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A Convergent Perturbation Expansion in First-Quantized Electrodynamics*

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It is shown that a real physical problem exists which, when calculated in first-quantized electrodynamics, possesses a convergent perturbation expansion. The result is demonstrated by proving the analyticity in a region of nonzero radius about the origin in the complex coupling-constant plane, of the transition probability for pair creation by two electromagnetic fields. Some singularities in the complex plane are located, which limit the radius of convergence only for a discrete set of values for the energies of the electromagnetic fields which define the problem.

INTRODUCTION

PERTURBATION theory has played a fundamental role in the development of quantum field theory. Although the existence of large coupling constants for the strong interactions has now led to the development of methods which avoid it, perturbation theory is still the backbone of quantum electrodynamics. As such, the question of the convergence of perturbation theory has been the subject of considerable discussion (and controversy) in the literature.[1]

The investigation of this paper is directed towards the demonstration that a real problem exists which leads to a perturbation series that will converge within the framework of Dirac theory, i.e., a non-second-quantized theory. The procedure employed is to use the known solution[2] for the interaction of two plane-wave electromagnetic fields in which one of the fields is treated as a perturbation, but the other may have arbitrary strength. The analytic properties of the transition probability as a function of the field-strength parameter of this second field are then examined to determine the radius of convergence of a power series in this parameter. This power series is the perturbation expansion for this c-number theory. It is shown that, except for a denumerable set of values of the expansion parameter, the series has a nonzero radius of convergence.

PROCEDURE

The problem considered in ALL was the pair production resulting from the interaction of two

* Based on portions of a thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy at the University of Maryland, 1958.

[1] F. J. Dyson, Phys. Rev. **85**, 631 (1952); C. A. Hurst, Proc. Cambridge Phil. Soc. **48**, 625 (1952); W. Thirring, Helv. Phys. Acta **26**, 33 (1953); A. Petermann, Arch. Sci. Phys. Nat. **6**, 5 (1953); Phys. Rev. **89**, 1160 (1953); R. Utiyama and T. Imamura, Prog. Theoret. Phys. (Kyoto) **9**, 431 (1953); M. Fierz, *Proceedings of the Fifth Annual Rochester Conference on High-Energy Physics*, (Interscience Publishers, Inc., New York, 1955), p. 67. D. R. Yennie and S. Gartenhaus, Proceedings of the Midwest Conference on Theoretical Physics, St. Louis, Missouri, 30 (1958); A. Buccafurri and E. R. Caianiello, Nuovo cimento **8**, 170 (1958).

[2] H. R. Reiss, J. Math. Phys. **3**, 59 (1962). Since the title of this paper is "Absorption of Light by Light," it will be referred to hereafter as ALL.

plane-wave electromagnetic fields propagating in opposite directions. Any other angle of collision of the two fields can be obtained by Lorentz transformation, with the obvious exception of the case of parallel propagation, for which there is no interaction. The fields were taken to be plane polarized, and the two independent cases of parallel or perpendicular relative polarization of the fields were calculated. The results from these two cases are quite similar, and their analytic properties are the same, so only one of these cases will be treated here.

The probability for the creation of an electron pair per unit volume per unit time by the head-on collision of a plane wave of frequency ω and arbitrary strength, with a weak plane wave of frequency $\tilde{\omega}$, with the two waves polarized perpendicular to each other, is[2]

$$W = \frac{m^4\tilde{z}}{8\pi^4}\sum_{q=q_0}^{\infty}(\alpha q w)^{\frac{1}{2}}\int_0^1\frac{d\lambda}{(1-\lambda)^{\frac{1}{2}}}\int_0^{\pi/2}d\nu\left[\frac{z}{\alpha\lambda+1+z}I_{11}^2-\frac{\alpha\lambda\cos^2\nu}{qw}I_0^2\right]. \quad (1)$$

The convention is employed that $\hbar = c = 1$. The parameter z is the perturbation expansion parameter, since it is $z = \frac{1}{2}(ae/m)^2$; where a is the amplitude of the vector potential for the plane wave of arbitrary strength, and e and m are the electron charge and mass. The parameter $\tilde{z}$ refers to the weak plane wave. The quantity $w = \omega\tilde{\omega}/m^2$ is the product of the photon energies of the two fields, measured in units of electron mass, and α is an abbreviation for $qw - 1 - z$. The functions I_{11}^2 and I_0^2 are defined in terms of the family of integrals

$$I_n = \int_0^{2\pi}d\theta(\cos n\theta)\times\exp\left[iq(b_1\sin\theta+\tfrac{1}{2}b_2\sin 2\theta+\theta)\right]. \quad (2)$$

I_{11}^2 is defined to be

$$I_{11}^2 = 2I_1^2 - I_0^2 - I_0I_2, \quad (3)$$

so that it is not actually a square of any I_n integral, although it is a quadratic combination of them. The quantities in the exponential function in the I_n integrals are

$$b_1 = 2(2z\alpha\lambda)^{\frac{1}{2}}(\alpha\lambda+1+z)^{-1}\sin\nu$$
$$b_2 = z(\alpha\lambda+1+z)^{-1}. \quad (4)$$

Finally, the lower limit on the sum over q in Eq. (1) is $q_0 = [(1+z)/w]$, where the square bracket is defined to mean the smallest integer containing $(1+z)/w$.

Equation (1) is identical to Eq. (16) of ALL, but with a change of integration variables to simplify the type of analysis required here. The integration variables used in ALL were ζ and p_1, which are related to λ and ν by

$$\zeta = m^2(\alpha\lambda+1+z) \qquad p_1 = m(\alpha\lambda)^{\frac{1}{2}}\sin\nu$$
$$\lambda = (\zeta/m^2 - 1 - z)/\alpha$$
$$\nu = \arcsin\left[(p_1/m)(\zeta/m^2-1-z)^{-\frac{1}{2}}\right],$$

with the Jacobian

$$\partial(\zeta, p_1)/\partial(\lambda,\nu) = m^3(\alpha^3\beta)^{\frac{1}{2}}\cos\nu.$$

The convergence of a perturbation expansion of Eq. (1) is to be investigated. The expansion parameter is z, which is proportional to the square of the electron charge. In principle, a perturbation expansion should be in powers of e rather than e^2; but examination of Eq. (1) shows that $z^{1/2}$ occurs only in b_1, given in Eq. (4). From a theorem proved in ALL, both I_0^2 and I_{11}^2 are even in b_1, so that any expansion of W in powers of $z^{1/2}$ would lead to a series in powers of z.

In view of the familiar Cauchy-Taylor theorem that the necessary and sufficient condition for a function to be expansible in a power series is that it should be analytic in a region, the analytic behavior of W as a function of z will be examined in the neighborhood of the origin in the complex z plane. Since it has not been found possible to locate the singularity closest to the origin, the technique employed is to show that there exists a nonzero radius of convergence, without establishing the upper bound to this radius. In Eq. (1), W is given as a series in the index q, which is unrelated to the perturbation series. It will be shown that the terms in the q series are analytic and that the q sum converges uniformly in a certain region. It then follows that W is analytic in that region. The uniform convergence property of the q series is demonstrated by finding a uniform bound for the general term in the q series such that the sum of the uniform bounds is convergent.

SINGULARITIES

The dependence on z of the lower limit of the q sum in Eq. (1) is given by

$$q_0 = [(1+z)/w].$$

This means that for some fixed value of w, as z is increased the value of $(1+z)/w$ must eventually pass through an integer value. When this happens a new term of nonzero value is added to W, so that the derivative of W with respect to z is singular at

such a value of z, and W is thus not an analytic function of z at such a point.

When $z = 0$, then $q_0 = [1/w]$. There will be no singularity until z increases from zero sufficiently that

$$(1 + z)/w = [1/w],$$

or when

$$z = w[1/w] - 1. \tag{5}$$

Equation (5) thus represents a limit on the radius of convergence of a perturbation expansion. To make the algebraic behavior of Eq. (5) more manifest, set

$$1/w = q_0 - \delta, \qquad 0 \leq \delta < 1.$$

Then, from Eq. (5)

$$z = \delta/(q_0 - \delta), \qquad 0 \leq \delta < 1. \tag{6}$$

Between consecutive discontinuities, Eq. (6) represents a hyperbola in z and δ, which rapidly approaches a straight line for large values of the parameter q_0.

