depend on the assumption of locality. We shall now consider some additional conclusions which can be drawn if we take into account the locality condition (16).

From the work of Jost[22] it is well known that in a local field theory based on our general assumptions there exists an antiunitary involution Θ_0, which can be interpreted physically as an inversion transformation, or TCP-transformation (with respect to the origin in Minkowski space). This operator satisfies the conditions

$$\Theta_0{}^2 = I, \quad \Theta_0\Omega = \Omega, \quad \Theta_0 U(M, x)\Theta_0 = U(M, -x), \tag{54a}$$

and

$$\Theta_0\varphi(x)\Theta_0 = \varphi(-x), \tag{54b}$$

where the last relation refers specifically to the case of a Hermitian scalar field.

We shall introduce another antiunitary involution J, defined by

$$J = U(R(\mathbf{e}_3, \pi), 0)\Theta_0 = \Theta_0 U(R(\mathbf{e}_3, \pi), 0) \tag{55}$$

where, as before, $R(\mathbf{e}_3, \pi)$ denotes the rotation by angle π about the 3-axis. It is easily seen that

$$J^2 = \mathrm{I}, \quad J\Omega = \Omega, \quad JU(M, x)J = U(\mathcal{J}M\mathcal{J}, \mathcal{J}x) \tag{56a}$$

where $\mathcal{J}$ is defined in (47). Furthermore, $JD_1 = D_1$, and

$$J\varphi[f]J = \varphi[f^j]^* \text{ on } D_1 \tag{56b}$$

for any $f \in \mathcal{S}(R^4)$, and where $f^j(x) = f(\mathcal{J}x)$.

We consider the third relation in (56a) for the case of a (real) velocity transformation in the 3-direction. We have

$$JV(t)J = V(t), \quad \text{all real } t. \tag{57a}$$

From this relation, and from the fact that J is an antiunitary involution, we readily conclude that

$$JD_K = D_K, \quad J(K_3, D_K)J = -(K_3, D_K), \tag{57b}$$
$$JD_V(\lambda) = D_V(-\lambda), \quad J(V(\tau), D_V(\lambda))J = (V(\tau^*), D_V(-\lambda)) \tag{57c}$$

for any complex $\tau = \rho + i\lambda$, ρ and λ real.

As the formula (52) suggests, the complex velocity transformations $V(i\pi)$ and $V(-i\pi)$ will be of particular interest. We shall employ the special notation

$$D_+ = D_V(\pi), \quad D_- = D_V(-\pi) \tag{58}$$

for the domains of these operators, and $(V(i\pi), D_+)$ and $(V(-i\pi), D_-)$ are thus self-adjoint. We then have

$$D_+ = JD_- = V(-i\pi)D_-, \quad D_- = JD_+ = V(i\pi)D_+, \tag{59a}$$

and

$$J(V(i\pi), D_+)J = (V(-i\pi), D_-),$$
$$J(V(-i\pi), D_-)J = (V(i\pi), D_+). \tag{59b}$$

The antiunitary involution J can be regarded as associated with the pair of wedges W_R and W_L, or, if we like, with their common "edge," whereas the involution Θ_0 is associated with a point, the origin of Minkowski space. J is the Hilbert space object corresponding to the involution $\mathcal{J}$ on Minkowski space, as revealed by (56b). We note that if $\text{supp}(f) \subset W_R$, then $\text{supp}(f^j) \subset W_L$, and vice versa. Conjugation with J thus maps operators locally associated with the right wedge W_R into operators locally associated with the left wedge W_L. We also note that

$$JU(\Lambda)J = U(\Lambda), \quad \text{all } \Lambda \in \bar{L}_0(W_R), \tag{60}$$

where $\bar{L}_0(W_R)$ is the group of all Poincaré transformations which map W_R *onto* W_R.

We shall next consider an extension of Lemma 10 which incorporates the condition that the field be local.

Lemma 11: Let $\{R_n | n = 1, \ldots, \infty\}$ be a *fixed* set of bounded, open, nonempty subsets of W_R, constructed as

in Lemma 10. Let $\mathcal{Q}$ be the linear span of the identity operator I and all operators (Q, D_1) of the form

$$Q = \varphi[f_1]\varphi[f_2]\cdots\varphi[f_n] \tag{61}$$

where $\{f_k | k = 1, \ldots, n\}$ is any n-tuplet of test functions such that $f_k \in \mathcal{S}(R^4)$ and $\mathrm{supp}(f_k) \subset R_k$, for $k = 1, \ldots, n$.

Then:

(a) The linear manifold $D_q = \mathcal{Q}\Omega$ is dense in the Hilbert space $\mathcal{H}$, and $D_{qc} = \mathrm{span}\{c(K_3)D_q | c(s) \in \mathcal{D}(R^1)\}$ is a core for every operator $(V(\tau), D_V(\mathrm{Im}(\tau)))$.

(b) $(Q^*, D_1) \in \mathcal{Q}$ if $(Q, D_1) \in \mathcal{Q}$.

(c) If $(Q, D_1) \in \mathcal{Q}$ and $c(s) \in \mathcal{D}(R^1)$, then

$$V(i\pi)c(K_3)Q\Omega = c(K_3)JQ^*\Omega. \tag{62}$$

Proof: (1) The assertions (a) follow directly from Lemmas 4 and 7.

(2) The assertion (b) is trivial if Q is a multiple of I. If Q is of the special form (61) we have

$$\begin{aligned} Q^\dagger &= \varphi[f_n^\dagger]\cdots\varphi[f_2^\dagger]\varphi[f_1^\dagger] \\ &= \varphi[f_1^\dagger]\varphi[f_2^\dagger]\cdots\varphi[f_n^\dagger], \end{aligned} \tag{63}$$

where the second member is equal to the third in view of the locality condition (16), and in view of the relationships between the supports of the functions f_k, as stated in part (a) of Lemma 10. Since $(Q^*, D_1) = (Q^\dagger, D_1)$, we see that $(Q^*, D_1) \in \mathcal{Q}$.

(3) The relation (62) is trivial if Q is a multiple of I. For Q of the special form (61) we have, in view of (63),

$$JQ^\dagger J = \varphi[f_1^j]\varphi[f_2^j]\cdots\varphi[f_n^j]. \tag{64}$$

Since $Q^*\Omega = Q^\dagger\Omega$ the relation (62) then follows from (64) and from (52) in Lemma 10. This, in effect, proves the assertion (c).

To an n-tuplet $(x_1, \ldots, x_n)$ such that $x_k \in R_k$ for $k = 1, \ldots, n$, corresponds the n-tuplet $(x_1, x_2 - x_1, x_3 - x_2, \ldots, x_n - x_{n-1})$, which is a so-called Jost point.[23] We note here that there is a very close connection between our considerations and Jost's beautiful proof of the TCP-theorem.[22] In a sense the key point is the fact that the complex Lorentz transformations $V(\mathbf{e}_3, i\lambda)$, for $\lambda \in (0, \pi)$, map the wedge region W_R into the forward imaginary tube V_{+i}. This fact, and the associated connection between complex Lorentz transformations and the inversion transformation, were discovered by Jost, and form the basis of his proof.

We are now in a position to state and prove the key theorem. For the definition of the algebras $\mathcal{P}(W_R)$ and $\mathcal{P}(W_L)$ we refer to our general definition [in Sec. II, immediately following Eq. (15)] of the algebra $\mathcal{P}(R)$, for any open $R \subset \mathcal{M}$. The algebra $\mathcal{P}(W_R)$, respectively the algebra $\mathcal{P}(W_L)$, can be regarded as consisting of field operators locally associated with the wedge region W_R, respectively the region W_L.

Theorem 1: (a) The algebras $\mathcal{P}(W_R)$ and $\mathcal{P}(W_L)$ are $*$-algebras with the antilinear involution $(X, D_1) \to (X^*, D_1)$. They commute on D_1, i. e.,

$$[X, Y]\psi = 0 \tag{65}$$

for all $\psi \in D_1$ and for all $X \in \mathcal{P}(W_R)$, $Y \in \mathcal{P}(W_L)$.

(b) The vacuum vector Ω is cyclic and separating for both $\mathcal{P}(W_R)$ and $\mathcal{P}(W_L)$.

(c) With $V(t) = U(V(\mathbf{e}_3, t), 0)$ (a velocity transformation in the 3-direction),

$$V(t)\mathcal{P}(W_R)V(t)^{-1} = \mathcal{P}(W_R), \quad V(t)\mathcal{P}(W_L)V(t)^{-1} = \mathcal{P}(W_L) \tag{66}$$

for all real t, and with J defined by (55),

$$J\mathcal{P}(W_R)J = \mathcal{P}(W_L). \tag{67}$$

(d) With D_+ and D_- defined as in (58),

$$\mathcal{P}(W_R)\Omega \subset D_+, \quad \mathcal{P}(W_L)\Omega \subset D_-. \tag{68a}$$

For any $X \in \mathcal{P}(W_R)$

$$V(i\pi)X\Omega = JX^*\Omega \tag{68b}$$

and for any $Y \in \mathcal{P}(W_L)$

$$V(-i\pi)Y\Omega = JY^*\Omega. \tag{68c}$$

(e) The condition

$$C_R X\Omega = X^*\Omega, \quad \text{all } X \in \mathcal{P}(W_R), \tag{69a}$$

defines an *antilinear* operator $(C_R, \mathcal{P}(W_R)\Omega)$, and the condition

$$C_L Y\Omega = Y^*\Omega, \quad \text{all } Y \in \mathcal{P}(W_L), \tag{69b}$$

defines an *antilinear* operator $(C_L, \mathcal{P}(W_L)\Omega)$.

These two operators satisfy the relations

$$(C_R, \mathcal{P}(W_R)\Omega)^{**} = (C_L, \mathcal{P}(W_L)\Omega)^* = (JV(i\pi), D_+), \tag{69c}$$

$$(C_L, \mathcal{P}(W_L)\Omega)^{**} = (C_R, \mathcal{P}(W_R)\Omega)^* = (JV(-i\pi), D_-). \tag{69d}$$

Proof: (1) The assertions (a) and (c) are trivial. That Ω is a cyclic vector for the algebras follows from the Reeh–Schlieder theorem. That Ω is separating for $\mathcal{P}(W_R)$ follows readily from the commutation relation (65), and from the fact that Ω is cyclic for $\mathcal{P}(W_L)$. In a similar manner we conclude that Ω is separating for $\mathcal{P}(W_L)$.[24]

(2) We now consider the assertions (d) and (e). We note that our formulation is tautological in the sense that the assertions (d) are trivially implied by the assertions (e). We presented the matter in this manner because we wanted the relations (68b) and (68c) to stand out as clearly as possible.

For didactic reasons we shall first prove the assertions (d), independently of the considerations in (e). Let a set $\mathcal{Q}$ of operators, and a domain D_{qc}, be constructed exactly as in Lemma 11. We note that $\mathcal{Q} \subset \mathcal{P}(W_R)$.

Let $Q \in \mathcal{Q}$, $X \in \mathcal{P}(W_R)$, and $c(s) \in \mathcal{D}(R^1)$. We introduce the integral representation (44) of the operator $c(K_3)$, and we note that

$$c^*(-K_3) = \int_{-\infty}^{\infty} d\hat{c}^*(t)V(t) \tag{70a}$$

where $\hat{c}(t)$ is given by (44b).

We consider the following string of equalities:

$$\begin{aligned} &\langle X\Omega \,|\, V(i\pi)c(K_3)Q\Omega\rangle \\ &\quad = \langle X\Omega \,|\, c(K_3)JQ^*\Omega\rangle = \langle X\Omega \,|\, Jc^*(-K_3)Q^*\Omega\rangle \\ &\quad = \langle c^*(-K_3)Q^*\Omega \,|\, JX\Omega\rangle \end{aligned}$$

$$= \int_{-\infty}^{\infty} dt \hat{c}(t) \langle V(t) Q^* V(t)^{-1} \Omega \,|\, (JXJ)\Omega \rangle$$

$$= \int_{-\infty}^{\infty} dt \hat{c}(t) \langle (JXJ)^* \Omega \,|\, V(t) Q V(t)^{-1} \Omega \rangle$$

$$= \langle JX^* \Omega \,|\, c(K_3) Q \Omega \rangle. \tag{70b}$$

The first two members are equal in view of (62) in Lemma 11. The equality of the second and the third members follows from (57b), and since J is an antiunitary involution these expressions are equal to the fourth member. The equality of the fourth and fifth members follows from (70a). The integrands in the fifth and sixth members are equal because the operator $V(t)Q^\dagger V(t)^{-1} \in \mathcal{P}(W_R)$ commutes with the operator $JXJ \in \mathcal{P}(W_L)$ on D_1. The equality of the last two members follows from (44a).

In view of the construction of the domain D_{qc} we conclude from (70b) that if η is any vector in D_{qc}, then

$$\langle X\Omega \,|\, V(i\pi)\eta \rangle = \langle JX^* \Omega \,|\, \eta \rangle. \tag{70c}$$

Since D_{qc} is a core for $(V(i\pi), D_+)$ (by Lemma 11), it follows from (70c) that $X\Omega \in D_+$, and that (68b) holds.

The relation (68c) and the second relation in (68a) then follows trivially from (67) and (59b).

(3) The assertions (e) involve antilinear operators, and since the theory of such operators might appear less familiar than the theory of linear operators we shall make a few remarks about the subject. Let (A, D_a) be an antilinear operator, defined on a dense domain D_a. The adjoint $(A, D_a)^* = (A^*, D_a{}^*)$ of (A, D_a) is defined as follows. A vector η is in the domain $D_a{}^*$ of the adjoint if and only if there exists a vector $\zeta(\eta)$ such that $\langle \eta \,|\, A\xi \rangle = \langle \xi \,|\, \zeta(\eta) \rangle$ for every $\xi \in D_a$. The operator A^* on $D_a{}^*$ is then defined by $A^*\eta = \zeta(\eta)$, and it is also antilinear. The operator (A, D_a) is closable if and only if its adjoint is densely defined, and if it is closable its closure $(A, D_a)^{**}$ is the adjoint of the adjoint $(A^*, D_a{}^*)$. The properties of an antilinear operator (A, D_a) can be conveniently studied in terms of the *linear* operator $(L, D_a) = (J_0 A, D_a) = J_0 (A, D_a)$, where J_0 is an arbitrary *antiunitary* operator. We then have $(A, D_a)^* = (L^* J_0, J_0^{-1} D(L^*))$. The operator (A, D_a) is closable if and only if (L, D_a) is closable, and if it is closable, then $(A, D_a)^{**} = J_0^{-1} (L, D_a)^{**}$. The well-known polar decomposition theorem for linear operators has a counterpart for antilinear operators, as we easily see in view of the above. We note that the formulas (69c) and (69d) explicitly describe the polar decompositions of the adjoints and closures of the "adjointing operators" C_R and C_L defined by (69a) and (69b).

(4) After this digression we consider the assertions (e). It follows at once from the definition (69a), and from (68b) that

$$(JV(i\pi), D_+) \supset (C_R, \mathcal{P}(W_R)\Omega), \tag{71a}$$

and if we take the closures of both members in (71a) we obtain

$$(JV(i\pi), D_+) \supset (C_R, \mathcal{P}(W_R)\Omega)^{**} \tag{71b}$$

since $(V(i\pi), D_+)$ is self-adjoint and $(JV(i\pi), D_+)$ therefore is closed.

We shall now show that

$$(C_R, \mathcal{P}(W_R)\Omega)^{**} \supset (JV(i\pi), D_{qc}). \tag{71c}$$

Let η be any vector in the domain of $(C_R, \mathcal{P}(W_R)\Omega)^*$. Let $Q \in \mathcal{Q}$, and $c(s) \in \mathcal{D}(R^1)$. We again introduce the integral representation (44) for the operator $c(K_3)$, and we consider the string of equalities:

$$\langle C_R{}^* \eta \,|\, c(K_3) Q\Omega \rangle$$

$$= \int_{-\infty}^{\infty} dt \hat{c}(t) \langle C_R{}^* \eta \,|\, V(t) Q V(t)^{-1} \Omega \rangle$$

$$= \int_{-\infty}^{\infty} dt \hat{c}(t) \langle V(t) Q^* V(t)^{-1} \Omega \,|\, \eta \rangle$$

$$= \langle c^*(-K_3) Q^* \Omega \,|\, \eta \rangle = \langle JV(i\pi) c(K_3) Q\Omega \,|\, \eta \rangle. \tag{71d}$$

The equality of the second and third members follows from the fact that $V(t) Q V(t)^{-1} \Omega$ is in the domain of the antilinear operator $(C_R, \mathcal{P}(W_R)\Omega)$. The reasoning behind the other steps is similar to the reasoning in (2) above. In view of the construction of the domain D_{qc} the equalities (71d) imply (71c).

Since D_{qc} is a core for $(V(i\pi), D_+)$, we have

$$(JV(i\pi), D_+) = (JV(i\pi), D_{qc})^{**} \tag{71e}$$

and it follows from (71b) and (71e) that

$$(C_R, \mathcal{P}(W_R)\Omega)^{**} = (JV(i\pi), D_+). \tag{71f}$$

The analogous relation

$$(C_L, \mathcal{P}(W_L)\Omega)^{**} = (JV(-i\pi), D_-) \tag{71g}$$

is most easily proved by considering the conjugation of both members in (71f) by J. The remaining relations in (69c) and (69d) follow trivially from (71f) and (71g), and from the relation

$$(JV(i\pi), D_+)^* = (JV(-i\pi), D_-). \tag{71h}$$

This completes the proof of the theorem. We conclude this section with some remarks which we hope will further clarify the situation.

Concerning the relations (69c) and (69d) we note the following. If we are given two algebras, denoted $\tilde{\mathcal{P}}(W_R)$ and $\tilde{\mathcal{P}}(W_L)$, which satisfy the conditions (a) and (b), and the relation (67), of Theorem 1 (for some antiunitary involution J), and if we define the "adjointing operators" $\tilde{C}_R$ and $\tilde{C}_L$ by (69a) and (69b), then it can be shown that these antilinear operators are closable, and that

$$(\tilde{C}_L, \tilde{\mathcal{P}}(W_L)\Omega)^* \supset (\tilde{C}_R, \tilde{\mathcal{P}}(W_R)\Omega)^{**}. \tag{72}$$

However, it *cannot* be concluded that the inclusion in (72) can be replaced by equality. We can see this as follows (within the framework of quantum field theory). Suppose that the two algebras had been defined "wrongly" in such a way that they were actually equal to two algebras which in our notation are written as $\mathcal{P}(W_R')$, respectively $\mathcal{P}(W_L')$, where $W_L' = \mathcal{J} W_R'$, and where W_R' is a wedge properly included in W_R, and obtained from W_R through a translation. The conditions (a) and (b), and the relation (67), of Theorem 1 would then be satisfied, and the relation (72) would hold. The two members in (72) are, however, not equal, because the "wrong" algebras are "too small." It is significant that the "wrong" algebras, constructed as above, also do not

satisfy the relations (66), which say that the algebras are invariant under all velocity transformations $V(t)$.

As the above considerations indicate, it is easy to construct a large set of *distinct* closed extensions of $(C_R, \mathcal{P}(W_R)\Omega)$. Let W_R'' be any wedge obtained by a translation of W_R, and such that $W_R'' \supset W_R$. We define the operator $(C_R'', \mathcal{P}(W_R'')\Omega)$ in analogy with (69a), and we then have $(C_R'', \mathcal{P}(W_R'')\Omega) \supset (C_R, \mathcal{P}(W_R)\Omega)$, with a corresponding inclusion relation for the closures. It is easily seen that the closures are distinct if $W_R'' \neq W_R$.

Lemma 11 states facts about the field operators which are of crucial importance in the proof of Theorem 1. However, if we consider the role played by this lemma in the proof, it might seem miraculous that one can draw general conclusions about *all* the operators in $\mathcal{P}(W_R)$ from the properties of operators in a particular set $\mathcal{Q}$ which are locally associated with a family of regions $\{R_n \mid n = 1, \ldots, \infty\}$ which does not cover W_R. Now it should be noted that the construction of the domain D_{qc} involves operators in $V(t)\mathcal{Q}V(t)^{-1}$, for any real t, but it is still the case that the set of regions $\{V(\mathbf{e}_3, t)R_n \mid n = 1, \ldots, \infty, t \in R^1\}$ does not cover W_R either. A closer examination of this issue reveals that the "potency" of the set $\mathcal{Q}$ ultimately depends on the geometrical fact that if x is *any* point of W_R, then $\{V(\mathbf{e}_3, t)x \mid t \in R^1\}^{cc} = W_R$, where the superscript cc denotes the causal complement of the causal complement.

Finally, we note that since $\mathcal{Q} \subset \mathcal{P}(W_R)$ it follows, in view of (68b) in Theorem 1, that the factor $c(K_3)$ in both members of (62) in Lemma 11 is in fact "unnecessary": The relation also makes sense if $c(K_3)$ is replaced by 1. We introduced this factor in order to have simple proofs of Lemmas 10 and 11.

V. ON SOME ALGEBRAIC QUESTIONS CONNECTED WITH THEOREM 1.

This section is a mathematical preliminary to our discussion of physical duality conditions in the next section. The questions which we shall discuss are related to the issues of Theorem 1, although one might say that we are here more concerned with the properties of the triplet (Ω, J, K_3) than with the quantum fields.

We shall first be concerned with the characterization of operators in general (bounded or unbounded) which satisfy relations such as (68b) and (68c) in Theorem 1.

Lemma 12: Let $\mathcal{U}(W_R)$ be the set of all closable operators $(X, D(X))$ such that $\Omega \in D(X) \cap D(X^*)$, and such that $X\Omega \in D_+$ and

$$V(i\pi)X\Omega = JX^*\Omega. \tag{73a}$$

Let $\mathcal{U}(W_L)$ be the set of all closable operators $(Y, D(Y))$, such that $\Omega \in D(Y) \cap D(Y^*)$, and such that $Y\Omega \in D_-$ and

$$V(-i\pi)Y\Omega = JY^*\Omega. \tag{73b}$$

Then:

(a) $(X, D(X))^* = (X^*, D(X^*)) \in \mathcal{U}(W_R)$ if $(X, D(X)) \in \mathcal{U}(W_R)$ and $(Y, D(Y))^* = (Y^*, D(Y^*)) \in \mathcal{U}(W_L)$ if $(Y, D(Y)) \in \mathcal{U}(W_L)$.

(b)

$$J\mathcal{U}(W_R)J = \mathcal{U}(W_L), \quad J\mathcal{U}(W_L)J = \mathcal{U}(W_R), \tag{74}$$

i.e., $(X, D(X)) \in \mathcal{U}(W_R)$ if and only if $(JXJ, JD(X)) \in \mathcal{U}(W_L)$.

(c)

$$V(t)\mathcal{U}(W_R)V(t)^{-1} = \mathcal{U}(W_R), \quad V(t)\mathcal{U}(W_L)V(t)^{-1} = \mathcal{U}(W_L) \tag{75}$$

for all real t.

(d) Let $\mathcal{U}_b(W_R)$ denote the set of all *bounded* operators in $\mathcal{U}(W_R)$, and let $\mathcal{U}_b(W_L)$ denote the set of all *bounded* operators in $\mathcal{U}(W_L)$. Then

$$\mathcal{U}_b(W_R)\Omega = \mathcal{U}(W_R)\Omega = D_+, \quad \mathcal{U}_b(W_L)\Omega = \mathcal{U}(W_L)\Omega = D_-. \tag{76}$$

(e) The relation

$$\langle X^*\Omega \mid Y\Omega\rangle = \langle Y^*\Omega \mid X\Omega\rangle \tag{77}$$

holds for all operators $(X, D(X)) \in \mathcal{U}(W_R)$, $(Y, D(Y)) \in \mathcal{U}(W_L)$.

If a closable operator $(X, D(X))$ is such that $\Omega \in D(X) \cap D(X^*)$, then $(X, D(X)) \in \mathcal{U}(W_R)$ if and only if (77) holds for all $(Y, D(Y)) \in \mathcal{U}(W_L)$.

If a closable operator $(Y, D(Y))$ is such that $\Omega \in D(Y) \cap D(Y^*)$, then $(Y, D(Y)) \in \mathcal{U}(W_L)$ if and only if (77) holds for all $(X, D(X)) \in \mathcal{U}(W_R)$.

(f)

$$\mathcal{P}(W_R) \subset \mathcal{U}(W_R), \quad \mathcal{P}(W_L) \subset \mathcal{U}(W_L). \tag{78}$$

Proof: (1) The assertions (a) and (b) are trivial if we take into account the relations (59a) and (59b). The assertion (c) is completely trivial.

(2) We prove the assertions (d) by exhibiting explicit mappings of D_+ into $\mathcal{U}_b(W_R)$ and of D_- into $\mathcal{U}_b(W_L)$. For any $\xi \in D_+$, let the bounded operator $Z_+(\xi)$ be defined by

$$Z_+(\xi) = |\xi\rangle\langle\Omega| + |\Omega\rangle\langle JV(i\pi)\xi| - \langle\Omega \mid \xi\rangle |\Omega\rangle\langle\Omega|. \tag{79a}$$

If we note that $\langle\Omega \mid \xi\rangle = \langle JV(i\pi)\xi \mid \Omega\rangle$, we easily see that the mapping $\xi \to Z_+(\xi)$ is a linear mapping of D_+ into $\mathcal{U}_b(W_R)$ such that

$$Z_+(\xi)\Omega = \xi, \quad Z_+(\xi)^*\Omega = JV(i\pi)\xi. \tag{79b}$$

This proves the equalities at left in (76). The equalities at right in (76) are proved in a similar manner, through a consideration of the mapping $\eta \to Z_-(\eta)$, where $\eta \in D_-$ and

$$Z_-(\eta) = |\eta\rangle\langle\Omega| + |\Omega\rangle\langle JV(-i\pi)\eta| - \langle\Omega \mid \eta\rangle |\Omega\rangle\langle\Omega|. \tag{79c}$$

(3) We next consider the assertions (e) in the lemma. Let $(X, D(X)) \in \mathcal{U}(W_R)$ and $(Y, D(Y)) \in \mathcal{U}(W_L)$. It follows from the relations (73) that

$$\begin{aligned}\langle X^*\Omega \mid Y\Omega\rangle &= \langle JV(i\pi)X\Omega \mid Y\Omega\rangle = \langle V(-i\pi)JX\Omega \mid Y\Omega\rangle \\ &= \langle JX\Omega \mid V(-i\pi)Y\Omega\rangle = \langle JX\Omega \mid JY^*\Omega\rangle \\ &= \langle Y^*\Omega \mid X\Omega\rangle\end{aligned} \tag{80}$$

which proves the formula (77).

(4) Now let $(X, D(X))$ be a closable operator such that $\Omega \in D(X) \cap D(X^*)$. The condition that (77) hold for all

$(Y, D(Y)) \in \mathcal{U}(W_L)$ is, in view of part (d) of the lemma, equivalent to the condition that

$$\langle X^*\Omega \,|\, \eta\rangle = \langle JV(-i\pi)\eta \,|\, X\Omega\rangle \tag{81}$$

for every $\eta \in D_-$. It is easily seen that Eq. (81) is equivalent to the equation

$$\langle J\eta \,|\, JX^*\Omega\rangle = \langle V(i\pi)J\eta \,|\, X\Omega\rangle. \tag{82}$$

Since $JD_- = D_+$, and since $(V(i\pi), D_+)$ is self-adjoint, we conclude that if (81), and hence (82), holds for every $\eta \in D_-$, then $X\Omega \in D_+$, and (73a) holds, i. e., $(X, D(X))$ is in the set $\mathcal{U}(W_R)$.

In the same manner we prove the last assertion in part (e).

(5) The assertion (f) in the lemma is a paraphrase of the assertions (d) in Theorem 1. This completes the proof.

It should be noted that the sets $\mathcal{U}(W_R)$ and $\mathcal{U}(W_L)$ are *not* algebras, and in fact not even linear manifolds. The sets $\mathcal{U}_b(W_R)$ and $\mathcal{U}_b(W_L)$ of bounded operators are not algebras either, but linear manifolds which are easily seen to be weakly closed. That an operator X is included in one of the sets $\mathcal{U}(W_R)$ or $\mathcal{U}(W_L)$ is, in a sense, not a very restrictive condition: It is only a condition on the vectors $X\Omega$ and $X^*\Omega$. We found it convenient to introduce these sets since we will be dealing with operators which have properties such as those considered in the lemma.

We next consider some criteria for operators to be in these sets.

Lemma 13: (a) Let $(X, D(X))$ be closable, and such that $\Omega \in D(X) \cap D(X^*)$. Then $(X, D(X)) \in \mathcal{U}(W_R)$ if and only if there exists a set $\mathcal{C}_L \subset \mathcal{U}(W_L)$ such that $\mathrm{span}\{\mathcal{C}_L\Omega\}$ is a core for $(V(-i\pi), D_-)$, and such that the relation

$$\langle X^*\Omega \,|\, Y\Omega\rangle = \langle Y^*\Omega \,|\, X\Omega\rangle \tag{83}$$

holds for all $(Y, D(Y)) \in \mathcal{C}_L$.

(b) Let $(Y, D(Y))$ be closable, and such that $\Omega \in D(Y) \cap D(Y^*)$. Then $(Y, D(Y)) \in \mathcal{U}(W_L)$ if and only if there exists a set $\mathcal{C}_R \subset \mathcal{U}(W_R)$ such that span $\{\mathcal{C}_R\Omega\}$ is a core for $(V(i\pi), D_+)$, and such that the relation (83) holds for all $(X, D(X)) \in \mathcal{C}_R$.

(c) Let $(X, D(X))$ be closable, and such that $\Omega \in D(X) \cap D(X^*)$. Then $(X, D(X)) \in \mathcal{U}(W_R)$ if and only if there exists a set $\mathcal{Q}_L \subset \mathcal{U}(W_L)$ such that span $\{\mathcal{Q}_L\Omega\}$ is dense in the Hilbert space $\mathcal{H}$, and

$$V(t)\mathcal{Q}_L V(t)^{-1} = \mathcal{Q}_L, \quad \text{all real } t, \tag{84a}$$

and such that the relation (83) holds for all $(Y, D(Y)) \in \mathcal{Q}_L$.

In particular, $(X, D(X)) \in \mathcal{U}(W_R)$ if and only if (83) holds for every $(Y, D_1) \in \mathcal{P}_0(W_L)$.

(d) Let $(Y, D(Y))$ be closable, and such that $\Omega \in D(Y) \cap D(Y^*)$. Then $(Y, D(Y)) \in \mathcal{U}(W_L)$ if and only if there exists a set $\mathcal{Q}_R \subset \mathcal{U}(W_R)$ such that $\mathrm{span}\{\mathcal{Q}_R\Omega\}$ is dense in the Hilbert space $\mathcal{H}$, and

$$V(t)\mathcal{Q}_R V(t)^{-1} = \mathcal{Q}_R, \quad \text{all real } t, \tag{84b}$$

and such that the relation (83) holds for all $(X, D(X)) \in \mathcal{Q}_R$.

In particular, $(Y, D(Y)) \in \mathcal{U}(W_L)$ if and only if (83) holds for every $(X, D_1) \in \mathcal{P}_0(W_R)$.

Proof: (1) We consider the assertion (a). In view of the discussion in step (4) of the proof of the preceding lemma, we can restate the condition on X as follows: The relation (82) holds for all η in a core of $(V(-i\pi), D_-)$. Now, if D' is a core for $(V(-i\pi), D_-)$, then JD' is a core for $(V(i\pi), D_+)$, and we thus conclude, with reference to (82), that $X\Omega \in D_+$, and that (73a) holds. In an analogous manner we prove the assertion (b) in the lemma.