The summand in q contains as a factor $\alpha^{1/2}$, which is an irrational function of z. To see if it really introduces a branch point at $z = qw - 1$, or if the rest of the summand contributes a further $\alpha^{1/2}$ factor, set $u = \alpha^{1/2}$ and examine the parity of the various terms in u which arise from elimination of z in favor of u. The b_1 function is odd in u, but it is known that I_0^2 and I_{11}^2 are even functions of b_1, and depend otherwise only on even powers of u, so they are also even functions of u. The only other appearance of u is its direct occurrence as a factor in the summand. The integration operations indicated in the summand cannot introduce any additional odd factors of u, so there is a real branch point at $u = 0$, i.e., at $z = qw - 1$. Since this condition holds for every q term, the radius in z is limited by $z = q_0 w - 1$. This is identical with Eq. (5), so the branch point at $\alpha = 0$ has given no new limitation on the region of analyticity.

The integrations over λ and ν and those involved in I_0^2 and I_{11}^2 can introduce no singularities which do not already exist in the integrands. This is true by the theorem which states that if, for any definite integral the integrand is a continuous function of z and of the integration variable over the entire closed interval of integration, for z within some closed region, and if the integrand is analytic in z within this region for the entire integration interval, then the integral is analytic in z within the entire region. The I_0^2 and I_{11}^2 functions have integrands which are exponential functions, so the continuity and analyticity conditions are satisfied everywhere except at the pole which occurs in both b_1 and b_2 at

$$z = -1 - qw\lambda/(1 - \lambda). \tag{7}$$

From Eq. (7), as λ increases from 0 to 1, z moves along the negative real axis from -1 and approaches $-\infty$. This pole in the exponential function cannot be removed by any of the integrations or the summation, so a line of singularities exists along the negative real z axis from -1 to $-\infty$. It is interesting to compare this behavior with the results of another investigation[3] in which the q series in Eq. (1) was split into a finite part consisting of all the smaller indices, and an infinite remainder series starting at a very large q value. This last part was evaluated using the asymptotic results valid for real z and very large q, and then the total result for W was extended into the complex z plane. This approximation for W was found to be analytic everywhere in the complex plane cut along the negative real line from -1 to $-\infty$, except for the point given by Eq. (5).

For fixed q, the ν integrand is analytic in z in the entire finite z plane with the exception of negative real z less than -1, and before integration, the I_0^2 and I_{11}^2 integrands are continuous in ν (and λ). Hence the ν integrand is continuous in ν (and λ) and the result of the ν integration is analytic in the finite z plane and continuous in λ. The λ integral is then also analytic in the finite z plane. Therefore, any given term in the q sum is analytic in z except when $z = qw - 1$, or when z is real and ≤ -1.

UNIFORM BOUNDS

The establishment of a bound for the general term in the q sum hinges upon finding bounds for I_0 and I_1. These functions, Eq. (2) with Eq. (4), exhibit rapid oscillations in the integrand, particularly for large q, so that no bound (which will lead to a convergent q sum) is immediately evident from Eq. (2). If, however, the path of integration in θ can be deformed into the complex θ plane to coincide (at least in part) with the paths of steepest descent from the saddle points which exist there, then the imaginary part of the exponential function in the integrand of Eq. (2) is constant, and a bound can be found simply from the largest value of the real part of the exponential function on the path of integration, i.e., at one (or more) of the saddle points.

[3] H. R. Reiss, Ph.D. Thesis, University of Maryland (1958); NAVORD Report 6180, U. S. Naval Ordnance Laboratory (1958).

Write I_0 as

$$I_0 = \int_C d\theta \exp [qf(\theta)],$$

where

$$f(\theta) = i(b_1 \sin \theta + \tfrac{1}{2}b_2 \sin 2\theta + \theta), \tag{8}$$

and C represents a suitable contour which will shortly be specified in detail, and which is obtained by deformation of the original path along the real axis from 0 to 2π. $f(\theta)$ has the property

$$f(\pi - \theta) = -f(\pi + \theta) + 2\pi i \tag{9}$$

so that any saddle point which is found shows the existence of another saddle point at a location symmetrical with respect to inversion through the point $\theta = \pi$. The condition $f'(\theta) = 0$ locates the saddle points at

$$\cos \theta_{sp} = -\frac{b_1}{4b_2} \pm \left[\left(\frac{b_1}{4b_2}\right)^2 - \frac{(1 - b_2)}{2b_2}\right]^{\frac{1}{2}},$$

or, from Eq. (4) at

$$\cos \theta_{sp} = -(\alpha\lambda \sin^2 \nu/2z)^{\frac{1}{2}} \pm i[(\alpha\lambda \cos^2 \nu + 1)/2z]^{\frac{1}{2}}. \tag{10}$$

Equation (10) defines four saddle points. It will be proved below that $|\cos \theta_{sp}| > 1$, so none of these saddle points can occur on the real axis. The symmetry condition Eq. (9) states that two of the saddle points must be in the upper half-plane, and the other two in the lower half-plane.

Let θ_r and θ_i be the real and imaginary parts of θ. Then the real part of $f(\theta)$ is, from Eq. (8),

$$\begin{aligned}\operatorname{Re} f(\theta) = {} & -\beta_1 \cos \theta_r \sinh \theta_i - \gamma_1 \sin \theta_r \cosh \theta_i \\ & - \tfrac{1}{2}\beta_2 \cos 2\theta_r \sinh 2\theta_i \\ & - \tfrac{1}{2}\gamma_2 \sin 2\theta_r \cosh 2\theta_i - \theta_i,\end{aligned} \tag{11}$$

where b_1 and b_2 have been split into real and imaginary parts by

$$b_1 = \beta_1 + i\gamma_1, \qquad b_2 = \beta_2 + i\gamma_2.$$

On the real axis,

$$(\partial/\partial\theta_i) \operatorname{Re} f(\theta) = -\beta_1 \cos \theta_r - \beta_2 \cos 2\theta_r - 1, \qquad \theta_i = 0, \tag{12}$$

which suggests that if β_1 and β_2 are sufficiently small, $\operatorname{Re} f(\theta)$ will decrease for all θ_r if the path of integration on the real axis is displaced upwards into the upper half-plane. The extrema of the right-hand side of Eq. (12) occur for

$$\theta_r = 0, \pi, \arccos (-\beta_1/4\beta_2).$$

It will be required that Eq. (12) must be negative for all these extrema. For both $\theta_r = 0$ and $\theta_r = \pi$, this is assured by

$$|b_1| + |b_2| < 1. \tag{13}$$

For $\theta_r = \arccos (-\beta_1/4\beta_2)$ the condition becomes

$$\tfrac{1}{8} |b_1^2|/|b_2| + |b_2| < 1. \tag{14}$$

In general, however, $|b_1|$ can be bounded in terms of $|b_2|$, since from Eq. (4),

$$\frac{b_1^2}{b_2} = 8 \frac{\alpha\lambda \sin^2 \nu}{\alpha\lambda + 1 + z}$$

so that, for $|z| < 1$,

$$|b_1^2| < 8 |b_2|. \tag{15}$$

Equation (15) is always true for $|z| < 1$. If Eq. (13) is to be satisfied also, then

$$|b_2| < 5 - 2(6)^{\frac{1}{2}}. \tag{16}$$

If, on the other hand, Eqs. (15) and (14) are to be true simultaneously, then

$$|b_2| < 1/9.$$

A bound on $|b_2|$ has immediate significance for $|z|$, since it follows from Eq. (4) that

$$|z| < |b_2|/(1 + |b_2|).$$

Therefore, Eq. (16) will be accepted as a restriction of $|b_2|$, since it is the more stringent of the two possible bounds. Thus, only

$$|z| < \tfrac{1}{2} - 6^{-\frac{1}{2}} \tag{17}$$

shall be considered.