(2) The premises in part (c) of the lemma can be restated as follows: The relation

$$\langle JV(t)\eta \,|\, JX^*\Omega\rangle = \langle V(i\pi)JV(t)\eta \,|\, X\Omega\rangle \tag{85a}$$

holds for all real t, and all η in the dense set $D'' = \mathrm{span}\{\mathcal{Q}_L\Omega\}$. Let $c(s) \in \mathcal{D}(R^1)$. In view of (85a) and the relations (44a) and (44b) we then have

$$\begin{aligned}\langle Jc(K_3)\eta \,|\, JX^*\Omega\rangle &= \int_{-\infty}^{\infty} dt\hat{c}(t)\langle JV(t)\eta \,|\, JX^*\Omega\rangle \\ &= \int_{-\infty}^{\infty} dt\hat{c}(t)\langle V(i\pi)JV(t)\eta \,|\, X\Omega\rangle = \langle V(i\pi)Jc(K_3)\eta \,|\, X\Omega\rangle\end{aligned} \tag{85b}$$

for all $\eta \in D''$. In view of Lemma 7 the set $D_c'' = \mathrm{span}\{c(K_3)\eta \,|\, c(s) \in \mathcal{D}(R^1), \eta \in D''\}$ is a core for $(V(-i\pi), D_-)$, and the equality of the first and fourth members in (85b) then implies, and in step (1) above, that $(X, D(X)) \in \mathcal{U}(W_R)$.

In particular, these considerations hold for the case when $\mathcal{Q}_L = \mathcal{P}_0(W_L)$.

The assertions (d) are proved in an analogous manner.

We shall next consider the situation which arises when a subset of one of the sets $\mathcal{U}(W_R)$ or $\mathcal{U}(W_L)$ is an algebra. The following lemma is a preliminary for this study.

Lemma 14: Let $X_1, X_2 \in \mathcal{U}(W_R)$ be two *bounded* operators with the property that

$$X_1V(t)X_2^*V(t)^{-1} \in \mathcal{U}(W_R), \quad \text{all real } t. \tag{86}$$

Then

$$X_1(JX_2J)\Omega = (JX_2J)X_1\Omega. \tag{87}$$

Proof: (1) Let $Y \in \mathcal{U}_b(W_L)$. The condition (86) then implies that

$$\langle Y\Omega \,|\, X_1V(t)X_2^*\Omega\rangle = \langle V(t)X_2V(t)^{-1}X_1^*\Omega \,|\, Y^*\Omega\rangle \tag{88a}$$

for all real t. After a simple transformation of the right member, on the basis of the relations (73a) and (73b), we obtain from (88a) the relation

$$\langle Y\Omega \,|\, X_1V(t)X_2^*\Omega\rangle = \langle V(-t-i\pi)Y\Omega \,|\, JX_2JV(i\pi - t)X_1\Omega\rangle. \tag{88b}$$

(2) In view of the properties of the exponential function $V(\tau) = \exp(-i\tau K_3)$ discussed in Sec. III (immediately preceding Lemma 7), we note that the three vector-valued functions of τ given by

$$X_1V(\tau)X_2^*\Omega, \quad JX_2JV(i\pi - \tau)X_1\Omega, \tag{89a}$$

and

$$V(-\tau^* - i\pi)Y\Omega \tag{89b}$$

are all well defined and strongly continuous on the closed strip $0 \leq \mathrm{Im}(\tau) \leq \pi$ in the complex τ-plane. The functions in (89a) are strongly analytic functions of τ on the corresponding open strip, and the function in (89b) is a strongly analytic function of τ^* on the open strip $0 > \mathrm{Im}(\tau^*) > -\pi$. It follows that the function $f(\tau)$ defined by

$$f(\tau) = \langle Y\Omega \,|\, X_1 V(\tau) X_2^* \Omega\rangle - \langle V(-\tau^* - i\pi)Y\Omega \,|\, JX_2 JV(i\pi - \tau)X_1\Omega\rangle \tag{89c}$$

is continuous on the closed strip $0 \leq \mathrm{Im}(\tau) \leq \pi$ and an analytic function of τ on the open strip $0 < \mathrm{Im}(\tau) < \pi$. By (88b) we have $f(t) = 0$ for all real t, and it follows that $f(\tau) = 0$ throughout the closed strip. In particular, we have $f(i\pi) = 0$, which, in view of (89c) and the relation (73a), implies that

$$\langle Y\Omega \,|\, X_1 JX_2\Omega\rangle = \langle Y\Omega \,|\, JX_2 JX_1\Omega\rangle \tag{89d}$$

for all $Y \in \mathcal{U}_b(W_L)$. Since $\mathcal{U}_b(W_L)\Omega$ is dense in the Hilbert space $\mathcal{H}$ by Lemma 12 the relation (87) follows.

We shall now consider von Neumann algebras of bounded operators. If $\mathcal{B}$ is any set of bounded operators we denote the commutant of $\mathcal{B}$ by $\mathcal{B}'$, and we write $\mathcal{B}''$ for $(\mathcal{B}')'$.

Theorem 2: Let $\mathcal{A}_R \subset \mathcal{U}(W_R)$ be a von Neumann algebra such that $\mathcal{A}_R\Omega$ is dense in the Hilbert space $\mathcal{H}$, and such that

$$V(t)\mathcal{A}_R V(t)^{-1} = \mathcal{A}_R, \quad \text{all real } t. \tag{90}$$

Let the von Neumann algebra $\mathcal{A}_L$ be defined by $\mathcal{A}_L = J\mathcal{A}_R J$. Then:

(a)

$$\mathcal{A}_R' = J\mathcal{A}_R J = \mathcal{A}_L \subset \mathcal{U}(W_L),$$
$$\mathcal{A}_L' = J\mathcal{A}_L J = \mathcal{A}_R \subset \mathcal{U}(W_R). \tag{91}$$

(b) The vector Ω is cyclic and separating for $\mathcal{A}_R$ and $\mathcal{A}_L$.

(c) For any real t,

$$V(t)\mathcal{A}_L V(t)^{-1} = \mathcal{A}_L. \tag{92}$$

(d) The linear manifold $\mathcal{A}_R\Omega$ is a core for $(V(i\pi), D_+)$, and hence also for the antilinear operator $(JV(i\pi), D_+)$.

The linear manifold $\mathcal{A}_L\Omega$ is a core for $(V(-i\pi), D_-)$, and hence also for the antilinear operator $(JV(-i\pi), D_-)$.

The linear manifold $\{\mathcal{A}_R\Omega\} \cap \{\mathcal{A}_L\Omega\}$ is dense in the Hilbert space $\mathcal{H}$, and a core for the operators $(V(i\pi), D_+)$ and $(V(-i\pi), D_-)$.

(e) The von Neumann algebra $\mathcal{A}_R$ is "maximal" in the sense that if $\mathcal{A}$ is any von Neumann algebra with Ω as a *separating* vector, and such that $\mathcal{A}_R \subset \mathcal{A}$, and such that $V(t)\mathcal{A}V(t)^{-1} = \mathcal{A}$ for all real t, then $\mathcal{A} = \mathcal{A}_R$. The algebra $\mathcal{A}_R$ is "minimal" in the sense that if $\mathcal{A}$ is a von Neumann algebra with Ω as a *cyclic* vector, and such that $\mathcal{A} \subset \mathcal{A}_R$, and such that $V(t)\mathcal{A}V(t)^{-1} = \mathcal{A}$ for all real t, then $\mathcal{A} = \mathcal{A}_R$.

The algebra $\mathcal{A}_L$ is "maximal" and "minimal" in the same sense.

(f) The von Neumann algebra $\mathcal{A}_R$ is also "maximal within $\mathcal{U}(W_R)$" in the sense that if $\mathcal{A}$ is any von Neumann algebra such that $\mathcal{A}_R \subset \mathcal{A} \subset \mathcal{U}(W_R)$, then $\mathcal{A} = \mathcal{A}_R$.

The algebra $\mathcal{A}_L$ is "maximal within $\mathcal{U}(W_L)$" in the analogous sense.

Proof: (1) We note that the premises of Lemma 14 are satisfied by any two operators in $\mathcal{A}_R$. Let $X_1, X_2, X_3 \in \mathcal{A}_R$. In view of the lemma we have the following string of equalities:

$$JX_2JX_1X_3\Omega = X_1X_3JX_2\Omega = (X_1J)JX_3JX_2\Omega = X_1JX_2JX_3\Omega. \tag{93a}$$

Since, by the premises of the theorem, the set $\{X_3\Omega \,|\, X_3 \in \mathcal{A}_R\}$ is dense in $\mathcal{H}$, we conclude that $[(JX_2J), X_1] = 0$, for any two $X_1, X_2 \in \mathcal{A}_R$, and hence we have $J\mathcal{A}_R J \subset \mathcal{A}_R'$.

(2) The premises of part (d) of Lemma 13 are satisfied for any $Y \in \mathcal{A}_R'$ with $Q_R = \mathcal{A}_R$, and it follows that $\mathcal{A}_R' \subset \mathcal{U}(W_L)$. In view of the conclusion in step (1) above we thus have

$$\mathcal{A}_L = J\mathcal{A}_R J \subset \mathcal{A}_R' \subset \mathcal{U}(W_L). \tag{93b}$$

(3) Since $\mathcal{A}_R\Omega$ is dense, the set $J\mathcal{A}_R'J\Omega$ is also dense, in view of (93b). The condition (90) implies that $V(t)\mathcal{A}_R'V(t)^{-1} = \mathcal{A}_R'$, and hence that $V(t)(J\mathcal{A}_R'J)V(t)^{-1} = J\mathcal{A}_R'J$, for all real t. Since it follows from (93b) that $J\mathcal{A}_R'J \subset \mathcal{U}(W_R)$, we conclude, by the same reasoning as in step (1) above, that

$$\mathcal{A}_R' = J(J\mathcal{A}_R'J)J \subset (J\mathcal{A}_R'J)' = J\mathcal{A}_R''J = J\mathcal{A}_R J. \tag{93c}$$

The relations (91) then follow trivially from (93b) and (93c). From what has been said we also conclude that (92) holds.

(4) We prove the assertions (d) on the basis of (92) and (90). Let $c(s) \in \mathcal{D}(R^1)$, and let $X \in \mathcal{A}_R$. We define the operator X_c by

$$X_c = \int_{-\infty}^{\infty} dt \hat{c}(t) V(t) X V(t)^{-1} \tag{94a}$$

where $\hat{c}(t)$ is given in (44b). We obviously have $X_c \in \mathcal{A}_R$, and furthermore

$$X_c\Omega = c(K_3)X\Omega. \tag{94b}$$

We then conclude, in view of Lemma 7, that the linear manifold $D_A = \{X_c\Omega \,|\, X \in \mathcal{A}_R, c(s) \in \mathcal{D}(R^1)\}$ is a core for *every* operator $(V(z), D_V(\mathrm{Im}(z)))$.

For every $Y \in \mathcal{A}_L$, and any $c(s) \in \mathcal{D}(R^1)$, we define Y_c by the integral at right in (94a), with X replaced by Y. We then have $Y_c \in \mathcal{A}_L$, and

$$Y_c\Omega = c(K_3)Y\Omega = (V(i\pi)c(K_3))(JY^*J)\Omega \tag{94c}$$

where the second member is equal to the third in view of (73b). Since $JY^*J \in \mathcal{A}_R$, and since $\exp(s\pi)c(s) \in \mathcal{D}(R^1)$, we conclude that $D_A = \{Y_c\Omega \,|\, Y \in \mathcal{A}_L, c(s) \in \mathcal{D}(R^1)\}$. Since $\mathcal{A}_R\Omega \subset D_+$ and $\mathcal{A}_L\Omega \subset D_-$, the assertions (d) now follow trivially from the properties of the manifold D_A.

(5) The vector Ω is a cyclic vector for $\mathcal{A}_R$ by the premises, and also, trivially, a cyclic vector for $\mathcal{A}_L$. In view of (91) it follows that Ω is a separating vector for both $\mathcal{A}_R$ and $\mathcal{A}_L$.

(6) We next consider the assertion in part (e) of the theorem. If $\mathcal{A}$ is any von Neumann algebra with Ω as a separating vector, and such that $\mathcal{A}_R \subset \mathcal{A}$, and such that $V(t)\mathcal{A}V(t)^{-1} = \mathcal{A}$ for all real t, then $\mathcal{A}' \subset \mathcal{A}'_R \subset \mathcal{U}(W_L)$, and Ω is a cyclic vector for $\mathcal{A}'$, and hence for $J\mathcal{A}'J \subset \mathcal{U}(W_R)$. Furthermore, $V(t)(J\mathcal{A}'J)V(t)^{-1} = J\mathcal{A}'J$. The von Neumann algebra $J\mathcal{A}'J$ thus satisfies the premises of the present theorem, and it follows from the already established relations (91) that $J\mathcal{A}J = \mathcal{A}'$, and from this relation it readily follows that $\mathcal{A} = \mathcal{A}_R$, as asserted.

Suppose now that $\mathcal{A}$ is a von Neumann algebra with Ω as a *cyclic* vector, and such that $\mathcal{A} \subset \mathcal{A}_R$, and such that $V(t)\mathcal{A}V(t)^{-1} = \mathcal{A}$ for all real t. Then $\mathcal{A}$ satisfies the premises of the present theorem. In particular, $\mathcal{A}$ is "maximal," which implies that $\mathcal{A} = \mathcal{A}_R$.

In a similar fashion we show that $\mathcal{A}_L$ is "maximal" and "minimal."

(7) To prove the assertion (f) we consider the string of equalities (93a). Suppose that $X_1, X_3 \in \mathcal{A}_R$, and suppose that X_2 is an element of a von Neumann algebra $\mathcal{A}$ such that $\mathcal{A}_R \subset \mathcal{A} \subset \mathcal{U}(W_R)$. It is easily seen that the premises of Lemma 14 are satisfied by the pair of operators (X_1X_3) and X_2, and also by the pair of operators X_3 and X_2. It follows that the equalities in (93a) also hold in the present case, and we conclude, as in step (1) of the proof, that $JX_2J \in \mathcal{A}'_R$, i.e., $J\mathcal{A}J \subset \mathcal{A}'_R$. It follows that $\mathcal{A} \subset J\mathcal{A}'_RJ = \mathcal{A}_R$, and hence we have $\mathcal{A} = \mathcal{A}_R$, as asserted. This completes the proof of the theorem.

It should be noted that this theorem as such has little to do with the quantum field. It is of physical interest only if the algebra $\mathcal{A}_R$ is in some sense "generated" by field operators in $\mathcal{P}(W_R)$. We are not here asserting that such an algebra $\mathcal{A}_R$ actually exists. This issue will be discussed in the next section.

At this point we wish to discuss the relationship between our considerations and the Tomita–Takesaki theory of modular Hilbert algebras.[13,25] Within the framework of this theory one is able to draw some highly interesting conclusions about the structure of von Neumann algebras. The main theorem (from our point of view) is due to Tomita, and we shall state the facts in the following form.

Let $\mathcal{A}$ be a von Neumann algebra (of operators on a separable Hilbert space) which has a cyclic and separating vector Ω, and let $\mathcal{A}'$ denote its commutant. Then there exists a unique antiunitary involution J, and a unique self-adjoint operator (K, D_K), which satisfy the following conditions:

$$\text{(a)}\quad J\Omega = \Omega, \quad \Omega \in D_K, \quad K\Omega = 0; \tag{95a}$$

$$\text{(b)}\quad J\mathcal{A}J = \mathcal{A}'; \tag{95b}$$

$$\text{(c)}\quad JD_K = D_K, \quad J(K, D_K)J = (-K, D_K); \tag{95c}$$

$$\text{(d)}\quad \exp(-itK)\mathcal{A}\exp(itK) = \mathcal{A}, \quad \exp(-itK)\mathcal{A}'\exp(itK) = \mathcal{A}', \tag{95d}$$

for all real t, and the one-parameter group of unitary operators $\exp(-itK)$ is thus, acting by conjugation, a group of automorphisms of $\mathcal{A}$ and of $\mathcal{A}'$.

(e) If $(C, \mathcal{A}\Omega)$ is the antilinear operator defined by

$$CX\Omega = X^*\Omega, \quad \text{all } X \in \mathcal{A}, \tag{95e}$$

then

$$(J\exp(\pi K), D_+) = (C, \mathcal{A}\Omega)^{**} \tag{95f}$$

where D_+ is the linear manifold such that $(\exp(\pi K), D_+)$ is self-adjoint.