The negative property of Eq. (12) requires that any path which crosses the real axis must be such that $\operatorname{Re} f(\theta)$ decreases as the path goes from the lower to the upper half-plane. In particular, any path of constant imaginary part which passes through a saddle point with $\theta_i > 0$, and which crosses the real axis, must be a path of steepest ascent from the saddle point. Therefore, any path of steepest descent from a saddle point with $\theta_i > 0$ must lie wholly within the upper half-plane. From Eq. (11), as $\theta_i \to +\infty$,

$$\operatorname{Re} f(\theta) \to \infty, \qquad \beta_2 \cos 2\theta_r + \gamma_2 \sin 2\theta_r < 0$$

$$\operatorname{Re} f(\theta) \to -\infty, \qquad \beta_2 \cos 2\theta_r + \gamma_2 \sin 2\theta_r > 0.$$

Since the trigonometric functions of argument $2\theta_r$ possess two separated regions in an interval of length 2π where they take on a given sign, then these relations state that there will be two regions in θ_r where $\operatorname{Re} f(\theta) \to \infty$, separated by two regions where $\operatorname{Re} f(\theta) \to -\infty$. The curve of steepest descent from one of the saddle points in the upper half-plane must then go from one region where $\operatorname{Re} f(\theta) \to -\infty$ at $\theta_i \to \infty$, through the saddle point, to the other

region where Re $f(\theta) \to -\infty$ at $\theta_i \to \infty$, thus enclosing one of the regions where Re $f(\theta) \to \infty$. Hence, one branch of the path of steepest ascent from this same saddle point can ascend between the two branches of the path of steepest descent to the region at $\theta_i \to \infty$ where Re $f(\theta) \to \infty$; but the other branch of this path of steepest ascent is excluded from reaching any other such region in the upper half-plane, because both these regions are enclosed by paths of steepest descent which cannot be crossed. Hence, the second branch of the path of steepest ascent must cross the real axis into the lower half-plane.

All the comments above which refer to paths of steepest descent (or ascent) from saddle points in the upper half-plane, apply as well to paths of steepest ascent (or descent) from saddle points in the lower half-plane. The geometry of these paths may be clarified by Fig. 1, where the particular location of the saddle points is not of significance, but the qualitative behavior of the paths through the saddle points is the feature of interest. It can be shown that any one complete path of steepest descent in the upper half-plane can have no more than two intersections with a line of constant θ_i. To show this, note first that the imaginary part of $f(\theta)$ is

$$\text{Im } f(\theta) = \beta_1 \sin \theta_r \cosh \theta_i - \gamma_1 \cos \theta_r \sinh \theta_i + \tfrac{1}{2}\beta_2 \sin 2\theta_r \cosh 2\theta_i - \tfrac{1}{2}\gamma_2 \cos 2\theta_r \sinh 2\theta_i + \theta_r$$

so that, for constant θ_i, the partial derivative with respect to θ_r of Im $f(\theta)$ has the form

$$(\partial/\partial\theta_r) \text{ Im } f(\theta) = a_1 \sin \theta_r + a_2 \cos \theta_r + a_3 \sin 2\theta_r + a_4 \cos 2\theta_r + a_5. \tag{18}$$

This is equivalent to the expression

$$(\partial/\partial\theta_r) \text{ Im } f(\theta) = e^{-2i\theta_r} G(e^{i\theta_r}), \tag{19}$$

where $G(\exp i\theta_r)$ is a polynomial of fourth degree in $\exp i\theta_r$. Equation (19) can vanish only when G does, which will happen for at most four values in the interval $0 \leq \theta_r < 2\pi$. Thus Im $f(\theta)$ can have no more than four extrema as a function of θ_r in $0 \leq \theta_r < 2\pi$. Since Im $f(\theta)$ is continuous in θ_r, it can therefore take on any particular value at most at only four points in $0 \leq \theta_r < 2\pi$. For any constant θ_i which is greater than the lowest point on a curve of steepest descent from a saddle point in the upper half-plane, the curve of steepest descent will cross the line of constant θ_i at least twice. Since the curve of steepest ascent from the same saddle point goes from $\theta_i = +\infty$ to $\theta_i = -\infty$, it must cross the same line of constant θ_i at least once. Hence, the line of constant θ_i is crossed at least three times by curves along which Im $f(\theta)$ has the same saddle point value. If, however, one of the lines of constant Im $f(\theta)$ should oscillate with θ_r, and loop back across the line of constant θ_i, then five crossings would occur by curves with the same value of Im $f(\theta)$. This is impossible, so the paths of steepest descent from the saddle points in the upper half-plane cannot oscillate, but must increase monotonically towards $\theta_i \to \infty$ as θ_r departs from the location of the minimum in the steepest descent curve.

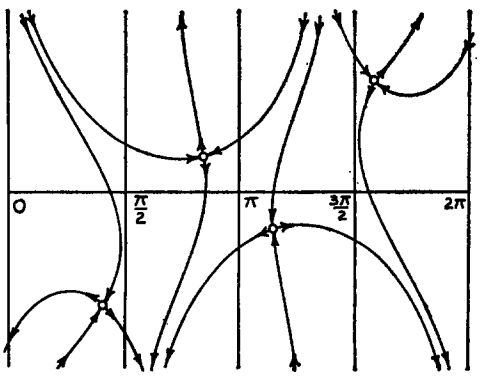

FIG. 1. Geometry of the saddle points and paths of steepest ascent and descent from them. Small circles show the saddle-point locations. Arrows on the curves indicate the direction of increasing Re $f(\theta)$.

It has now been shown that there are two saddle points in the upper half-plane; that the paths of steepest descent from these saddle points are wholly contained in the upper half plane; and that these paths cannot oscillate across a line of constant θ_i. Consequently, sufficient information is at hand to make plausible the specific choice of a path of integration in the complex θ plane. This path is to be such that the largest value of Re $f(\theta)$ which occurs along it is to occur at a saddle point, and the total length of the path is to be finite. A path with these properties can be constructed from a combination of the paths of steepest descent from the saddle points and a line of constant θ_i, which θ_i is to coincide with the larger of the θ_i coordinates of the two saddle points in the upper half plane. With reference to Fig. 2, starting at the lower-lying saddle point, the path of steepest descent is followed to the point at the intersection of this path with the line of constant θ_i, then the line of constant θ_i is followed to the second saddle point, the path of steepest descent followed to its intersection with the line of constant θ_i, and the line of constant

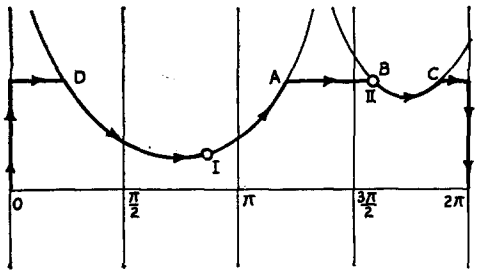

FIG. 2. Path of integration in the complex θ plane. Circles labeled I and II mark the saddle point locations. Heavy arrowed lines show the path of integration.

θ_i followed to the path of steepest descent from the first saddle point, which is followed to the saddle point itself. The language of this description takes tacit cognizance of the periodicity of the I_0 (and I_1) integrands, so that the lines $\theta = 0$ and $\theta = 2\pi$ are viewed as being identical. In terms of the labeling of Fig. 2, the path of integration is to be I to A to II (or B) to C to D to I, with an obvious modification if the second saddle point should be at C rather than where shown. A link with the original path of integration may be established by a line from the origin along $\theta = 0$ to the new path, and another line along $\theta = 2\pi$ from the new path to $\theta_i = 0$. Contributions to the integral from these additions to the path will cancel because of the periodicity of the integrand.

To find how Re $f(\theta)$ varies along the path, note that $(\partial/\partial\theta_r)$ Re $f(\theta)$ for constant θ_i gives an expression identical in form to Eq. (18). Hence there are no more than four extrema in $(\partial/\partial\theta_r)$ Re $f(\theta)$ for constant θ_i. Consider $\theta_i = \theta_{im} + \Delta$, where θ_{im} is the θ_i coordinate of saddle point II in Fig. 2, and Δ represents a small upward displacement. Take the points A through D in Fig. 2 to be at $\theta_i = \theta_{im} + \Delta$, so that II and B are no longer coincident. There must be a maximum with respect to θ_r in Re $f(\theta)$ between D and A, and another between B and C. Because of the limitation to four extrema at constant θ_i, no more than these two maxima can occur. In particular, since there can be no maximum between A and B, the highest point in terms of Re $f(\theta)$ on the path segment AB is at either A or B, and this highest point is of necessity smaller than the larger of the two saddle-point values. This conclusion is true for any $\Delta > 0$, so from the continuity of $f(\theta)$ it remains true when $\Delta \to 0$. Similar considerations apply to the path segment CD, so it must be true that

$$|e^{\alpha f(\theta)}| \leq |e^{\alpha f(\theta_{sp})}|$$

along the entire path, where θ_{sp} denotes that saddle point in the upper half-plane which has the larger value of Re $f(\theta)$.

The total path length involved can be bounded by observing that the paths of steepest descent cannot cross the real axis, and θ_i must therefore decrease by less than θ_{im} in going from $\theta_i = \theta_{im}$ to the lowest point on the steepest descent curve. The path length would then be bounded by $2\pi + 4\theta_{im}$ except for one possible complication. Although it was shown that a path of steepest descent cannot oscillate across a line of constant θ_i, similar considerations show that there can be one such oscillation across a line of constant θ_r. Thus, to account for this possibility, the path length is bounded by $6\pi + 4\theta_{im}$.

It now remains to place a bound on Re $f(\theta_{sp})$. From the definition of $f(\theta)$, Eq. (8),

$$\text{Re } f(\theta_{sp}) = -\text{Im } (b_1 \sin \theta_{sp}) - \text{Im } (\tfrac{1}{2} b_2 \sin 2\theta_{sp}) - \theta_{i sp}.$$

A upper bound on this is given by

$$\text{Re } f(\theta_{sp}) < |b_1 \sin \theta_{sp}| + |\tfrac{1}{2} b_2 \sin 2\theta_{sp}| - \theta_{i sp}. \tag{20}$$

The first two terms in Eq. (20) are most readily investigated in terms of their squares. It is most convenient to start with the second term, and to regard its square as a product of $|b_2 \cos^2 \theta_{sp}|$ and $|b_2 \sin^2 \theta_{sp}|$.

From Eqs. (4) and (10), it follows that

$$|b_2 \cos^2 \theta_{sp}| \leq \tfrac{1}{2} |\alpha\lambda + 1 + z|^{-1} [|\alpha\lambda \cos 2\nu + 1| + 2 \sin \nu \, |(\alpha\lambda)^{\frac{1}{2}}(\alpha\lambda \cos^2 \nu + 1)^{\frac{1}{2}}|]. \tag{21}$$

With the notation

$$\bar{\alpha} = qw - 1 + |z|$$

then $|\alpha| \leq \bar{\alpha}$, and

$$|\alpha\lambda \cos 2\nu + 1| \leq \bar{\alpha}\lambda \, |\cos 2\nu| + 1$$

$$|(\alpha\lambda)^{\frac{1}{2}}(\alpha\lambda \cos^2 \nu + 1)^{\frac{1}{2}}| \leq (\bar{\alpha}\lambda)^{\frac{1}{2}}(\bar{\alpha}\lambda \cos^2 \nu + 1)^{\frac{1}{2}}$$

$$|\alpha\lambda + 1 + z| \geq \bar{\alpha}\lambda + 1 - |z|.$$

Thus Eq. (21) can be rewritten

$$|b_2 \cos^2 \theta_{sp}| \leq \tfrac{1}{2}(\bar{\alpha}\lambda + 1 - |z|)^{-1}[\bar{\alpha}\lambda \, |\cos 2\nu| + 1 + 2 \sin \nu (\bar{\alpha}\lambda)^{\frac{1}{2}}(\bar{\alpha}\lambda \cos^2 \nu + 1)^{\frac{1}{2}}]. \tag{22}$$

Viewed as a function of ν, the numerator on the right-hand side of Eq. (22) has extrema when

$$\nu = \tfrac{1}{2}\pi, \qquad \bar{\alpha}\lambda \cos 2\nu + 1 = \pm 2^{-\frac{1}{2}}(\bar{\alpha}\lambda + 1),$$

where the ambiguous sign is given by the sign of $\cos 2\nu$. These extrema give the values

$$[(\bar{\alpha}\lambda)^{\frac{1}{2}} + 1]^2, \qquad 2^{\frac{1}{2}}(\bar{\alpha}\lambda + 1), \qquad 2 + 2^{\frac{1}{2}}(\bar{\alpha}\lambda + 1)$$

for the square bracket in Eq. (22). Since the last value is the largest of the three for all values of $\bar{\alpha}\lambda$, it is always true that

$$|b_2 \cos^2 \theta_{sp}| \leq (\bar{\alpha}\lambda + 1 - |z|)^{-1}[1 + 2^{-\frac{1}{2}}(\bar{\alpha}\lambda + 1)]. \quad (23)$$

As a function of λ, Eq. (23) attains its maximum value when $\lambda = 0$. Then

$$|b_2 \cos^2 \theta_{sp}| \leq (1 - |z|)^{-1}(1 + 2^{-\frac{1}{2}}) \quad (24)$$

represents a bound which is a function of $|z|$ only. The denominator in Eq. (24) is always positive in view of the restriction imposed by Eq. (17).

Starting from

$$|b_2 \sin^2 \theta_{sp}| \leq \tfrac{1}{2} |\alpha\lambda + 1 + z|^{-1} [|\alpha\lambda \cos 2\nu + 1 + 2z| + 2 \sin \nu |(\alpha\lambda)^{\frac{1}{2}}(\alpha\lambda \cos^2 \nu + 1)^{\frac{1}{2}}|],$$

It follows in the same way as above that

$$|b_2 \sin^2 \theta_{sp}| \leq (1 - |z|)^{-1}(1 + 2^{-\frac{1}{2}} + |z|). \quad (25)$$

The first term on the right-hand side in Eq. (20) can be bounded in terms of Eq. (25) by use of Eq. (15), since then,

$$|b_1^2 \sin^2 \theta_{sp}| < 8 |b_2 \sin^2 \theta_{sp}|. \quad (26)$$

Since the saddle points through which the path of integration is taken lie above the real axis, then the third term in Eq. (20) will subtract from the contribution of the first two terms, and an upper bound on Re $f(\theta_{sp})$ follows from taking a lower bound for θ_{isp}. If $\cos \theta$ is written in terms of its real and imaginary parts,

$$\text{Re} \cos \theta = \cos \theta_r \cosh \theta_i$$
$$\text{Im} \cos \theta = -\sin \theta_r \sinh \theta_i,$$

a straightforward derivation leads to

$$\cosh 2\theta_i = |\cos \theta|^2 \pm [|\cos \theta|^4 - 2 \text{Re} (\cos^2 \theta) + 1]^{\frac{1}{2}}. \quad (27)$$

Since

$$|\cos^2 \theta| \geq |\text{Re} (\cos^2 \theta)|,$$

then

$$[|\cos^2 \theta|^2 - 2 \text{Re} (\cos^2 \theta) + 1]^{\frac{1}{2}} \geq [(|\cos^2 \theta| - 1)^2]^{\frac{1}{2}}.$$

It will appear below that $|\cos \theta| \geq 1$. This removes the sign ambiguity in Eq. (27), and gives

$$\cosh 2\theta_i \geq 2 |\cos^2 \theta| - 1. \quad (28)$$

To place a lower bound on $|\cos \theta|$ at the saddle points, it is convenient to write $\cos \theta_{sp}$ from Eq. (10) as

$$\cos \theta_{sp} = (2z)^{-\frac{1}{2}}(-A \pm iB). \quad (29)$$

Then it follows that

$$|\cos^2 \theta_{sp}| = (2 |z|)^{-1}[AA^* + BB^* \pm 2 \text{Im} (A^*B)]. \quad (30)$$

From the definitions of A and B as given by Eqs. (29) and (10), it is readily shown that

$$AA^* \geq \bar{\alpha}\lambda \sin^2 \nu$$

and

$$BB^* \geq \bar{\alpha}\lambda \cos^2 \nu + 1,$$

so that

$$AA^* + BB^* \geq \bar{\alpha}\lambda + 1. \quad (31)$$

To place a bound on Im (A^*B), where

$$A^*B = \lambda^{\frac{1}{2}} \sin \nu [|\alpha| \lambda \cos^2 \nu + \alpha^*]^{\frac{1}{2}}, \quad (32)$$

it may be observed that, in general,

$$\text{Im} (u^{\frac{1}{2}}) = 2^{-\frac{1}{2}}[|u| - \text{Re} (u)]^{\frac{1}{2}} < 2^{-\frac{1}{2}} |\text{Im} (u)|^{\frac{1}{2}},$$

when Re $(u) > 0$. Within the bounds already imposed on $|z|$, it is possible to make Re $(A^*B) > 0$ by just choosing q large enough. Thus, from Eq. (32),

$$\text{Im} (A^*B) < 2^{-\frac{1}{2}}\lambda^{\frac{1}{2}} \sin \nu \, |\text{Im} (z)|^{\frac{1}{2}}.$$