We note here that the operator $\exp(2\pi K)$ is traditionally denoted by Δ in papers on the subject: Our notation in terms of the operator K is specific for this paper, and motivated by our physical considerations.

The existing proofs of Tomita's theorem can hardly be regarded as trivial. Given the von Neumann algebra $\mathcal{A}$ and the cyclic and separating vector Ω, the operators J and Δ [and also the operator K by $2\pi K = \ln(\Delta)$] are in fact determined through (95f), which describes the polar decomposition of the closure of the antilinear operator $(C, \mathcal{A}\Omega)$. With this construction it is easily shown that the relations (95a) and (95c) hold, but the relations (95b) and (95d) are entirely nontrivial. In this paper we do not depend on Tomita's theorem, but we wanted to point out its relevance to our discussion. In particular our Theorem 2 is within the purview of the Tomita–Takesaki theory. In a sense this theorem contains nothing new, but we wanted to state the facts in this form for later reference, and also to prove these facts in an elementary way directly from the particular set of premises which arises naturally from our physical considerations. In our case the existence of J and K is not the issue since we are given the triplet (Ω, J, K_3) to start with. If we now compare the situation described in Theorem 2 with the situation described in Tomita's theorem we see that our operators J and $K = K_3$ are precisely the operators which in Tomita's theorem are determined by the algebra $\mathcal{A} = \mathcal{A}_R$.

Let us also note here that there are similarities between our discussion of Lemma 14 and Theorem 2, and the work of Haag, Hugenholtz, and Winnink,[26] and the work of Kastler, Pool, and Thue Poulsen.[27]

If we consider Theorem 1 we note some further analogies with the Tomita–Takesaki theory, although it should be noted that Theorem 1 concerns unbounded operators, rather than bounded operators as in Tomita's theorem. The definition (69a) is thus analogous to the definition (95e) above, and the relation (69c) is analogous to (95f). The relation (67) has a tenuous connection with (95b), but it should be noted that it is not proper to regard the algebra $\mathcal{P}(W_L)$ as the "commutant" of $\mathcal{P}(W_R)$: These algebras are rather analogous to some pair of algebras which generate the algebras $\mathcal{A}$ and $\mathcal{A}'$.

The connection between the duality condition in quantum field theory and Tomita's theorem has been discussed previously by Eckmann and Osterwalder, in their discussion of the duality condition for a *free* field.[7] We shall comment further on this in Sec. VII.

We conclude this section with an addendum to Theorem 2.

Lemma 15: Let $\mathcal{A}_R$ be a von Neumann algebra which satisfies the premises of Theorem 2. Then $\mathcal{A}_R$ and $\mathcal{A}_L = J\mathcal{A}_RJ = \mathcal{A}'_R$ are factors.

Proof: That the algebras $\mathcal{A}_R$ and $\mathcal{A}_L$ are *factors* means that their centers are equal to the set $\{cI\}$ of all complex multiples of the identity. In the case at hand this condition is equivalent to the statement $\mathcal{A}_R \cap \mathcal{A}_L = \{cI\}$.

Let $Z \in \mathcal{A}_R \cap \mathcal{A}_L$. Since Z is then an element of the set $U(W_R) \cap U(W_L)$, it follows from (73a) and (73b) that

$$V(i\pi)Z\Omega = JZ^*\Omega = V(-i\pi)Z\Omega. \tag{96a}$$

This implies that $V(i\pi)Z\Omega \in D_+$, and that

$$V(2\pi i)Z\Omega = \exp(2\pi K_3)Z\Omega = Z\Omega, \tag{96b}$$

which implies that $Z\Omega$ is an eigenvector of K_3, with eigenvalue 0. It is easily seen (and well known) that under our general assumptions about the nature of the representation of $\bar{L}_0$ carried by the Hilbert space $\mathcal{H}$, the only eigenvector of K_3 is the vacuum vector Ω. It follows from the above that $Z\Omega = c\Omega$, for some complex number c, and hence that $Z = cI$. This proves the lemma.

VI. THE DUALITY CONDITION FOR THE WEDGE REGIONS W_R AND W_L

In this section we shall consider conditions under which the operators in $\mathcal{P}(W_R)$ "generate" a von Neumann algebra $\mathcal{A}_R$ which satisfies the premises of Theorem 2. The basic idea is very simple. We try to construct $\mathcal{A}_R$ as the "commutant" of a suitable subset of operators in $\mathcal{P}(W_L)$. The execution of this idea is, however, beset with "technical" difficulties which derive from the fact that the operator in $\mathcal{P}(W_L)$ are in general unbounded. Furthermore, we are faced with the unfortunate situation that practically nothing is known about the nature of these operators as mathematical objects. It is, for instance, not known at present whether the field operators $\varphi[f]$, with f real, have any *local* self-adjoint extensions in a sense which will be discussed later. In our discussion we wish to avoid making assumptions which might later turn out to be too restrictive. For this reason we do not try to define the algebra $\mathcal{A}_R$ in terms of the commutant of *all* the operators in the set $\mathcal{P}(W_L)$, but instead in terms of the commutant of the field operators $\varphi[f]$, with $\mathrm{supp}(f) \subset W_L$.

We begin with some general considerations about the commutant of a subset of $\mathcal{P}(\mathcal{H})$.

Lemma 16: Let $\mathcal{J}$ be a subset of $\mathcal{P}(\mathcal{H})$, such that $(X^*, D_1) \in \mathcal{J}$ for all $(X, D_1) \in \mathcal{J}$. Let K_f be the set of all *bounded* operators Q such that

$$QD_1 \subset D(X^{**}), \quad [Q, X^{**}]\psi = 0 \tag{97a}$$

for all $\psi \in D_1$, and all $(X, D_1) \in \mathcal{J}$. Then:

(a)

$$QD(X^{**}) \subset D(X^{**}), \quad [Q, X^{**}]\psi = 0 \text{ for all } \psi \in D(X^{**}), \tag{97b}$$

$$Q^*D(X^*) \subset D(X^*), \quad [Q^*, X^*]\phi = 0 \text{ for all } \phi \in D(X^*), \tag{97c}$$

for all $(X, D_1) \in \mathcal{J}$.

(b) The set K_f is a weakly closed algebra. The set $\mathcal{A}_f = K_f \cap K_f^* = \{Q \mid Q, Q^* \in K_f\}$ is a von Neumann algebra. This algebra is precisely equal to the set of all bounded operators Q such that

$$(X, D_1)^{**}Q \supset Q(X, D_1)^{**}, \quad (X, D_1)^*Q \supset Q(X, D_1)^* \tag{98}$$

for all $(X, D_1) \in \mathcal{J}$.

(c) If G is any unitary operator such that $GD_1 = D_1$ and $G\mathcal{J}G^{-1} \subset \mathcal{J}$, then $G^{-1}\mathcal{A}_f G \subset \mathcal{A}_f$.

(d) Let $\mathcal{P}_f$ be the polynomial algebra (on D_1) generated by $\mathcal{J}$. Then

$$\langle X^*\phi \mid Q\psi\rangle = \langle Q^*\phi \mid X\psi\rangle \tag{99}$$

for any $X \in \mathcal{P}_f$, any $Q \in \mathcal{A}_f$, and any $\phi, \psi \in D_1$.

We omit the proofs since the above lemma is merely a summary of trivial and well-known facts. That $\mathcal{A}_f$ is a von Neumann algebra if all operators Q in this set satisfies (98) was shown by von Neumann,[28] and the conditions (98) correspond to his conditions that the *bounded* operators Q and Q^* commute with the closable operator (X, D_1). We note here that K_f need not be a von Neumann algebra, i. e., Q^* is not necessarily included in K_f for every $Q \in K_f$. This circumstance derives from the fact that the adjoints of the operators in $\mathcal{J}$ are not necessarily included in the set of all closures of the operators in $\mathcal{J}$. If it happens to be the case that $(X^\dagger, D_1)^* = (X, D_1)^{**}$ for all $(X, D_1) \in \mathcal{J}$, then $K_f = K_f^* = \mathcal{A}_f$.

We shall define the commutants of sets of field operators in terms of the conditions (98), and we are now prepared to state a somewhat lengthy theorem concerning the commutants of field operators associated with either one of the wedge regions W_R and W_L.

Theorem 3: Let $\mathcal{A}_c(W_R)$ be the von Neumann algebra of all bounded operators Q such that

$$\begin{aligned} &Q(\varphi[f], D_1)^{**} \subset (\varphi[f], D_1)^{**}Q, \\ &Q(\varphi[f], D_1)^{*} \subset (\varphi[f], D_1)^{*}Q \end{aligned} \tag{100}$$

for all $f \in \mathcal{S}(R^4)$ such that $\mathrm{supp}(f) \subset W_L$.

Similarly, let $\mathcal{A}_c(W_L)$ be the von Neumann algebra of all bounded operators Q such that (100) holds for all $f \in \mathcal{S}(R^4)$ such that $\mathrm{supp}(f) \subset W_R$.

Then:

(a)

$$\mathcal{A}_c(W_R) \subset \mathcal{A}_c(W_L)', \quad \mathcal{A}_c(W_L) \subset \mathcal{A}_c(W_R)'. \tag{101}$$

(b)

$$\mathcal{A}_c(W_R) = U(R(\mathbf{e}_1, \pi), 0)\mathcal{A}_c(W_L)U(R(\mathbf{e}_1, \pi), 0)^{-1} \tag{102a}$$

where $R(\mathbf{e}_1, \pi)$ denotes the rotation by angle π about the 1-axis.

Let $\sigma(W_R)$ be the semigroup of all elements in the Poincaré group $\bar{L}_0$ which map W_R *into* W_R. Similarly, let $\sigma(W_L) = \{\Lambda^{-1} \mid \Lambda \in \sigma(W_R)\}$ be the semigroup of all elements in the group $\bar{L}_0$ which map W_L *into* W_L. Then

$$U(\Lambda)\mathcal{A}_c(W_R)U(\Lambda)^{-1} \subset \mathcal{A}_c(W_R), \quad \text{all } \Lambda \in \sigma(W_R), \tag{102b}$$

and

$$U(\Lambda)\mathcal{A}_c(W_L)U(\Lambda)^{-1} \subset \mathcal{A}_c(W_L), \quad \text{all } \Lambda \in \sigma(W_L). \tag{102c}$$

The set $\bar{L}_0(W_R) = \sigma(W_R) \cap \sigma(W_L)$ is the group of all ele-

ments of $\bar{L}_0$ which map W_R *onto* W_R and W_L *onto* W_L, and we have

$$U(\Lambda)\mathcal{A}_c(W_R)U(\Lambda)^{-1}=\mathcal{A}_c(W_R),\quad U(\Lambda)\mathcal{A}_c(W_L)U(\Lambda)^{-1}=\mathcal{A}_c(W_L) \tag{102d}$$

for all $\Lambda\in\bar{L}_0(W_R)$. In particular,

$$V(t)\mathcal{A}_c(W_R)V(t)^{-1}=\mathcal{A}_c(W_R),\quad V(t)\mathcal{A}_c(W_L)V(t)^{-1}=\mathcal{A}_c(W_L) \tag{102e}$$

for all real t.

(c)

$$\mathcal{A}_c(W_R)=J\mathcal{A}_c(W_L)J. \tag{102f}$$

(d) The relations

$$\langle X^*\phi\,|\,Y\psi\rangle=\langle Y^*\phi\,|\,X\psi\rangle,\quad \text{all } \phi,\psi\in D_1, \tag{103}$$

hold for all $X\in\mathcal{A}_c(W_R)$ and all $Y\in\mathcal{P}(W_L)$.

The relations (103) also hold for all $X\in\mathcal{P}(W_R)$ and all $Y\in\mathcal{A}_c(W_L)$.

(e) With the notation in Lemma 12 we have $\mathcal{A}_c(W_R)\subset\mathcal{U}_b(W_R)$ and $\mathcal{A}_c(W_L)\subset\mathcal{U}_b(W_L)$, and hence $\mathcal{A}_c(W_R)\Omega\subset D_+$, $\mathcal{A}_c(W_L)\Omega\subset D_-$, and

$$V(i\pi)X\Omega=JX^*\Omega,\quad \text{all } X\in\mathcal{A}_c(W_R), \tag{104a}$$

$$V(-i\pi)Y\Omega=JY^*\Omega,\quad \text{all } Y\in\mathcal{A}_c(W_L). \tag{104b}$$

(f) If it is the case, *in addition*, that $\mathcal{A}_c(W_R)\Omega$ is dense in the Hilbert space $\mathcal{H}$, then the algebra $\mathcal{A}_R=\mathcal{A}_c(W_R)$ satisfies all the premises of Theorem 2 and Lemma 15, and, with reference to the notation in Theorem 2, $\mathcal{A}_L=\mathcal{A}_c(W_L)$. In particular, the algebras $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ are *factors*, and they satisfy the *duality condition*

$$\mathcal{A}_c(W_R)=\mathcal{A}_c(W_L)'. \tag{105}$$

Proof: (1) That $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ are indeed von Neumann algebras follows from Lemma 16. We temporarily postpone the proof of the relations (101) (of which either one implies the other). The assertions (b) and (c) of the theorem are all trivial. We consider the assertions in part (d). From Lemma 16 it follows that (103) holds for all $X\in\mathcal{A}_c(W_R)$ and all $Y\in\mathcal{P}_0(W_L)$. In view of Lemma 1 these relations also hold for all $Y\in\mathcal{P}(W_L)$ and all $X\in\mathcal{A}_c(W_R)$, as asserted. Analogous considerations apply to the second assertion (d).

(2) The assertions (e) now follow trivially from Lemma 13 and part (d) of the theorem [setting $\phi=\psi=\Omega$ in (103)].

(3) Having established part (e) we conclude from (102e) and (102f), on the basis of Lemma 14, that

$$[X,Y]\Omega=0 \tag{106a}$$

for all $X\in\mathcal{A}_c(W_R)$ and all $Y\in\mathcal{A}_c(W_L)$.

Let $x\in W_R$, and let $X(x)=T(x)XT(x)^{-1}$. We then have $\Lambda(\mathrm{I},x)\in\sigma(W_R)$, i.e., $\Lambda(\mathrm{I},x)W_R\subset W_R$, and hence $X(x)\in\mathcal{A}_c(W_R)$ whenever $X\in\mathcal{A}_c(W_R)$. For any such $X(x)$ the relation (106a) thus holds for any $Y\in\mathcal{A}_c(W_L)$, with $X(x)$ substituted for X.

Let $R=W_R\cap\Lambda(\mathrm{I},x)W_L$. This region is open and nonempty for any $x\in W_R$. It is easily seen that if $Q=[X(x),Y]$, with $X(x)$ and Y as above, then the conditions (100) hold for any $f\in\mathcal{S}(R^4)$ such that $\mathrm{supp}(f)\subset R$. By Lemma 16 we then conclude that

$$\langle Z_1\Omega\,|\,[X(x),Y]Z_2\Omega\rangle=\langle Z_2^*Z_1\Omega\,|\,[X(x),Y]\Omega\rangle=0 \tag{106b}$$

for any $Z_1,Z_2\in\mathcal{P}_0(R)$. Since $\mathcal{P}_0(R)\Omega$ is dense it follows that $[X(x),Y]=0$, for all $x\in W_R$. Since the point $x=0$ is on the boundary of W_R, and since $X(x)$ is a strongly continuous function of x [in view of the strong continuity of the function $T(x)$] we conclude that $[X,Y]=0$. This proves the assertions (a) of the Theorem.

(4) The assertions (f) follow trivially from Theorem 2 and Lemma 15. This completes the proof of the theorem.