This, in turn, may be replaced by

$$\text{Im} (A^*B) < (\lambda |z|/2)^{\frac{1}{2}}.$$

When this result is combined with Eq. (31), and inserted into Eq. (30), then

$$|\cos^2 \theta_{sp}| > (2 |z|)^{-1}[\bar{\alpha}\lambda + 1 - (2\lambda |z|)^{\frac{1}{2}}]. \quad (33)$$

As a function of λ, the right-hand side of Eq. (33) achieves a minimum when

$$\lambda^{\frac{1}{2}} = \bar{\alpha}^{-1}(|z|/2)^{\frac{1}{2}},$$

so that

$$|\cos^2 \theta_{sp}| > (2 |z|)^{-1}(1 - |z|/2\bar{\alpha}). \quad (34)$$

With the upper bound on $|z|$ as dictated by Eq. (17), Eq. (34) requires that $|\cos \theta_{sp}| > 1$, which justifies Eq. (28). The bound given by Eq. (34) now establishes a lower bound on θ_{isp} from Eq. (28) as

$$\theta_{isp} > \tfrac{1}{2} \text{arccosh} [|z|^{-1} - 1 - (2\bar{\alpha})^{-1}]. \quad (35)$$

Finally, Eq. (20) can be restated in terms of $|z|$. By combining Eqs. (24)–(26) and (35), the result is obtained that

$$\text{Re } f(\theta_{sp}) < (1 - |z|)^{-\frac{1}{2}}(1 + 2^{-\frac{1}{2}} + |z|)^{\frac{1}{2}} \cdot [8^{\frac{1}{2}} + (1 - |z|)^{-\frac{1}{2}}(1 + 2^{-\frac{1}{2}})^{\frac{1}{2}}] - \tfrac{1}{2} \text{arccosh} (|z|^{-1} - 1). \quad (36)$$

The $(2\bar{\alpha})^{-1}$ term in the argument of the inverse hyperbolic function in Eq. (35) has been omitted in Eq. (36) in view of its vanishing significance for large q. The result thus obtained is dependent on $|z|$ alone. The aim of this part of the investigation

has been to find the conditions under which Re $f(\theta_{sp}) < 0$. The right-hand side of Eq. (36) is equal to zero for

$$|z| < 4 \times 10^{-5} \tag{37}$$

and hence Re $f(\theta_{sp}) < 0$ for values of $|z|$ less than this limit.

It is now possible to express the result for the bound on I_0.

$$|I_0| < (6\pi + 4\theta_{im})e^{-qK}, \tag{38}$$

where K is found from Eq. (36), and can be taken to be positive. To show that θ_{im} in Eq. (38) causes no difficulty, rewrite e^{-qK} as

$$e^{-qK} \geq e^{-(q-1)K} \times \exp\left[\mathrm{Re}\,(ib_1 \sin\theta + i\tfrac{1}{2}b_2 \sin 2\theta) - \theta_{isp}\right].$$

Suppose that the maximum value of Re $f(\theta_{sp})$ occurs for the saddle point at $\theta_{isp} = \theta_{im}$ (i.e., at saddle point II in Fig. 2). Then

$$\theta_{im} \exp\left[\mathrm{Re}\,(ib_1 \sin\theta_{sp} + i\tfrac{1}{2}b_2 \sin 2\theta_{sp}) - \theta_{isp}\right] = e^{K'}\theta_{im}e^{-\theta_{im}}$$

where K' is known to be bounded by a finite constant, and $\theta_{im}e^{-\theta_{im}} \leq 1/e$. If the maximum value of Re $f(\theta_{sp})$ occurs at the saddle point where $\theta_{isp} < \theta_{im}$ (i.e., at saddle point I in Fig. 2), then since the preceding work has shown that Re $f(\theta_{sp})$ is bounded by Eq. (36) for both saddle points, the difference between Re $f(\theta_{sp})$ at each of the saddle points is certainly bounded, and

$$\theta_{im} \exp\left[\mathrm{Re}\,(ib_1 \sin\theta_{sp} + i\tfrac{1}{2}b_2 \sin 2\theta_{sp}) - \theta_{isp}\right] < e^{K}e^{K'}\theta_{im}e^{-\theta_{im}}.$$

Since

$$6\pi e^{-K} < 6\pi < e^{K'+1}, \qquad 4\theta_{im}e^{-K} < 4e^{K'+1}$$

then

$$|I_0| < 5e^{K'+1}e^{-(q-1)K} = 5e^{K'+K+1}e^{-qK}, \tag{39}$$

where K is the negative of the right-hand side of Eq. (36), and

$$K' = -K + \tfrac{1}{2}\,\mathrm{arccosh}\,(|z|^{-1} - 1).$$

An upper bound, Eq. (38), has now been determined for I_0. This bound was established by the selection of a suitable contour passing through two of the saddle points possessed by the exponential function in the integrand of I_0. Now that a bound is known for $|I_0|$ a bound for $|I_1|$ is directly implied, though it is more convenient to treat I_1 in combination with the factors with which it is associated in I_{11}^2. I_0^2 occurs in Eq. (1) multiplied by a factor $\alpha\lambda \cos^2 \nu/qw$. Because this factor is bounded,

$$|\alpha\lambda \cos^2 \nu|/qw \leq \bar{\alpha}\lambda \cos^2 \nu/qw < 1,$$

then the total contribution of the I_0^2 term after the double integration over λ and ν is performed, is bounded by $\pi/2$ times the square of Eq. (39). The I_{11}^2 term in Eq. (1) occurs with the factor b_2. From the definition of I_{11}^2 given in Eq. (3), and after I_2 has been eliminated in favor of I_0 and I_1 through an integration by parts, it then follows that

$$|b_2 I_{11}^2| \leq |1 - b_2|\,|I_0^2| + |b_1|\,|I_0|\,|I_1| + 2\,|b_2|\,|I_1^2|. \tag{40}$$

For the first term

$$|1 - b_2| \leq (\bar{\alpha}\lambda + 1)/(\bar{\alpha}\lambda + 1 - |z|) \leq (1 - |z|)^{-1}. \tag{41}$$

Since I_1 differs from I_0 only in that an additional $\cos\theta$ term appears in the integrand, an upper bound for I_1 may be arrived at by multiplying I_0 by the maximum value which $\cos\theta$ can attain along the path of integration. Thus, the third term in Eq. (40) requires that a bound be placed on $|b_2||\cos\theta|^2$. In general,

$$|\cos\theta| \leq |\cos\theta_r \cosh\theta_i| + |\sin\theta_r \sinh\theta_i| < 2\cosh\theta_i.$$

The maximum θ_i encountered along the integration path is θ_{im}, which corresponds to one of the saddle points. Hence

$$|\cos\theta|^2 < 2\{1 + |\cos\theta_{sp}|^2 + [1 + |\cos\theta_{sp}|^2 - (2\,\mathrm{Re}\cos\theta_{sp})^2]^{\frac{1}{2}}\} < 4(1 + |\cos\theta_{sp}|^2).$$

However, it has already been shown [Eq. (24)] that

$$|b_2|\,|\cos^2\theta_{sp}| \leq (1 - |z|)^{-1}(1 + 2^{-\frac{1}{2}}).$$

Also, in view of Eq. (16), an upper bound δ can be imposed on $|b_2|$. This bound δ must be such that $\delta \leq 5 - 2 \times 6^{1/2}$, but $\delta > |z|\,(1 - |z|)^{-1}$ to be consistent with $|z| < |b_2|\,(1 + |b_2|)^{-1}$. Hence,

$$|b_2|\,|\cos\theta|^2 < 4\,\delta + 4(1 - |z|)^{-1}(1 + 2^{-\frac{1}{2}}). \tag{42}$$

Then an upper bound is established for the second term in Eq. (40), since

$$|b_1|^2\,|\cos\theta|^2 < 8\,|b_2|\,|\cos\theta|^2. \tag{43}$$

Finally, then, $|b_2 I_{11}^2|$ is bounded in terms of $|I_0^2|$ by

$$|b_2 I_{11}^2| < C'\,|I_0^2|, \tag{44}$$

where C' is a constant resulting from the use of Eqs. (41)–(43) in Eq. (40). The end result of integrating over λ and ν is to multiply Eq. (44) by π.

From Eq. (1), the q sum contains a factor $(\alpha qw)^{1/2}$ multiplying the double integral over λ and ν. Thus, with

$$|\alpha^{\frac{1}{2}}| \leq \bar{\alpha}^{\frac{1}{2}} < (qw)^{\frac{1}{2}}$$

$$|(\alpha qw)^{\frac{1}{2}}| < qw,$$

if the general term of the q sum is written as $F_q(z)$, it has now been shown that

$$|F_q(z)| < Cqe^{-(q-1)2K},$$

where C is a constant. The exponent K is known to be positive for sufficiently small $|z|$. Specifically, since the bound on $|z|$ given by Eq. (37) is less than the upper bound imposed on $|z|$ by Eq. (17), then positive real constants Z and K_0 can be defined such that $Z < 4 \times 10^{-5}$ and K_0 is twice the negative of the right-hand side of Eq. (36) with Z substituted for $|z|$, whereby

$$|F_q(z)| < Cqe^{-(q-1)K_0} \tag{45}$$

for all $|z| \leq Z$.

The total transition probability W, Eq. (1), is given by a constant times a sum over q. Each term $F_q(z)$ in the series is an analytic function of z in the region given in Eq. (5), excluding the negative real axis from -1 to $-\infty$. Since the $F_q(z)$ are uniformly bounded as shown in Eq. (45), and the sum of these uniform bounds converges, then the sum over q is an analytic function of z in the region $|z| \leq Z_0$, where $Z_0 \leq Z$ and $Z_0 < w[1/w] - 1$. W is thus an analytic function of z in $|z| \leq Z_0$, and therefore possesses a convergent power series expansion in z in this region.

CONCLUSIONS

It has been demonstrated that a real physical problem in electrodynamics exists which has a convergent expansion in powers of the electromagnetic coupling constant. This demonstration is for the case of a non-second-quantized theory. Two limitations are imposed upon the radius of convergence. One limitation [Eq. (5)] is in terms of the energies of the two plane-wave fields in the problem, and goes to zero for a discrete set of values of the field energies. The other limitation [Eq. (37)], is given as a numerical upper bound on the radius of convergence. This upper bound, however, is not a least upper bound, but it depends on the details of the bounding procedure. The significant result is that there is a nonzero radius of convergence for the perturbation expansion.

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Green's Distributions and the Cauchy Problem for the Iterated Klein-Gordon Operator

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An explicit form of the homogeneous Green's function for the multi-dimensional iterated Klein-Gordon operator is obtained. By a direct calculation from its Fourier representation, the Green's function is expressed as a one-dimensional, infinite integral of the Sonine type. Although this integral is classically divergent when the order of the operator is less than the number of space dimensions, it can be treated rigorously under these conditions using the concepts of distribution analysis. A generalized Sonine integral is developed and the result applied to obtaining an explicit expression for the Green's function, which is now to be regarded as a distribution in the sense of Schwartz. Using a distribution introduced for this purpose, the Green's function is written in a form which explicitly displays its singularities on the light cone. The well-known difference between even- and odd-dimensional spaces is reflected in the nature of these singularities. The singularities appearing for an odd number of space dimensions consist of a finite linear combination of derivatives of the Dirac delta function $\delta(s^2)$ where s is the space-time distance. The highest derivative appearing is of order $\frac{1}{2}(n - 2l - 1)$ with n giving the number of space dimensions and $2l$ giving the order of the operator. The singular part for even-dimensional spaces consists of a polynomial in $1/s$ of degree $n - 2l + 1$. No singularities appear when the order of the operator is greater than the number of dimensions. The general solution of Cauchy's problem for the iterated Klein-Gordon operator is obtained in convolution form. An explicit solution for the ordinary Klein-Gordon equation is presented in a form which exhibits separately the contributions due to the singular part and the regular part of the Green's function.

1. INTRODUCTION

THE problem of Cauchy for the Klein-Gordon equation

$$(\Box + \mu^2)\varphi(x) = 0 \tag{1}$$

in multi-dimensional spaces has been studied extensively.[1-4] The field is uniquely determined by the differential equation for all space-time if it is known on a space-like surface along with its first derivative normal to the surface. For convenience, we choose the space-like manifold to be the plane of zero time. The Cauchy initial value problem then consists of finding a unique solution $\varphi(x)$ in terms of φ and $\partial\varphi/\partial t$ taken at time $t = 0$.

The available methods of solving the Cauchy problem all lead to integral representations of $\varphi(x)$ which must be given some generalized interpretation. Explicit expressions for the general solution in terms of ordinary integrals and functions are obtained only by means of special techniques. Hadamard[2] for example, introduced the concept of "finite part" of an improper integral. In the case of even-dimensional spaces he obtained directly an explicit solution, while in the case of odd-dimensional spaces he was forced to use the more indirect "method of descent."

Riesz[3] has developed a theory of fractional integrals of functions of several variables and applied this theory to the solution of the Cauchy problem. He introduces multi-dimensional integrals of the Riemann-Liouville type whose kernels are modified elementary solutions or "Riesz potentials"[4] depending on a complex parameter. Using Green's identity, the soultion of the Cauchy problem is obtained by analytic continuation with respect to the parameter. The cases of even- and odd-dimensional spaces are treated on an equal footing, although after the analytic continuation is carried out, quite different formulas are obtained for the two cases.

In modern field theory the method of Fourier integrals is widely used, chiefly because of the direct physical interpretation of the Fourier transform in momentum space. The general solution for the field $\varphi(x)$ can be expressed, in terms of the Cauchy data, as convolutions generated by the propagator or homogeneous Green's function $\Delta(x)$. However, due to the singular character of the Green's function, some generalized interpretation must be given to $\Delta(x)$. Such an interpretation is of course available in the theory of distributions developed by Schwartz.[5]

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[1] R. Courant and D. Hilbert, *Methoden der Mathematischen Physik* (Springer-Verlag, Berlin, Germany, 1937), Band I, II.

[2] J. Hadamard, *Lectures on Cauchy's Problem in Linear Partial Differential Equations* (Yale University Press, New Haven, Connecticut, 1923).

[3] M. Riesz, Acta Math. **81**, 1 (1949).

[4] N. E. Fremberg, Comm. Sem. Math. Univ. Lund, **7** (1946).

[5] L. Schwartz, *Theorie des distributions*, (Hermann & Cie, Paris, France, 1950-51), Vols. I and II.

In this paper we consider the Cauchy problem for the iterated Klein-Gordon equation

$$(\Box + \mu^2)^l \varphi(x) = 0 \tag{2}$$

in multi-dimensional spaces and its associated homogeneous Green's function $\Delta_{n,l}(x)$. The d'Alembert operator $\Box$ is taken in the form

$$\Box = \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x_1^2} - \cdots - \frac{\partial^2}{\partial x_n^2}, \tag{3}$$

where n gives the number of space dimensions, and l is to be considered a positive integer. Since the wave equation (2) is of order $2l$, the Cauchy data now consist of $\partial^i \varphi / \partial t^i$ taken at zero time for all $= 0, 1, \cdots, 2l - 1$.

The Green's function is determined from its Fourier representation. After some angular integrations, $\Delta_{n,l}(x)$ is expressed (cf. Sec. 2) as a one-dimensional, infinite integral of the type investigated by Sonine.[6] Using Sonine's result, it is shown that this integral is divergent when the order of Eq. (2) is less than the number of space dimensions. It becomes apparent, then, that the Green's function cannot be considered a function in the ordinary sense for general values of n and l. As is well known, such singular functions occurring in physics can be treated rigorously only in connection with the concepts of distribution analysis.

We therefore show (cf. Sec. 3) how the Sonine integral can be generalized by defining it as a distribution in the sense of Schwartz. The Green's function may then be evaluated directly from its Fourier representation and explicit expressions (cf. Sec. 4) obtained for general n and l. Of course the Green's function itself is now to be regarded as a (tempered) distribution. This treatment involves the introduction of a distribution (cf. Sec. 3) whose properties are particularly convenient when investigating the singularities of the Green's function.