We note that the assertions (b) in the theorem correspond to geometrical conditions which obviously have to be satisfied if we wish to regard $\mathcal{A}_c(W_R)$ as locally associated with W_R and $\mathcal{A}_c(W_L)$ as locally associated with W_L. In a theory in which a physical TCP-operator exists, as is the case here, the condition (102f) must also hold. The commutation relations implied by (101) correspond to a *minimal* condition of "physical independence" of the operators in $\mathcal{A}_c(W_R)$ from the operators in $\mathcal{A}_c(W_L)$. We note that the result (101) is analogous to a well-known theorem of Borchers concerning the local nature of a field which is local relative to a local irreducible field.[14] The relations (103) in part (d) are "commutation relations" between the bounded operators in the von Neumann algebras and the unbounded operators in $\mathcal{P}(\mathcal{H})$ in a sense which is weaker than the sense in which Q commutes with $\varphi[f]$ in (100). The assertions (d) can be restated as follows[29]:

$$X(Y^*,D_1)\subset(Y,D_1)^*X \tag{107a}$$

for all $X\in\mathcal{A}_c(W_R)$ and all $Y\in\mathcal{P}(W_L)$, and

$$Y(X^*,D_1)\subset(X,D_1)^*Y \tag{107b}$$

for all $Y\in\mathcal{A}_c(W_L)$ and all $X\in\mathcal{P}(W_R)$.

In the following we shall call a pair of von Neumann algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ a pair of *local wedge-algebras* if and only if they satisfy all the relations (101)—(103) which the algebras $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ satisfy. It follows that a pair of local wedge-algebras *also* satisfies the relations (104), by the same reasoning as in the proof of Theorem 3. Note that neither the duality condition (105), nor the commutation relations (100), are implied in the notion of a pair of local wedge-algebras.

With respect to the duality condition (105) the situation is as follows. The algebras $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ are uniquely determined by the field $\varphi(x)$, and it is then a matter of "checking" whether these algebras are sufficiently large in the sense that $\mathcal{A}_c(W_R)\Omega$ is dense in the Hilbert space $\mathcal{H}$. We do not know at this time whether $\mathcal{A}_c(W_R)\Omega$ is dense in general, i.e., with *no* additional assumptions about the field. It seems to us that in a physical theory described in terms of local observables and a local quantum field $\varphi(x)$ it must be the case that there exists a von Neumann algebra $\mathcal{A}(W_R)$, generated by the observables associated with the region W_R, and similarly an algebra $\mathcal{A}(W_L)$, and such that these algebras satisfy the conditions (a)—(d) in Theorem 3. In addition, we might require that the family of observables

associated with W_R is sufficiently large so that $\mathcal{A}(W_R)\Omega$ is dense in $\mathcal{H}$. As an example of the kind of considerations which are relevant here we refer to the work of Licht on "strict localization."[30] If the algebra $\mathcal{A}(W_R)$ satisfies the above conditions, then $\mathcal{A}(W_R) \subset \mathcal{U}(W_R)$ and the relation (104a) holds because $\mathcal{A}(W_R)$ is a local wedge-algebra, and since $\mathcal{A}(W_R)\Omega$ is dense, it follows that the duality condition $\mathcal{A}(W_R)' = \mathcal{A}(W_L)$ holds.

If it is the case that $\mathcal{A}_c(W_R)\Omega$ is dense we would define the "algebra of observables" $\mathcal{A}(W_R)$ by $\mathcal{A}(W_R) = \mathcal{A}_c(W_R)$, with reference to the construction in Theorem 3. If $\mathcal{A}_c(W_R)\Omega$ is *not* dense, the algebra $\mathcal{A}(W_R)$, if it exists, would have to be defined differently. *One* possibility is the following. It might be the case that $\mathcal{A}(W_R)$ could be defined in a satisfactory manner as the commutant of some other subset of $\mathcal{P}(W_L)$ which is "better behaved" than the set of operators $\varphi[f]$ in $\mathcal{P}(W_L)$. Since we feel that we have no basis for a rational choice we shall not discuss this possibility. Another possibility is that there might exist, within the framework of the particular theory, natural extensions of the field operators $\varphi[f]$. We could then try to define $\mathcal{A}(W_R)$ as the commutant of the extensions of the operators $\varphi[f]$ in $\mathcal{P}(W_L)$, if it so happens that $\mathcal{A}(W_R)\Omega$ is dense for this choice. We shall consider a particular case of this situation below. The general problem of how to define algebras of bounded operators in terms of the unbounded field operators has been discussed by many authors, and what we say below is not particularly novel.[1,16,29-31]

We shall now consider four particular conditions on the quantum field which seem to us to be interesting to contemplate. Each one of these conditions guarantees the existence of local von Neumann algebras which satisfy the duality condition (105) (for the wedge regions W_R and W_L).

Condition I: The linear manifold $\mathcal{A}_c(W_R)\Omega$ is dense in the Hilbert space $\mathcal{H}$, where $\mathcal{A}_c(W_R)$ is the von Neumann algebra constructed from the field as in Theorem 3.

Condition II: For any open nonempty subset R of Minkowski space the linear manifold $\mathcal{C}(R)\Omega$ is dense in the Hilbert space $\mathcal{H}$, where $\mathcal{C}(R)$ is the von Neumann algebra of all bounded operators Q such that

$$\begin{aligned} &Q(\varphi[f], D_1)^{**} \subset (\varphi[f], D_1)^{**}Q, \\ &Q(\varphi[f], D_1)^{*} \subset (\varphi[f], D_1)^{*}Q \end{aligned} \tag{108}$$

for all $f \in \mathcal{S}(R^4)$ such that $\mathrm{supp}(f) \subset (\bar{R})^c$, where $(\bar{R})^c$ denotes the causal complement of the closure of R.

Condition III: The quantum field $\varphi(x)$ has a *local self-adjoint extention* in the following sense. To each $f \in \mathcal{S}(R^4)$ corresponds a *closed* operator $(\overline{\varphi}[f], D(f))$ such that:

(a)

$$(\overline{\varphi}[f], D(f))^* = (\overline{\varphi}[f^*], D(f^*)), \tag{109a}$$

$$(\overline{\varphi}[f], D(f)) \supset (\varphi[f], D_1) \tag{109b}$$

for all $f \in \mathcal{S}(R^4)$. The operator $(\overline{\varphi}[f], D(f))$ is thus self-adjoint if f is real.

(b) If $r(x) \in \mathcal{S}(R^4)$ is *real*, and if $f(x) \in \mathcal{S}(R^4)$ such that $\mathrm{supp}(r) \subset (\mathrm{supp}(f))^c$, then

$$F(\overline{\varphi}[f], D(f)) \subset (\overline{\varphi}[f], D(f))F \tag{110}$$

for any spectral projection F of the self-adjoint operator $(\overline{\varphi}[r], D(r))$.

(c) For any $f \in \mathcal{S}(R^4)$, $\Lambda \in \overline{L}_0$,

$$U(\Lambda)(\overline{\varphi}[f], D(f))U(\Lambda)^{-1} = (\overline{\varphi}[\Lambda f], D(\Lambda f)). \tag{111}$$

Condition IV: Condition III holds, with

$$(\overline{\varphi}[f], D(f)) = (\varphi[f], D_1)^{**} \tag{112}$$

for all $f \in \mathcal{S}(R^4)$.

The Condition II trivially implies the Condition I, and we have $\mathcal{C}(W_R) = \mathcal{A}_c(W_R)$, $\mathcal{C}(W_L) = \mathcal{A}_c(W_L)$. Both conditions thus imply the duality condition (105) for the wedge regions. We shall consider further implications of Condition II in the next section.

Condition III is (as far as we know) much stronger than the condition that every operator $(\varphi[f], D_1)$, with $f \in \mathcal{S}(R^4)$ and f real, has a self-adjoint extension. The conditions (110) and (111) can be interpreted as the conditions that the extension of the field is also a local scalar field. Condition IV is the most restrictive of the conditions. It, in effect, states that the quantum field $\varphi(x)$ has a *unique* local, covariant, self-adjoint extension, given by (112).

Theorem 4: Condition III is assumed. Let $\mathcal{A}(W_R)$ be the set of all bounded operators Q such that

$$Q(\overline{\varphi}[f], D(f)) \subset (\overline{\varphi}[f], D(f))Q \tag{113}$$

for all $f \in \mathcal{S}(R^4)$ such that $\mathrm{supp}(f) \subset W_L$. Let $\mathcal{A}(W_L)$ be the set of all bounded operators Q such that (113) holds for all $f \in \mathcal{S}(R^4)$ such that $\mathrm{supp}(f) \subset W_R$. Then:

(a) $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ are von Neumann algebras with the vacuum vector Ω as a cyclic and separating vector. Both algebras are factors, and they satisfy the duality condition

$$\mathcal{A}(W_R)' = \mathcal{A}(W_L). \tag{114}$$

(b) If $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ are defined as in Theorem 3, then

$$\mathcal{A}_c(W_R) \subset \mathcal{A}(W_R), \quad \mathcal{A}_c(W_L) \subset \mathcal{A}(W_L), \tag{115}$$

and equality obtains if and only if $\mathcal{A}_c(W_R)\Omega$ is dense in $\mathcal{H}$.

(c) The algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ form a pair of local wedge-algebras, i.e., they satisfy all the conditions (a)—(e) in Theorem 3 which the algebras $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ satisfy.

(d) Let $\mathcal{G}(W_R)$ be the set of all spectral projections of all operators $(\overline{\varphi}[f], D(f))$, with f real, $f \in \mathcal{S}(R^4)$, and $\mathrm{supp}(f) \subset W_R$. Similarly, let $\mathcal{G}(W_L)$ be the set of all spectral projections of all operators $(\overline{\varphi}[f], D(f))$, with f real, $f \in \mathcal{S}(R^4)$, and $\mathrm{supp}(f) \subset W_L$. Then

$$\mathcal{A}(W_R) = \mathcal{G}(W_R)'', \quad \mathcal{A}(W_L) = \mathcal{G}(W_L)''. \tag{116}$$

Proof: (1) We first note that in view of (109a) the set $\mathcal{A}(W_R)$, as defined in terms of (113), is the commutant of a set of operators which is closed under the formation of the adjoint. Hence $\mathcal{A}(W_R)$, and similarly $\mathcal{A}(W_L)$, are von Neumann algebras.

From the relation (111), which describes the action of the Poincaré group (by conjugation) on the extended field, it trivially follows that the algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ satisfy all the relations (102a)–(102e) in Theorem 3, and, in particular,

$$V(t)\mathcal{A}(W_R)V(t)^{-1}=\mathcal{A}(W_R),\quad V(t)\mathcal{A}(W_L)V(t)^{-1}=\mathcal{A}(W_L) \tag{117}$$

for all real t. Note, however, that the relation (102f) in part (c) of Theorem 3 *does not* follow trivially from (111).

(2) Let $\psi, \phi \in D_1$, and let $f \in \mathcal{S}(R^4)$, $\mathrm{supp}(f) \subset W_L$. For any $X \in \mathcal{A}(W_R)$ we have

$$\begin{aligned}\langle\psi|X\varphi[f]\phi\rangle &= \langle\psi|\bar{\varphi}[f]X\phi\rangle = \langle\psi|\bar{\varphi}[f^*]^*X\phi\rangle \\ &= \langle\bar{\varphi}[f^*]\psi|X\phi\rangle = \langle\varphi[f^*]\psi|X\phi\rangle.\end{aligned} \tag{118a}$$

From the equality of the first and last members of (118a) it readily follows that the relations

$$\langle X^*\psi|Y\phi\rangle = \langle Y^*\psi|X\phi\rangle,\quad \text{all } \phi,\psi \in D_1, \tag{118b}$$

hold for all $X \in \mathcal{A}(W_R)$ and all $Y \in \mathcal{P}(W_L)$. In a similar manner, we conclude that (118b) also hold for all $X \in \mathcal{P}(W_R)$ and all $Y \in \mathcal{A}(W_L)$. As in the proof of Theorem 3 we conclude that

$$\mathcal{A}(W_R) \subset \mathcal{U}_b(W_R),\quad \mathcal{A}(W_L) \subset \mathcal{U}_b(W_L). \tag{118c}$$

(3) Trivially we have $\mathcal{G}(W_R)'' \subset \mathcal{A}(W_R)$ and $\mathcal{G}(W_L)'' \subset \mathcal{A}(W_L)$. We shall show that Ω is a cyclic vector of the von Neumann algebra $\mathcal{G}(W_R)''$.

Let $\{R_n | n = 1, \ldots, \infty\}$ be a set of subsets of W_R, constructed as in Lemma 10. Let $\{f_k | k = 1, \ldots, n\}$ be an n-tuplet of *real* test functions such that $f_k \in \mathcal{S}(R^4)$ and $\mathrm{supp}(f_k) \subset R_k$, for $k = 1, \ldots, n$. In view of the nature of the regions R_k it follows that the self-adjoint operators $(\bar{\varphi}[f_k], D(f_k))$, $k = 1, \ldots, n$, all commute with each other, in the sense that their spectral projections commute. Let $F_k(\lambda)$ be the spectral projection of $(\bar{\varphi}[f_k], D(f_k))$ corresponding to the interval $(-\lambda, \lambda)$, where $\lambda > 0$, and let the bounded operator $Q_k(\lambda)$ be given by $Q_k(\lambda) = \bar{\varphi}[f_k]F_k(\lambda)$, for each $k = 1, \ldots, n$. We then have

$$\begin{aligned}&F_1(\lambda)F_2(\lambda)\cdots F_n(\lambda)\varphi[f_1]\varphi[f_2]\cdots\varphi[f_n]\Omega \\ &\quad = Q_1(\lambda)Q_2(\lambda)\cdots Q_n(\lambda)\Omega\end{aligned} \tag{119a}$$

and hence

$$\text{s-}\lim_{\lambda\to+\infty} Q_1(\lambda)Q_2(\lambda)\cdots Q_n(\lambda)\Omega = \varphi[f_1]\varphi[f_2]\cdots\varphi[f_n]\Omega. \tag{119b}$$

The operators $Q_k(\lambda)$ are all included in $\mathcal{G}(W_R)''$, and since (119b) holds for any $n > 0$, and any choice of real test functions, we conclude that $\overline{\mathcal{G}(W_R)''\Omega} = \overline{Q\Omega}$, where Q is defined as in Lemma 11. By Lemma 11 it then follows that $\mathcal{G}(W_R)''\Omega$ is dense in $\mathcal{H}$, and hence $\mathcal{A}(W_R)\Omega$ is also dense.

(4) It is trivially the case that $V(t)\mathcal{G}(W_R)''V(t)^{-1} = \mathcal{G}(W_R)''$ for all real t. We now note that both $\mathcal{A}(W_R)$ and $\mathcal{G}(W_R)''$ satisfy the premises of Theorem 2, with $\mathcal{A}_R = \mathcal{A}(W_R)$, or with $\mathcal{A}_R = \mathcal{G}(W_R)''$. It follows from this theorem, in view of $\mathcal{G}(W_R)'' \subset \mathcal{A}(W_R)$, that

$$\mathcal{G}(W_R)'' = \mathcal{A}(W_R) = J\mathcal{A}(W_R)'J = J\mathcal{G}(W_R)'J. \tag{120a}$$

Similar considerations apply to $\mathcal{A}(W_L)$ and $\mathcal{G}(W_L)$, and we thus establish the relations (116).

We trivially have $\mathcal{G}(W_R) \subset \mathcal{G}(W_L)'$, and hence $\mathcal{G}(W_R)'' \subset \mathcal{G}(W_L)'$. Similarly, $\mathcal{G}(W_L)'' \subset \mathcal{G}(W_R)'$, and it follows, in view of (120a), that $\mathcal{G}(W_R)'' = J\mathcal{G}(W_R)'J = \mathcal{G}(W_L)'$, i. e.,

$$\mathcal{A}(W_R) = J\mathcal{A}(W_L)J, \tag{120b}$$

which shows that J acts as asserted (and as expected) on the algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$, which have now been shown to form a pair of local wedge-algebras. The duality condition (114) follows trivially from (120a) and (120b).

(5) It remains to prove the relations (115). Let $X \in \mathcal{A}(W_R)$, $X_c \in \mathcal{A}_c(W_R)$, and let $f \in \mathcal{S}(R^4)$, $\mathrm{supp}(f) \subset W_L$. For any vectors $\phi, \psi \in D_1$ we have

$$\begin{aligned}\langle\psi|XX_c\varphi[f]\phi\rangle &= \langle\psi|X\varphi[f]^{**}X_c\phi\rangle = \langle\psi|X\bar{\varphi}[f]X_c\phi\rangle \\ &= \langle\psi|\bar{\varphi}[f]XX_c\phi\rangle = \langle\psi|\bar{\varphi}[f^*]^*XX_c\phi\rangle \\ &= \langle\bar{\varphi}[f^*]\psi|XX_c\phi\rangle = \langle\varphi[f^*]\psi|XX_c\phi\rangle.\end{aligned} \tag{121a}$$

From the equality of the first and the last members of (121a) it readily follows that

$$\langle Y^*\Omega|XX_c\Omega\rangle = \langle\Omega|XX_cY\Omega\rangle \tag{121b}$$

for any $Y \in \mathcal{P}_0(W_L)$. By Lemma 13 we conclude that $XX_c \in \mathcal{U}(W_R)$.

Since X and X_c are arbitrary elements of $\mathcal{A}(W_R)$ and $\mathcal{A}_c(W_R)$, and since $V(t)\mathcal{A}_c(W_R)V(t)^{-1} = \mathcal{A}_c(W_R)$, we conclude that $XV(t)X_c^*V(t)^{-1} \in \mathcal{U}(W_R)$. The operators X and X_c then satisfy the premises of Lemma 14, and it follows that

$$X(JX_cJ)\Omega = (JX_cJ)X\Omega. \tag{121c}$$

for any $X \in \mathcal{A}(W_R)$ and any $X_c \in \mathcal{A}_c(W_R)$. Since $\mathcal{A}(W_R)\Omega$ is dense in the Hilbert space it follows, by the same kind of reasoning as in step (1) of the proof of Theorem 2, that $[(JX_cJ), X] = 0$, which means that $J\mathcal{A}_c(W_R)J \subset \mathcal{A}(W_R)'$. In view of (120a) this implies the first relation (115). The second relation is obtained by conjugating the first by J.

This completes the proof of the theorem. We add a corollary which describes the situation under Condition IV. It is almost completely trivial in content.

Corollary to Theorem 4: Condition IV is assumed, and hence Condition III obtains. The quantum field has one and only one local self-adjoint extension $\bar{\varphi}(x)$, namely, $(\bar{\varphi}[f], D(f)) = (\varphi[f], D_1)^{**}$ for all $f \in \mathcal{S}(R^4)$. The domains D_0 and D_1 are cores for all operators $(\varphi[f], D_1)^*$, and

$$(\varphi[f], D_1)^* = (\varphi[f^*], D_1)^{**} = (\bar{\varphi}[f^*), D(f^*)). \tag{122}$$

With the notation in Theorems 3 and 4,

$$\mathcal{A}_c(W_R) = \mathcal{A}(W_R),\quad \mathcal{A}_c(W_L) = \mathcal{A}(W_L), \tag{123}$$

and all the conclusions in these theorems hold for the above algebras.

If we are allowed to speculate about the results in this section, we wish to say that we are inclined to believe that in a satisfactory local theory there ought to exist at least one field which satisfies Condition III, although this does not seem to be necessary for the duality condition to hold. It is well known that the general conditions on the field which we stated in Sec. II have to be amended with some conditions which guarantee that the

theory really describes physical particles. In particular, some kind of "dynamical principle" is sorely needed. It might, of course, be the case that Condition III is already implied by the minimal assumptions in Sec. II, but if this is not so we would like to believe that the condition at least holds in a properly amended theory. We can imagine a situation in which the local self-adjoint extension of the field is unique, without D_1 being a core for the extensions of the individual field operators $\varphi[f]$. Condition IV might thus be unduly restrictive. An even more restrictive condition, according to which Ω is an analytic vector for all Hermitian field operators $\varphi[f]$, has been discussed by Borchers and Zimmermann.[31] Such a condition cannot hold generally since it is violated by Wick polynomials of free fields, but it is conceivable that it could hold for one particular field in a particular theory. (It is well known that it does hold for a free field.)

Let us finally remark that most of our considerations up to this point also apply to a field theory in two-dimensional spacetime, in view of the special geometric properties of the wedge regions W_R and W_L.

VII. THE DUALITY CONDITION FOR A FAMILY OF BOUNDED REGIONS; LOCAL INTERNAL SYMMETRIES

The discussion in this section will be based on the assumption that there exists a pair of local wedge-algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$, which satisfy the duality condition $\mathcal{A}(W_R)' = \mathcal{A}(W_L)$.

These algebras thus in particular satisfy all the conditions (a)—(e) in Theorem 3, which the algebras $\mathcal{A}_c(W_R)$ and $\mathcal{A}_c(W_L)$ satisfy.

The operators in the von Neumann algebra $\mathcal{A}(W_R)$ can be regarded as "locally associated" with the region W_R. The existence of the wedge-algebras does not, however, guarantee (as far as we can see) that there exist non-trivial von Neumann algebras which can reasonably be regarded as associated with *bounded* regions in spacetime. In a satisfactory theory of local observables we would certainly require that there exists a sufficiently large set of bounded (self-adjoint) operators which correspond to measurements within some bounded regions in spacetime. Condition I on the field, discussed in the preceding section, would thus by itself appear too weak for a satisfactory theory, although it does guarantee the existence of the local wedge-algebras. As we shall see, either one of our Conditions II—IV does imply the existence of a set of truly "local" operators with reasonable properties. We note here that our particular conditions, although not physically unreasonable, are nevertheless quite arbitrary. We are not here asserting that anyone of these conditions *has* to hold, nor are we asserting that they guarantee that the theory has a physical interpretation which is satisfactory in *every* respect.

Let us now consider the definition of von Neumann algebras for other regions than the wedges W_R and W_L.

For any subset R of Minkowski space $\mathcal{M}$ we denote by ΛR the image of R under any element Λ of the Poincaré group $\bar{L}_0$. We define $\mathcal{W}$ as the set of all (open) wedge regions bounded by two intersecting characteristic planes, i.e.,

$$\mathcal{W} = \{\Lambda W_R \mid \Lambda \in \bar{L}_0\}. \tag{124a}$$

For every $W \in \mathcal{W}$ we define the von Neumann algebra $\mathcal{A}(W)$ by

$$\mathcal{A}(\Lambda W_R) = U(\Lambda)\mathcal{A}(W_R)U(\Lambda)^{-1}, \quad \text{all } \Lambda \in \bar{L}_0. \tag{124b}$$

We note that this definition is consistent since we assumed that $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ satisfy the relations (102a)—(102e) in Theorem 3.

It is natural to define von Neumann algebras for a suitable family of bounded regions in terms of intersections of the von Neumann algebras $\mathcal{A}(W)$. Since we hope to discuss these issues elsewhere in greater detail, and within a more general framework, we shall here restrict our considerations to a set of particularly simple bounded regions, namely, the so-called double cones. For any two points x_1 and x_2 in Minkowski space such that $x_2 \in V_+(x_1)$ [where $V_+(x_1)$ is the forward light cone with x_1 as apex], we define the double cone $C = C(x_1, x_2)$ by

$$C(x_1, x_2) = V_+(x_1) \cap V_-(x_2), \tag{125a}$$

where $V_-(x_2)$ is the backward light cone with x_2 as apex. The double cones so defined are thus open and non-empty. We denote by $\mathcal{D}_c$ the set of all double cones.

For any double cone C we define a von Neumann algebra $\mathcal{B}(\bar{C})$ by

$$\mathcal{B}(\bar{C}) = \cap \{\mathcal{A}(W) \mid W \in \mathcal{W}, W \supset \bar{C}\}. \tag{125b}$$

Here $\bar{C}$ denotes the closure of C. We prefer to regard $\mathcal{B}(\bar{C})$ as associated with the closed set $\bar{C}$, and hence the above notation.

We shall next extend the domain of the mapping $W \to \mathcal{A}(W)$ to include all *open* regions $\bar{C}^c$ which are the causal complements of closed double cones $\bar{C}$. For any $C \in \mathcal{D}_c$ we define the von Neumann algebra $\mathcal{A}(\bar{C}^c)$ by

$$\mathcal{A}(\bar{C}^c) = \{\mathcal{A}(W) \mid W \in \mathcal{W}, W \subset \bar{C}^c\}''. \tag{126}$$

We shall now state two theorems about the properties of the algebras which we have introduced above. The conclusions in the first of these do not depend on the duality condition, but follow fairly trivially from the relative locality of the wedge-algebras, and from the "geometrical" conditions in parts (b) and (c) of Theorem 3.

Theorem 5: Let $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ be a pair of von Neumann algebras such that

$$\mathcal{A}(W_R) \subset \mathcal{A}(W_L)' \tag{127}$$

and

$$\mathcal{A}(W_R) = J\mathcal{A}(W_L)J, \tag{128a}$$

$$\mathcal{A}(W_R) = U(R(\mathbf{e}_1, \pi), 0)\mathcal{A}(W_L)U(R(\mathbf{e}_1, \pi), 0)^{-1}, \tag{128b}$$

$$U(\Lambda)\mathcal{A}(W_R)U(\Lambda)^{-1} \subset \mathcal{A}(W_R), \quad \text{all } \Lambda \in \sigma(W_R), \tag{128c}$$

where $\sigma(W_R)$ is the semigroup of all Poincaré transformations which map W_R *into* W_R.

Let $\mathcal{A}(W)$ be defined by (124b), for any $W \in \mathcal{W}$. Let $\mathcal{B}(\bar{C})$ be defined by (125b), and let $\mathcal{A}(\bar{C}^c)$ be defined by

(126), for any double cone C. Then:

(a)

$$\mathcal{A}(\Lambda W) = U(\Lambda)\mathcal{A}(W)U(\Lambda)^{-1} \tag{129a}$$

for all $W \in \mathcal{W}$, all $\Lambda \in \bar{L}_0$;

$$\mathcal{B}(\Lambda \bar{C}) = U(\Lambda)\mathcal{B}(\bar{C})U(\Lambda)^{-1}, \tag{129b}$$

$$\mathcal{A}(\Lambda \bar{C}^c) = U(\Lambda)\mathcal{A}(\bar{C}^c)U(\Lambda)^{-1}, \tag{129c}$$

for all $C \in \mathcal{O}_c$, all $\Lambda \in \bar{L}_0$.

(b)

$$\mathcal{A}(\mathcal{J} W) = J\mathcal{A}(W)J, \tag{130a}$$

$$\mathcal{B}(\mathcal{J} \bar{C}) = J\mathcal{B}(\bar{C})J, \quad \mathcal{A}(\mathcal{J} \bar{C}^c) = J\mathcal{A}(\bar{C}^c)J \tag{130b}$$

for all $W \in \mathcal{W}$, $C \in \mathcal{O}_c$, and where $\mathcal{J}$ is given by (47).

(c)

$$\mathcal{A}(W) \supset \mathcal{A}(W_i), \quad \text{if } W, W_i \in \mathcal{W}, \ W \supset W_i, \tag{131a}$$

$$\mathcal{B}(\bar{C}) \supset \mathcal{B}(\bar{C}_i), \quad \mathcal{A}(\bar{C}^c) \subset \mathcal{A}(\bar{C}_i^c) \tag{131b}$$

for all $C, C_i \in \mathcal{O}_c$ such that $C \supset C_i$ (and hence $\bar{C}^c \subset \bar{C}_i^c$), and

$$\mathcal{B}(\bar{C}_1) \subset \mathcal{A}(W) \subset \mathcal{A}(\bar{C}_2^c) \tag{131c}$$

for all $W \in \mathcal{W}$, $C_1, C_2 \in \mathcal{O}_c$, such that $C_1 \subset W \subset \bar{C}_2^c$.

(d) The algebras $\mathcal{B}(\bar{C})$ are *local*, in the sense that

$$\mathcal{B}(\bar{C}_1) \subset \mathcal{B}(\bar{C}_2)' \tag{132a}$$

for any $C_1, C_2 \in \mathcal{O}_c$, such that $C_1 \subset \bar{C}_2^c$. Furthermore,

$$\mathcal{B}(\bar{C})' \supset \mathcal{A}(\bar{C}^c) \tag{132b}$$

for any $C \in \mathcal{O}_c$.

(e) The mapping $W \to \mathcal{A}(W)$ is *continuous from the outside* in the sense that

$$\mathcal{A}(W) = \cap \{\mathcal{A}(W_0) \,|\, W_0 \in \mathcal{W}, \ W_0 \supset \bar{W}\} \tag{133a}$$

and it is *continuous from the inside* in the sense that

$$\mathcal{A}(W) = \{\mathcal{A}(W_i) \,|\, W_i \in \mathcal{W}, \ \bar{W}_i \subset W\}''. \tag{133b}$$

The mapping $\bar{C} \to \mathcal{B}(\bar{C})$ is continuous from the outside in the sense that

$$\mathcal{B}(\bar{C}) = \cap \{\mathcal{B}(\bar{C}_0) \,|\, C_0 \in \mathcal{O}_c, \ \bar{C} \subset C_0\}. \tag{133c}$$

The mapping $\bar{C}^c \to \mathcal{A}(\bar{C}^c)$ is continuous from the inside in the sense that

$$\mathcal{A}(\bar{C}^c) = \{\mathcal{A}(\bar{C}_i^c) \,|\, C_i \in \mathcal{O}_c, \ C_i \supset \bar{C}\}''. \tag{133d}$$

Proof: (1) The assertions (a) and (b) are trivial. The relation (131a) follows trivially from (128c) and the definition (124b). The relations (131b) follow directly from the definitions (125b) and (126).

(2) We next consider the assertions in part (e) of the theorem. To prove (133a) it clearly suffices to prove this relation for the special case of $W = W_R$. For this case, let $\mathcal{A}$ denote the von Neumann algebra defined by the right member in (133a). We obviously have $\mathcal{A}(W_R) \subset \mathcal{A}$. Let $x \in W_R$. We then have $T(x)\mathcal{A}T(x)^{-1} \subset \mathcal{A}(W_R)$. Since the function $T(x)$ is strongly continuous, and since the point $x = 0$ is included in $\bar{W}_R$, we conclude that $\mathcal{A} = \mathcal{A}(W_R)$. Hence (133a) holds.

The relation (133b) follows readily from (133a). The relation (133c) follows from the definition (125b), and the relation (133d) follows from (133b) and the definition (126).

(3) The relation (131c) in part (b) of the theorem now follows trivially, in view of (133a).

(4) It remains to prove the assertions (d). Let C be a double cone, and let $W = \Lambda W_R$ be any wedge such that $W \subset \bar{C}^c$. Then $C \subset \Lambda W_L$, and it follows from (127) and (131c) that $\mathcal{B}(\bar{C})' \supset \mathcal{A}(\Lambda W_L)' \supset \mathcal{A}(W)$. In view of the definition (126) this implies the relation (132b). The relation (132a) then follows trivially from (132b) and (131c). This completes the proof of the theorem.

We note that the relations (131a) and (131b) are in fact implied by the relations (133b)—(133d), and our presentation is thus somewhat tautological. In view of the relation (133a), which says that the wedge-algebras are "continuous from the outside," we might well write $\mathcal{B}(\bar{W}) = \mathcal{A}(W)$ for any wedge W, corresponding to the idea that a wedge W is a limiting case of a double cone. We note here that the algebra $\mathcal{A}(\bar{C}^c)$ need *not* be continuous from the outside, and that the algebra $\mathcal{B}(\bar{C})$ need not be continuous from the inside, for any double cone C.