Various properties of the Green's function are presented in Sec. 4. The Green's function is written in a form which explicitly displays its singularities on the light cone. The remarkable contrast between spaces with an even and an odd number of dimensions is reflected in the nature of these singularities. For odd-dimensional spaces the singular part consists of a finite linear combination of derivatives of the Dirac delta function $\delta(s^2)$ where

$$s = (t^2 - x_1^2 - \cdots - x_n^2)^{1/2}$$

is the space-time distance. The highest derivative appearing in the linear combination is of order $\frac{1}{2}(n - 2l - 1)$. The singular part for spaces with an even number of dimensions, on the other hand, consists of a polynomial in $1/s$ of degree $n - 2l + 1$. In both cases, no singularities occur when the order of the differential equation is greater than the number of space dimensions. A number of interesting recurrence relations for the Green's function are also presented.

A complete set of homogeneous Δ-function solutions is required for constructing the field $\varphi(x)$ described by (2). Such a set of independent Δ-functions evidently consists of $\Delta_{n,p}(x)$ with $p = 1, 2, \cdots, l$. After investigating the initial conditions satisfied by these Green's functions at zero time, the general solution of the Cauchy problem for the iterated Klein-Gordon equation (2) is presented in convolution form (cf. Sec. 5). Since the Green's functions are distributions, this integral representation of $\varphi(x)$ may be expressed in terms of ordinary integrals and functions by means of the calculus of distributions. Further, Schwartz[5] has shown how the notion of convolution product can be extended to the convolution product of two distributions (when at least one of them has a bounded supporting set). Thus the field $\varphi(x)$ is interpreted as a distribution when the Cauchy data are themselves distributions instead of well-behaved functions.

It is interesting to carry out the convolution operation directly to obtain the explicit solution of the Cauchy problem for the Klein-Gordon equation (1). This is done in Sec. 6 where the general solution is obtained in a form which exhibits the contributions due to the singular part and the regular part of the Green's function. The explicit solution for the d'Alembert equation $\Box\varphi = 0$ is also given. Many of the expressions appearing here may be found scattered throughout the literature with varying degrees of generality.

2. THE GREEN'S FUNCTION

The Fourier representation of the homogeneous Green's function may clearly be written in the form

$$\Delta_{n,l}(x) = (2\pi)^{-n-1} \int \frac{e^{-ikx}\, dk}{(\mu^2 - k^2)^l}, \tag{4}$$

where

$$dk = dk_0\, dk_1 \cdots dk_n = dk_0\, d\mathbf{k},$$

$$kx = k_0 t - k_1 x_1 - \cdots - k_n x_n = k_0 t - \mathbf{k}\cdot\mathbf{x}.$$

[6] N. Sonine, Math. Ann. **16**, 1 (1880).

The integration in the k_0 plane is defined in the usual way[7]: It is to be carried out over a closed path C encircling both poles $k_0 = \pm(k^2 + \mu^2)^{1/2}$ in a clockwise direction. The variables $k_1, \cdots, k_n$ are then integrated from $-\infty$ to $+\infty$. The inhomogeneous Green's function $\bar{\Delta}_{n,l}(x)$ is obtained by taking the principal part of the k_0 integration over the singularities instead of integrating along the path C. The relation between the two Green's functions is given by the well-known formula

$$\Delta_{n,l}(x) = 2\epsilon(t)\,\bar{\Delta}_{n,l}(x), \tag{5}$$

where $\epsilon(t) = \text{sign}\,(t)$. From now on we will consider only the homogeneous Green's function since the inhomogeneous Green's function is easily obtained by means of (5).

The result of the k_0 integration over the path C in (4) is

$$\frac{1}{2\pi}\int_c \frac{e^{-ik_0 t}\,dk_0}{(\omega^2 - k_0^2)^l} = (\pi)^{\frac{1}{2}}\left(\frac{t}{2\omega}\right)^{l-\frac{1}{2}}\frac{J_{l-\frac{1}{2}}(\omega t)}{\Gamma(l)}, \tag{6}$$

where $\omega = (k^2 + \mu^2)^{1/2}$ and J is the Bessel function of the first kind [cf. Eq. (40)]. Introducing n-dimensional spherical coordinates in $\mathbf{k}$ space, we have

$$\Delta_{n,l} = \frac{\sigma_{n-1}(\pi)^{\frac{1}{2}}}{(2\pi)^n 2^{l-\frac{1}{2}}\Gamma(l)}\int_0^\infty \left(\frac{t}{\omega}\right)^{l-\frac{1}{2}} J_{l-\frac{1}{2}}(\omega t)k^{n-1}\,dk \times \int_0^\pi \sin^{n-2}\theta e^{ikr\cos\theta}\,d\theta, \tag{7}$$

where σ_n represents the surface area of the n-dimensional unit sphere,

$$\sigma_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}. \tag{8}$$

The integral over θ in (7) has the value[8]

$$(\pi)^{\frac{1}{2}}\Gamma\left(\frac{n-1}{2}\right)\left(\frac{kr}{2}\right)^{1-n/2} J_{n/2-1}(kr);$$

thus $\Delta_{n,l}$ may be written in the form

$$\Delta_{n,l} = \left(\frac{1}{2\pi}\right)^{(n-1)/2}\frac{\epsilon(t)}{2^l\Gamma(l)} \times \int_0^\infty \frac{J_{n/2-1}(kr)}{r^{n/2-1}}\left(\frac{|t|}{\omega}\right)^{l-\frac{1}{2}} J_{l-\frac{1}{2}}(\omega\,|t|)k^{n/2}\,dk. \tag{9}$$

The $\epsilon(t)$ appears because Eq. (6) represents a series of odd powers in time [cf. Eq. (64)].

The integral in (9) has the form of a Sonine integral,[8] namely,

$$\int_0^\infty \frac{J_\mu(bt)}{b^\mu}\frac{J_\nu[a(t^2+z^2)^{\frac{1}{2}}]}{(t^2+z^2)^{\nu/2}}\,a^\nu t^{\mu+1}\,dt = \begin{cases} 0, & a < b \\ [(a^2-b^2)^{\frac{1}{2}}/z]^{\nu-\mu-1}J_{\nu-\mu-1}[z(a^2-b^2)^{\frac{1}{2}}], & a > b, \end{cases} \tag{10}$$

where a and b are positive real numbers. To secure convergence, the restriction $\text{Re}\,\nu > \text{Re}\,\mu > -1$ is placed upon μ and ν. Using this result, one obtains (compare with Riesz[3] and Schwartz[5])

$$\Delta_{n,l} = \left(\frac{1}{2\pi}\right)^{(n-1)/2}\frac{\epsilon(t)h(s^2)}{2^l\Gamma(l)}\left(\frac{s}{\mu}\right)^{l-(n+1)/2} \times J_{l-(n+1)/2}(\mu s), \tag{11}$$

where $s = (t^2 - r^2)^{1/2}$ is the space-time distance and $h(a)$ is the Heaviside unit function: $h(a) = 1$ for $a > 0$ and $h(a) = 0$ for $a < 0$. The restriction for convergence becomes $2l > n - 1$. When this restriction is not obeyed, that is, when $2l < n$ (remembering that n and l are integers), the Sonine integral in Eq. (9) is divergent. It is clear, then, that the Green's function cannot be considered a function in the ordinary sense when the order of the differential equation is less than the number of space dimensions. For unrestricted values of the integers n and l the Fourier representation (4) must be given an extended interpretation. A natural interpretation from the standpoint of physics is provided by the theory of distributions.

3. SPECIAL DISTRIBUTIONS AND THE SONINE INTEGRAL

At first we summarize the basic definitions involved in distribution analysis; a detailed exposition is given by Schwartz.[5]

Briefly, distributions are continuous linear functionals on an appropriate topological vector space. Following Schwartz, we denote various spaces as follows:

(i) The space ($\mathfrak{D}$) consists of all (C^∞) functions on R^n with compact support.
(ii) The space of distributions ($\mathfrak{D}'$) is the dual of ($\mathfrak{D}$).
(iii) The space ($\mathfrak{S}$) consists of all (C^∞) functions on R^n that "decay rapidly at infinity."
(iv) The space of tempered distributions ($\mathfrak{S}'$) is the dual of ($\mathfrak{S}$).
(v) The space ($\mathfrak{D}_-$) is the space of all (C^∞) functions on R with support bounded on the

[7] W. E. Thirring, *Principles of Quantum Electrodynamics* (Academic Press Inc., New York, 1958).
[8] H. Bateman, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, II.

right, i.e., with support contained is some half-line $(-\infty, C)$.