Theorem 6: Let $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ be a pair of von Neumann algebras which satisfy all the premises of Theorem 5. It is assumed that these algebras satisfy the duality condition

$$\mathcal{A}(W_L) = \mathcal{A}(W_R)'. \tag{134}$$

Furthermore, it is assumed that Ω is a cyclic and separating vector for $\mathcal{A}(W_R)$, and that $\mathcal{A}(W_R) \subset \mathcal{U}(W_R)$, where $\mathcal{U}(W_R)$ is defined as in Lemma 12, and hence

$$V(i\pi)X\Omega = JX^*\Omega, \quad \text{all } X \in \mathcal{A}(W_R). \tag{135}$$

Let the von Neumann algebras $\mathcal{A}(W)$, $\mathcal{A}(\bar{C}^c)$, and $\mathcal{B}(\bar{C})$ be constructed as in Theorem 5. Then:

(a) The algebras $\mathcal{B}(\bar{C})$ and $\mathcal{A}(\bar{C}^c)$ satisfy the *duality condition*

$$\mathcal{B}(\bar{C})' = \mathcal{A}(\bar{C}^c). \tag{136}$$

(b) *If there exists* a double cone C_0 such that $\mathcal{B}(\bar{C}_0)\Omega$ is dense in the Hilbert space $\mathcal{H}$, then

$$\mathcal{A}(\bar{C}_1^c) = \{\mathcal{B}(\bar{C}) \,|\, C \in \mathcal{O}_c, \ \bar{C} \subset \bar{C}_1^c\}'' \tag{137a}$$

for every $C_1 \in \mathcal{O}_c$, and

$$\mathcal{A}(W) = \{\mathcal{B}(\Lambda \bar{C}_0) \,|\, \Lambda \in \bar{L}_0, \Lambda \bar{C}_0 \subset W\}'', \tag{137b}$$

$$\mathcal{A}(\bar{C}_1^c) = \{\mathcal{B}(\Lambda \bar{C}_0) \,|\, \Lambda \in \bar{L}_0, \Lambda \bar{C}_0 \subset \bar{C}_1^c\}'' \tag{137c}$$

for every $C_1 \in \mathcal{O}_c$, $W \in \mathcal{W}$. If, furthermore, $\bar{C}_0 \subset W_R$, then

$$\mathcal{A}(W_R) = \{V(t)\mathcal{B}(\bar{C}_0)V(t)^{-1} \,|\, t \in R^1\}''. \tag{137d}$$

(c) *If the quantum field satisfies Condition II*, and if $\mathcal{A}(W_R) = \mathcal{A}_c(W_R)$, with $\mathcal{A}_c(W_R)$ defined as in Theorem 3, then the pair of von Neumann algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L) = \mathcal{A}(W_R)'$ satisfies the premises of the present theorem. The vector Ω is a cyclic and separating vector for every algebra $\mathcal{B}(\bar{C})$, and for every algebra $\mathcal{A}(\bar{C}^c)$. The

relation (137a) holds, and the relations (137b) and (137c) hold for every $C_0 \in \mathcal{D}_c$.

If $C(R)$ is defined as in the statement of Condition II, then

$$\mathcal{B}(\bar{C}) \supset C(C) \tag{138}$$

for all $C \in \mathcal{D}_c$.

(d) *If the quantum field satisfies Condition III, or Condition IV*, then the pair of algebras $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$, defined as in Theorem 4, satisfies the premises of the present theorem, and Ω is a cyclic and separating vectors for every algebra $\mathcal{B}(\bar{C})$, and for every algebra $\mathcal{A}(\bar{C}^c)$. The relations (137a)—(137d) hold as in (b) above, for any $C_0 \in \mathcal{D}_c$.

Furthermore, if $\mathcal{G}(C)$ is the set of all spectral projections of all operators $(\bar{\varphi}[f], D(f))$, with f *real*, $f \in \mathcal{S}(R^4)$, and $\mathrm{supp}(f) \subset C$, then,

$$\mathcal{G}(C)'' \subset \mathcal{B}(\bar{C}) \tag{139}$$

and, for any $C_1 \in \mathcal{D}_c$,

$$\mathcal{A}(\bar{C}_1^c) = \{\mathcal{G}(C) \mid C \in \mathcal{D}_c, \bar{C} \subset \bar{C}_1^c\}''. \tag{140}$$

Proof: (1) All the conclusions of Theorem 5 hold. The duality condition (136) follows easily from the duality condition $\mathcal{A}(W_L) = \mathcal{A}(W_R)'$ for the wedge-algebras, if we note that

$$\begin{aligned}\mathcal{A}(\bar{C}^c) &= \{\mathcal{A}(\Lambda W_L) \mid \Lambda \in \bar{L}_0, \Lambda W_R \supset \bar{C}\}'' \\ &= (\cap \{\mathcal{A}(\Lambda W_L)' \mid \Lambda \in \bar{L}_0, \Lambda W_R \supset \bar{C}\})' = \mathcal{B}(\bar{C})',\end{aligned} \tag{141}$$

where the equality of the first and the second members follows from (133d) in Theorem 5.

(2) We next consider the assertions (b), assuming now that a C_0 in $\mathcal{D}_0$ exists, such that $\mathcal{B}(\bar{C}_0)\Omega$ is dense. Without loss of generality we can assume that $\bar{C}_0 \subset W_R$. Let $\mathcal{A}_R$ be equal to the *right* member in (137d). Then Ω is a cyclic vector for the von Neumann algebra $\mathcal{A}_R$, and it follows from the definition of this algebra that $V(t)\mathcal{A}_R V(t)^{-1} = \mathcal{A}_R$ for all real t. Since, obviously, $\mathcal{A}_R \subset \mathcal{A}(W_R) \subset \mathcal{U}(W_R)$, we conclude that $\mathcal{A}_R$ satisfies the premises of Theorem 2, and it follows from that theorem that $\mathcal{A}_R = \mathcal{A}(W_R)$. This proves the relation (137d). The relations (137a)—(137c) then follow trivially from (137d).

(3) The assertions (c) are completely trivial. We now consider the assertions (d). The crux of the matter is that $\mathcal{G}(C)''\Omega$ is dense for any double cone C. That this is so is established by the same kind of reasoning as in step (3) in the proof of Theorem 4, but with the modification that for any integer $n > 0$ the regions R_k, $k = 1, \ldots, n$, are selected as any set of n nonempty open sets in C such that the closures of any two of these regions are spacelike separated. Having thus shown that $\mathcal{G}(C)''\Omega$ is dense, we consider the case when the double cone C satisfies $\bar{C} \subset W_R$, and we define a von Neumann algebra $\mathcal{A}_R$ by

$$\mathcal{A}_R = \{V(t)\mathcal{G}(C)V(t)^{-1} \mid t \in R^1\}''. \tag{142}$$

The relation (139) is trivial, and we can now apply the reasoning in step (2) above to $\mathcal{A}_R$. We conclude that $\mathcal{A}_R = \mathcal{A}(W_R)$, and from this the relation (140) follows readily. This completes the proof of the theorem.

We feel that it is entirely proper to call the condition (136) a "duality condition," at least in the case when there exists a double cone C_0 such that $\mathcal{B}(\bar{C}_0)\Omega$ is dense in the Hilbert space $\mathcal{H}$. In this case we have the following situation. There exists a family of truly local operators, namely, the set of all the operators in all the algebras $\mathcal{B}(\bar{C})$, which is sufficiently large such that the local operators generate the algebras $\mathcal{A}(W)$ and $\mathcal{A}(\bar{C}^c)$ in the sense of (137a) and (137b). The algebra $\mathcal{A}(\bar{C}^c)$ in (136), which is associated with the unbounded region $\bar{C}^c$, is thus itself generated by "local observables," and this circumstance, in our opinion, adds luster to the duality condition. As we have seen this situation obtains if the field satisfies either one of Conditions II, III, or IV.

It should be noted, however, that even if the field satisfies Condition IV it is in general *not* the case that $\mathcal{B}(\bar{C}) = \mathcal{G}(C)''$, i. e., the local algebra $\mathcal{B}(\bar{C})$ need not be generated by the spectral projections of the self-adjoint operators $(\bar{\varphi}[f], D(f))$, with f *real*, $f \in \mathcal{S}(R^4)$, and $\mathrm{supp}(f) \subset C$. The duality condition in the case of a generalized free field has been studied by Landau,[8,32] and with reference to our discussion we can express the results as follows: For certain kinds of generalized free fields we have $\mathcal{B}(\bar{C}) \neq \mathcal{G}(C)''$. For a detailed discussion of this circumstance we refer to the work of Landau. The algebra $\mathcal{G}(C)''$ generated by the generalized field *alone* is thus "too small" to satisfy the duality condition. The situation is, however, entirely different if instead we consider the algebra generated (locally) by *all* the local generalized free fields which are local relative to the original field.

The duality condition for a free Hermitian scalar field was first proved by Araki,[2] by an entirely different method. The von Neumann algebras generated by a free field have been studied extensively.[6,7,29,33,34] It is well known that in this case the field operators $(\varphi[f], D_1)$, with f real, $f \in \mathcal{S}(R^4)$, are all essentially self-adjoint, and our Condition IV obtains. Furthermore, it is the case that $\mathcal{B}(\bar{C}) = \mathcal{G}(C)''$, for all double cones C. It should here be noted that Araki's proof of the duality condition, as well as the subsequent modified proofs by Osterwalder,[6] Eckmann and Osterwalder,[7] and by Landau,[8] hold for more general regions than double cones and wedges. The discussion in the work of Eckmann and Osterwalder is based on Tomita's theorem, but also on the very special properties of a free field, and it is not clear to us how the discussion could be generalized to the case of an arbitrary field. We also do not know at this time whether there is any simple "physical—geometrical" interpretation of the Tomita operators J and $V(i\pi)$ for a double cone, or for a more general region. The remarkably simple interpretation of these operators for the case of the wedge regions probably reflects the very special geometric properties of the pair W_R and W_L.

We shall conclude the present study with a discussion by local internal symmetries. Such symmetries were discussed by Landau and Wichmann,[35] within the framework of quantum field theory, and within the framework of the theory of local systems of algebras, and it was

shown that a local internal symmetry, as defined in that paper, commutes with all translations in the Poincaré group. It was shown by Landau,[36] and by Herbst,[37] that such symmetries also commute with the homogeneous Lorentz transformations under the additional assumption that asymptotic Fock spaces exist, i. e., that the theory has a sensible physical interpretation in terms of particle states.

The definition of a local internal symmetry G in the paper of Landau and Wichmann can be stated as follows, for the case of wedge regions: G is a unitary operator such that

$$G\Omega = \Omega, \quad G\mathcal{A}(W)G^{-1} \subset \mathcal{A}(\overline{W}^c)' \tag{143}$$

for all $W \in \mathcal{W}$. It should be noted that no duality condition was assumed in the quoted work, and it seems to us that the above definition can then be criticized: In particular, it could happen that the set of all symmetries so defined does not form a group. However, the above definition is satisfactory if the duality condition $\mathcal{A}(\overline{W}^c)' = \mathcal{A}(W)$ holds, because it is then easy to show that $G\mathcal{A}(W)G^{-1} = \mathcal{A}(W)$ for all $W \in \mathcal{W}$. In particular, it follows that the set of all local internal symmetries forms a group.

In view of the above we shall here define a local internal symmetry by replacing the second condition in (143) by the condition that $G\mathcal{A}(W)G^{-1} = \mathcal{A}(W)$, for all $W \in \mathcal{W}$.

Theorem 7: Let $\mathcal{A}(W_R)$ and $\mathcal{A}(W_L)$ be a pair of local wedge algebras, which satisfy the general premises of Theorem 6, and let $\mathcal{A}(W)$, $\mathcal{B}(\bar{C})$, and $\mathcal{A}(\bar{C}^c)$ be defined as in Theorems 5 and 6.

Let G be a unitary operator such that

$$G\Omega = \Omega, \quad G\mathcal{A}(W)G^{-1} = \mathcal{A}(W), \quad \text{all } W \in \mathcal{W}. \tag{144}$$

Then:

(a) The operator G commutes with the TCP-transformation, and with all Poincaré transformations, i. e.,

$$\Theta_0 G \Theta_0 = G, \quad U(\Lambda)GU(\Lambda)^{-1} = G, \quad \text{all } \Lambda \in \bar{L}_0. \tag{145}$$

(b) For all double cones C,

$$G\mathcal{B}(\bar{C})G^{-1} = \mathcal{B}(\bar{C}), \quad G\mathcal{A}(\bar{C}^c)G^{-1} = \mathcal{A}(\bar{C}^c). \tag{146}$$

(c) The set of all unitary operators G which satisfy the conditions (144) forms a group; the *group of all local internal symmetries*.

Proof: (1) The second condition (144) holds in particular for $W = W_R$. The algebra $\mathcal{A}_R = \mathcal{A}(W_R)$ satisfies the premises of Theorem 2, and in particular $\mathcal{A}(W_R)\Omega$ is a core for the self-adjoint operator $(V(i\pi), D_+)$. The conditions (144) trivially imply that $G^{-1}\mathcal{A}(W_R)\Omega = \mathcal{A}(W_R)\Omega$, and it follows that $\mathcal{A}(W_R)\Omega$ is also a core for the self-adjoint operator $(G^{-1}V(i\pi)G, G^{-1}D_+)$. Let $X \in \mathcal{A}(W_R)$. We then have

$$V(i\pi)GX\Omega = JGX^*\Omega = (JGJ)V(i\pi)X\Omega \tag{147a}$$

where the first two members are equal because $GXG^{-1} \in \mathcal{A}(W_R)$. We thus have

$$(G^{-1}V(i\pi)G, \mathcal{A}(W_R)\Omega) = (G^{-1}JGJ)(V(i\pi), \mathcal{A}(W_R)\Omega). \tag{147b}$$

Since $(G^{-1}V(i\pi)G, \mathcal{A}(W_R)\Omega)$ and $(V(i\pi), \mathcal{A}(W_R)\Omega)$ are essentially self-adjoint, and since $G^{-1}JGJ$ is unitary, it follows, by the polar decomposition theorem, that $G^{-1}D_+ = D_+$, $(V(i\pi), D_+) = (G^{-1}V(i\pi)G, D_+)$, and[38]

$$JG = GJ. \tag{148a}$$

(2) The same considerations apply to the algebra $\mathcal{A}(W)$ associated with any other wedge $W = \Lambda W_R$. The Tomita operator "J" for the algebra $\mathcal{A}(\Lambda W_R)$ is $U(\Lambda)JU(\Lambda)^{-1}$, and thus we have

$$U(\Lambda)JU(\Lambda)^{-1}G = GU(\Lambda)JU(\Lambda)^{-1} \tag{148b}$$

for all $\Lambda \in \bar{L}_0$. In view of the third relation (56a) we then have, after multiplication of both members in (148b) by J from the left,

$$U(\mathcal{J}\Lambda\mathcal{J}\Lambda^{-1})G = GU(\mathcal{J}\Lambda\mathcal{J}\Lambda^{-1}) \tag{148c}$$

for all $\Lambda \in \bar{L}_0$. It is easily seen that this implies that G commutes with all $U(\Lambda)$, and it then follows from (148a) that G also commutes with Θ_0.

(3) The remaining statements in the theorem are completely trivial.

In conclusion let us state that the considerations in this section can be generalized to other families of bounded regions. We chose to discuss these issues for double cones only, in order to avoid geometrical complications which might obscure the basically very simple mainline of argument.

ACKNOWLEDGMENTS

It is a pleasure for one of us (E. H. W.) to thank Dr. Lawrence J. Landau, and Dr. Konrad Osterwalder, for discussions about duality and related issues. We also wish to thank Drs. Landau and Osterwalder for sending us their manuscripts prior to publication.

*Work supported by the U.S. Atomic Energy Commission.
†This work is based in part on results presented in a thesis to be submitted by J. Bisognano in partial fulfillment of the requirements for the degree of Doctor of Philosophy at the University of California, Berkeley.
‡Work supported in part by the National Science Foundation under Grant GP-42249X.

[1]R. Haag and B. Schroer, J. Math. Phys. 3, 248 (1962).
[2]H. Araki, J. Math. Phys. 5, 1 (1964).
[3]M. Guenin and B. Misra, Helv. Phys. Acta 37, 267 (1964).
[4]L. Kraus, Z. Phys. 181, 1 (1964).
[5]S. Doplicher, R. Haag, and J. Roberts, Commun. Math. Phys. 13, 1 (1969); 15, 173 (1969).
[6]K. Osterwalder, Commun. Math. Phys. 29, 1 (1973).
[7]J. P. Eckmann and K. Osterwalder, J. Funct. Anal. 13, 1 (1973)..
[8]L. J. Landau, Comm. Math. Phys. 39, 49 (1974).
[9]A. S. Wightman, Phys. Rev. 101, 860 (1956).
[10]R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin, New York, 1964).
[11]R. Jost, *The General Theory of Quantized Fields* (American Mathematical Society, Providence, R.I., 1965).
[12]H. Reeh and S. Schlieder, Nuovo Cimento 22, 1051 (1961).
[13]M. Takesaki, *Tomita's Theory of Modular Hilbert Algebras and Its Applications* (Springer-Verlag, Berlin, 1970).
[14]H. J. Borchers, Nuovo Cimento 15, 784 (1960).
[15]See Ref. 10, Chap. 2.
[16]H. J. Borchers, Nuovo Cimento 24, 214 (1962).
[17]See Ref. 11, Chap. 4.
[18]See Ref. 10, Chap. 4, p. 138.
[19]See Ref. 11, p. 73. It should be noted that our choice of

independent variables is different (in a trivial way) from the choice in Jost's book.

[20]See Ref. 10, Chap. 2, p. 41. The extension to vector-valued tempered distributions is trivial.

[21]The question arises whether our definition (37) is really the "best possible." If the notion of causal complement is to correspond to a physical notion of causal independence one would like to require that the causal complement of any *open* region R contains the *interior* of R^c as defined in (37). There is hardly any physical basis for a more specific statement, and how the boundaries are handled is then only a question of mathematical convenience. For the discussion in this paper this issue is not important, but we have considered generalizations, and with these in mind it seemed to us that the definition (37) is appropriate.

[22]R. Jost, Helv. Phys. Acta 30, 409 (1957).

[23]See Ref. 10, Chap. 2, p. 70.

[24]This is, of course, well-known: See Ref. 10, p. 139.

[25]A. van Daele, J. Funct. Anal. 15, 378 (1974). This paper presents a simplified proof of Tomita's theorem.

[26]R. Haag, N. M. Hugenholtz, and M. Winnink, Commun. Math. Phys. 5, 215 (1967).

[27]D. Kastler, J.C.T. Pool, and E. Thue Poulsen, Commun. Math. Phys. 12, 175 (1969).

[28]J. von Neumann, Math. Ann. 102, 370 (1929).

[29]J. Langerholc and B. Schroer, Commun. Math. Phys. 1, 215 (1965).

[30]A. L. Licht, J. Math. Phys. 4, 1443 (1963).

[31]H. J. Borchers and W. Zimmermann, Nuovo Cimento 31, 1047 (1963).

[32]L. J. Landau, Ph. D. thesis, University of California, Berkeley, 1969 (unpublished).

[33]H. Araki, J. Math. Phys. 4, 1343 (1963).

[34]G.-F. Dell'Antonio, Commun. Math. Phys. 9, 81 (1968).

[35]L. J. Landau and E. H. Wichmann, J. Math. Phys. 11, 306 (1970).

[36]L. J. Landau, Commun. Math. Phys. 17, 156 (1970).

[37]I. W. Herbst, J. Math. Phys. 12, 2480 (1971).

[38]The conclusion in this step corresponds to a known result about von Neumann algebras: Compare with M. Sirugue and M. Winnink, Commun. Math. Phys. 19, 161 (1970).

Some restrictions on algebraically general vacuum metrics*

Carl H. Brans†

Joseph Henry Laboratories, Physics Department, Princeton University, Princeton, New Jersey 08540
(Received 18 November 1974)

Vacuum Einstein metrics of Petrov type I, general, are considered. It is shown that the only solution of this sort in which one of the Petrov scalars is zero is the trivial flat-space one. Further, it is shown that the point at which the four Petrov scalars vanish simultaneously (zero curvature tensor) cannot be included as a regular point of a neighborhood over which the scalars are functionally independent. In fact, for type I all derivatives of the Petrov scalars must vanish at a point at which the curvature tensor does so that this point cannot be a regular point of any nontrivial analytic solution.

This note discusses some properties of vacuum Einstein metrics which are algebraically and functionally general in the Petrov sense. The complex 2-form technique described by Debever[1] will be used since it is the most natural extension to differential geometry of the work of Petrov[2] in the tangent space at a fixed point. Using the Cartan real 1-form description we can write the metric in terms of a Lorentz-orthonormal form basis, ω^α, as

$$ds^2 = \eta_{\alpha\beta}\omega^\alpha\omega^\beta \quad (\alpha, \beta, \cdots = 0, 1, 2, 3), \tag{1}$$

where $\eta_{\alpha\beta} = \mathrm{diag}(-1, 1, 1, 1)$. The choice of such basis for a given metric is of course arbitrary up to Lorentz transformations at each point and an important geometric problem is to determine the extent to which this arbitrariness can be reduced. The procedure of Petrov attacks this problem by investigating the canonical form of the Weyl part of the curvature. In this procedure the use of the $SO(3, C)$ representation of the Lorentz group plays a central role, so it is natural to develop a formalism making use of it from the beginning. Thus replace the real form ω^α basis by complexified 2-form basis σ^a, defined by

$$\sigma^a = \omega^0 \wedge \omega^a + i\omega^b \wedge \omega^c, \quad (a, b, c) = \mathrm{cyclic}(1, 2, 3). \tag{2}$$

Thus, the Lorentz transformations of ω^α give rise to complex orthogonal transformation of the σ^a. Conversely, given a set of three complex 2-forms σ^a, it can be shown that they correspond to a real 1-form basis ω^α according to (2) if and only if they satisfy the conditions

$$\sigma^a \wedge \sigma^b = i\delta^{ab} I, \quad \sigma^a \wedge \bar{\sigma}^b = 0, \tag{3}$$

in which I is a real nonzero 4-form. The structure equations for real 1-forms are

$$d\omega^\alpha = \omega^\beta \wedge \omega^\alpha{}_\beta, \quad \omega_{\alpha\beta} + \omega_{\beta\alpha} = 0, \tag{4}$$

$$d\omega^\alpha{}_\beta + \omega^\alpha{}_\gamma \wedge \omega^\gamma{}_\beta = \Omega^\alpha{}_\beta, \tag{5}$$

where $\omega^\alpha{}_\beta$ are the connection forms and $\Omega^\alpha{}_\beta$ the curvature forms,

$$\Omega^\alpha{}_\beta = (1/2)R^\alpha{}_{\beta\gamma\mu}\omega^\gamma \wedge \omega^\mu. \tag{6}$$

These can then be translated into complexified form

$$d\sigma^a = X^b \wedge \sigma^c - X^c \wedge \sigma^b, \tag{7}$$

$$dX^a - X^b \wedge X^c = P^a{}_b\sigma^b + Q^a{}_b\bar{\sigma}^b, \tag{8}$$

where

$$X^a = \omega^b{}_c - i\omega^a{}_0. \tag{9}$$

The condition of being an Einstein empty space is then that $Q^a{}_b = 0$ and that $P^a{}_b$ be traceless. The Petrov classification consists of finding canonical forms for the symmetric matrix $P^a{}_b$ under complex orthogonal transformations of the basis σ^a.

In this paper we will be concerned with the type I, general, case in which $P^a{}_b$ can be diagonalized with distinct eigenvalues, thus uniquely determining the basis σ^a (up to inversions, of course). Hence assume that $P^a{}_b$ takes the form

$$P^a{}_b = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}, \quad \alpha + \beta + \gamma = 0, \tag{10}$$

so that the Eqs. (8) become

$$\begin{aligned} dX^1 - X^2 \wedge X^3 &= \alpha\sigma^1, \\ dX^2 - X^3 \wedge X^1 &= \beta\sigma^2, \\ dX^3 - X^1 \wedge X^2 &= \gamma\sigma^3. \end{aligned} \tag{11}$$

In some cases it is convenient to use a null basis, replacing the forms σ^a with ρ^a,

$$\begin{aligned} \rho^1 &= (\sigma^1 + i\sigma^2)/\sqrt{2}, \\ \rho^2 &= (-\sigma^1 + i\sigma^2)/\sqrt{2}, \\ \rho^3 &= i\sigma^3. \end{aligned} \tag{12}$$

The algebraic conditions (3) become

$$\rho^2 \wedge \rho^1 = \rho^1 \wedge \rho^2 = \rho^3 \wedge \rho^3 = -iI \neq 0, \tag{13}$$

and other products zero. Equation (13) can then be shown to be a necessary and sufficient condition that the ρ^a can be written

$$\begin{aligned} \sqrt{2}\,\rho^1 &= \mu \wedge \kappa, \\ \sqrt{2}\,\rho^2 &= \bar{\mu} \wedge \lambda, \\ 2\rho^3 &= -i(\mu \wedge \bar{\mu} + \kappa \wedge \lambda), \end{aligned} \tag{14}$$

where κ, λ are real null 1-forms, and μ is complex. In terms of the ω^α basis,

$$\begin{aligned} \kappa &= \omega^3 - \omega^0, \\ \lambda &= \omega^3 + \omega^0, \\ \mu &= \omega^1 + i\omega^2, \end{aligned} \tag{15}$$

and the metric can be written

$$ds^2 = \kappa\lambda + \mu\bar{\mu}. \tag{16}$$

The tangent vector basis dual to these 1-forms is, of course, directly related to the basis used in the Newman–Penrose (NP) formalism.[3] Thus, the exterior form equations used here are equivalent to the NP equations.

The structure equations can now be written

$$\begin{aligned} d\rho^1 &= Y^3 \wedge \rho^1 - Y^1 \wedge \rho^3, \\ d\rho^2 &= -Y^3 \wedge \rho^2 + Y^2 \wedge \rho^3, \\ d\rho^3 &= Y^1 \wedge \rho^2 - Y^2 \wedge \rho^1, \end{aligned} \tag{17}$$

where

$$\begin{aligned} Y^1 &= (X^1 + iX^2)/\sqrt{2}, \\ Y^2 &= (-X^1 + iX^2)/\sqrt{2}, \\ Y^3 &= iX^3. \end{aligned} \tag{18}$$

the Equation (11) becomes

$$\begin{aligned} dY^1 - Y^3 \wedge Y^1 &= \frac{(\beta - \alpha)}{2}\rho^2 + \frac{(\beta + \alpha)}{2}\rho^1, \\ dY^2 + Y^3 \wedge Y^2 &= \frac{(\beta - \alpha)}{2}\rho^1 + \frac{(\beta + \alpha)}{2}\rho^2, \\ dY^3 - Y^1 \wedge Y^2 &= \gamma\rho^3. \end{aligned} \tag{19}$$

The complete determination of the basis for the general type I case might be expected to correspond to some fairly strong restrictions on the solutions since there are no directional symmetries available. We will now consider some of these limitations.

In the first place, consider the case in which one of the eigenvalues is the negative of the other, say $\alpha = -\beta$, so that the third is zero, $\gamma = 0$. This might seem to be a natural alternative to the type D case in which two of the eigenvalues are equal to each other. This latter case includes the well known Schwarzschild and Kerr metrics and has been studied exhaustively by Kinnersley.[4] We find, however, that the $\alpha = -\beta$ condition cannot be met unless $\alpha = \beta = \gamma = 0$ as shown by the following theorem.

Theorem 1: The only solution to the vacuum Einstein equations for which one of the Petrov eigenvalues vanishes over a region is the trivial one (flat space–time over the region).

Proof: Assume that $\alpha = -\beta$ and $\gamma = 0$ so that the null-form equations become

$$\begin{aligned} dY^1 - Y^3 \wedge Y^1 &= \beta\rho^2, \\ dY^2 + Y^3 \wedge Y^2 &= \beta\rho^1, \\ dY^3 - Y^1 \wedge Y^2 &= 0. \end{aligned} \tag{20}$$

Taking exterior derivatives, and using (17) we get the Bianchi identities, one of which can be written

$$d\beta \wedge \rho^2 - 2\beta Y^3 \wedge \rho^2 + \beta Y^2 \wedge \rho^3 = 0. \tag{21}$$

Now consider the 1-form decomposition (14) and take the $\wedge$ product of (21) by $\bar{\mu}$ and λ separately to get

$$\beta Y^2 \wedge \kappa \wedge \lambda \wedge \bar{\mu} = \beta Y^2 \wedge \mu \wedge \bar{\mu} \wedge \lambda = 0, \tag{22}$$

which in turn gives

$$\beta Y^2 \wedge \rho^2 = 0, \tag{23}$$

or, if the geometry is nowhere flat in the region, $\beta \neq 0$,

$$Y^2 \wedge \rho^2 = 0. \tag{24}$$

Taking the exterior derivative of this equation, and using (20) and (17), we get

$$\beta\rho^1 \wedge \rho^2 = 0, \tag{25}$$

which contradicts (13) unless $\beta = 0$, thus completing the proof.

Next we consider what might be thought of as the "most general" Petrov type, namely, the situation in which two complex Petrov scalars are not only algebraically independent but also functionally independent. Specifically, we want to look at the case in which the real and imaginary parts of α and β constitute a set of four functionally independent scalar fields. It is clear that in this case these four fields can be used to determine a unique coordinate system. Thus, such a metric uniquely determines not only a preferred frame at each point, but also a preferred space–time coordinate system. In a certain sense it is the most unsymmetric possibility for Einstein metrics. We will now show that, if such a solution exists, it cannot contain the origin of the preferred coordinate system as a regular point.

Theorem 2: Let α and β be the Petrov scalars of a vacuum Einstein metric as described in (11), and $\alpha = u + iv$, $\beta = p + iq$, with u, v, p, q four real functions. These four functions cannot be functionally independent in any neighborhood of the point for which $u = v = p = q = 0$.

Proof: Take the exterior derivatives of the Eqs. (11) to produce the Bianchi identities

$$\begin{aligned} d\alpha \wedge \sigma^1 &= (\gamma - \alpha)X^2 \wedge \sigma^3 - (\beta - \alpha)X^3 \wedge \sigma^2, \\ d\beta \wedge \sigma^2 &= (\alpha - \beta)X^3 \wedge \sigma^1 - (\gamma - \beta)X^1 \wedge \sigma^3, \\ d\gamma \wedge \sigma^3 &= (\beta - \gamma)X^1 \wedge \sigma^2 - (\alpha - \gamma)X^2 \wedge \sigma^1. \end{aligned} \tag{26}$$

When these are evaluated at a point for which $\alpha = \beta = \gamma = 0$, they are easily seen to require

$$d\alpha = d\beta = d\gamma = 0, \tag{27}$$

thus contradicting the functional independence of α and β at this point.

A slight extension of the above argument results in

Theorem 3: The only type I solution for which α and β are analytic functions and which extends over a region containing a zero of the curvature tensor is the trivial flat space one.

For the Schwarzschild and Kerr metrics α and β do not vanish anywhere, depending on the usual radial coordinate like $1/r$.

ACKNOWLEDGMENT

The author is grateful to the Physics Department at Princeton University, particularly the Gravity Research Group, for their hospitality during the time when most of the work on this paper was done.

*Supported in part by a grant from the National Science Foundation.

†On leave from Loyola University, New Orleans, Louisiana, present address.

[1]R. Debever, Cahiers Phys. **168**, 303 (1964).
[2]A.Z. Petrov, Sci. Trans. Kazan State Univ. **114**, 55 (1954); or A.Z. Petrov, *Einstein Spaces* (Pergamon, New York, 1969).
[3]E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).
[4]W. Kinnersley, J. Math. Phys. **10**, 1195 (1969).

Erratum: Complex potential formulation of the axially symmetric gravitational field problem [J. Math. Phys. 15, 1409 (1974)]

Frederick J. Ernst

Department of Physics, Illinois Institute of Technology, Chicago, Illinois 60616
(Received 20 December 1974)

The second term in the numerator of Eq. (5) should be $+y^4 \sin^2\lambda$. The next to last term in Eq. (13b) should be $+\frac{1}{2}S_{tt*}B_0^*$. The exponent 2 should be deleted from the numerator of Eq. (42). "Covariance" is not spelled correctly in Ref. 9.

Erratum: The T operator and an inverse problem for nonlocal potentials [J. Math. Phys. 15, 1227 (1974)]

Te Hai Yao

Mathematics Department, Bedford College, Regent's Park, London NW1, England
(Received 2 December 1974)

(1) On p. 1231, line 16 on left side: $\psi(\xi = \xi\hat{\xi}; \mathbf{x})$ should be changed to $\xi\psi(\xi = \xi\hat{\xi}; \mathbf{x})$.

(2) On pp. 1228 and 1230: $\psi(\xi = \xi\hat{\xi}; \mathbf{x})$ should be changed to $\psi(\xi = \xi\hat{\xi}; \mathbf{x})$.