(vi) The space of distributions with support bounded on the left $(\mathfrak{D}'_+)$ is the dual of $(\mathfrak{D}_-)$.

A distribution $\mathfrak{T}$ is defined as a continuous linear functional $\mathfrak{T}\{\phi\}$ on $(\mathfrak{D})$. However, such a functional representation can be avioded[9] and it is sometimes convenient to omit the symbol ϕ. Every summable point function $\mathfrak{T}(x)$ can be associated with the distribution $\mathfrak{T}\{\phi\}$ given by

$$\mathfrak{T}\{\phi\} = \int_{-\infty}^{\infty} \mathfrak{T}(x)\phi(x)\,dx. \tag{12}$$

In practice, the usefulness of distributions is often enhanced by associating a "generalized" function with each distribution; Eq. (12) is then interpreted symbolically. (For other definitions of distributions and generalized functions see Korevaar,[10] Temple,[11] and Lighthill.[12]) Distributions can be differentiated without restriction. In $(\mathfrak{D}')$ derivatives are defined by

$$\mathfrak{T}^{(n)}\{\phi\} \equiv (-)^n \mathfrak{T}\{\phi^{(n)}\}, \tag{13}$$

so that every derivative of a distribution is again a distribution. In $(\mathfrak{S}')$ the Fourier transformation can be defined by means of Parseval's formula, and the Fourier transform of each tempered distribution is again a tempered distribution.[5] The Laplace transformation[13] is defined for distributions in $(\mathfrak{D}'_+)$.

The present investigation is based on a distribution obtained from the expression[5]

$$\mathfrak{H}_\beta(x) = h(x)x^{\beta-1}/\Gamma(\beta), \tag{14}$$

where β is a complex parameter. The functional associated with $\mathfrak{H}_\beta(x)$, namely,

$$\mathfrak{H}_\beta\{\phi\} = \frac{1}{\Gamma(\beta)} \int_0^\infty x^{\beta-1}\phi(x)\,dx, \tag{15}$$

makes sense (classically) only for $\operatorname{Re}\beta > 0$. However, the definition of $\mathfrak{H}_\beta$ can be extended to the entire finite β plane by setting

$$\mathfrak{H}_\beta\{\phi\} \equiv (-)^n \mathfrak{H}_{\beta+n}\{\phi^{(n)}\}, \tag{16}$$

where n is an integer such that $\operatorname{Re}\beta + n > 0$.

When β is neither zero nor a negative integer, the definition (16) is equivalent to taking Hadamard's[2] "finite part" of the integral in (15). When β is zero, the Dirac distribution

$$\mathfrak{H}_0\{\phi\} = \delta\{\phi\} = \phi(0) \tag{17}$$

is obtained. Since derivatives are given by

$$\mathfrak{H}_\beta^{(n)} = \mathfrak{H}_{\beta-n}, \tag{18}$$

we also have, in terms of the Dirac distribution,

$$\mathfrak{H}_{-n}\{\phi\} = \delta^{(n)}\{\phi\} = (-)^n\phi^{(n)}(0). \tag{19}$$

The set of elements $\mathfrak{H}_\beta$ constitutes the group of the Riemann-Liouville integral with

$$\mathfrak{H}_\mu * \mathfrak{H}_\nu = \mathfrak{H}_{\mu+\nu}, \tag{20}$$

the * indicating convolution product. Equation (18) may easily be extended to include *fractional* derivatives.

The product $x^n\mathfrak{H}_\beta$ for $n = 0, 1, 2, \cdots$ is defined by the formula

$$x^n\mathfrak{H}_\beta = (\beta)_n\mathfrak{H}_{\beta+n}, \tag{21}$$

where

$$(\beta)_n = \beta(\beta+1)\cdots(\beta+n-1), \quad (\beta)_0 = 1. \tag{22}$$

Making use of this product, we introduce the distribution $\mathbf{\Omega}_\beta(\alpha;\lambda)$ as

$$\mathbf{\Omega}_\beta(\alpha;\lambda) = {}_1F_2(1;\alpha+1,\beta+1;\lambda x)\,\mathfrak{H}_{\beta+1}/\Gamma(\alpha+1), \tag{23}$$

where α, β, and λ are complex parameters. Extensive use will be made of $\mathbf{\Omega}_\beta(\alpha;\lambda)$.

The hypergeometric series ${}_1F_2$ is given by

$${}_1F_2(c;a,b;z) = \sum_{m=0}^{\infty} \frac{(c)_m z^m}{m!\,(a)_m(b)_m}. \tag{24}$$

Except for certain integer values of the parameters for which the series terminates or fails to make sense, ${}_1F_2$ converges for all finite z. Using (21) and (24) we have immediately the expansion

$$\mathbf{\Omega}_\beta(\alpha;\lambda) = \sum_{m=0}^{\infty} \frac{\lambda^m \mathfrak{H}_{\beta+m+1}}{\Gamma(\alpha+m+1)}, \tag{25}$$

and in view of (16) we may write

$$\mathbf{\Omega}_\beta\{\phi\} \equiv (-)^n\mathbf{\Omega}_{\beta+n}\{\phi^{(n)}\}, \tag{26}$$

where n is an integer such that $\operatorname{Re}\beta + n + 1 > 0$. Clearly this distribution is well defined for all complex α, β, and λ.

Derivatives of $\mathbf{\Omega}_\beta$ are given by

$$\mathbf{\Omega}_\beta^{(n)} = \mathbf{\Omega}_{\beta-n} \tag{27}$$

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[9] H. Kronig, Math. Nachr. **9**, 129 (1953).

[10] J. Korevaar, Ned. Akad. Wetensch. Proc. **A58** (1955) (4 papers).

[11] G. Temple, Proc. Roy. Soc. (London) **A228**, 175 (1955).

[12] M. J. Lighthill, *An Introduction to Fourier Analysis and Generalized Functions* (Cambridge University Press, New York, 1958).

[13] J. Lavoine, *Calcul symbolique* (Centre National de la Recherche Scientifique, Paris, France, 1959).

which of course may be extended to fractional derivatives. Further, Let ${}_{\alpha\beta}\mathfrak{d}$ be an operator defined by

$$ {}_{\alpha\beta}\mathfrak{d} = x\frac{d^2}{dx^2} + (1 + \alpha - \beta)\frac{d}{dx}. \tag{28}$$

We obtain, as easy consequences of (25),

$$ {}_{\alpha\beta}\mathfrak{d}^n\mathbf{\Omega}_\beta(\alpha;\lambda) = \mathbf{\Omega}_{\beta-n}(\alpha - n;\lambda), \tag{29}$$

$$ \mathbf{\Omega}_{\beta-n}(\alpha - n;\lambda) = \lambda^n\mathbf{\Omega}_\beta(\alpha;\lambda) + \sum_{m=0}^{\infty}\frac{\lambda^{n-m-1}\mathfrak{H}_{\beta-m}}{\Gamma(\alpha - m)}, \tag{30}$$

where n is a positive integer. Equation (30) leads to the differential equation of second order

$$ ({}_{\alpha\beta}\mathfrak{d} - \lambda)\mathbf{\Omega}_\beta(\alpha;\lambda) = \mathfrak{H}_\beta/\Gamma(\alpha), \tag{31}$$

from which the homogeneous equation of third order

$$ (x\,d/dx + 1 - \beta)({}_{\alpha\beta}\mathfrak{d} - \lambda)\mathbf{\Omega}_\beta(\alpha;\lambda) = 0 \tag{32}$$

is evident.

Using the Laplace transform[13] of $\mathfrak{H}_\beta$,

$$ \mathfrak{L}\{\mathfrak{H}_\beta\} = \mathfrak{H}_\beta\{e^{-zx}\} = z^{-\beta}, \tag{33}$$

the Laplace transform of $\mathbf{\Omega}_\beta(\alpha;\lambda)$ is obtained:

$$ \begin{aligned}\mathfrak{L}\{\mathbf{\Omega}_\beta(\alpha;\lambda)\} &= \sum_{m=0}^{\infty}\frac{\lambda^m z^{-\beta-m-1}}{\Gamma(\alpha + m + 1)} \\ &= \frac{\gamma(\alpha;\lambda/z)e^{\lambda/z}}{\Gamma(\alpha)\lambda^\alpha z^{\beta-\alpha+1}},\end{aligned} \tag{34}$$

where γ is the incomplete gamma function.[8] Equation (34) reduces to

$$ \mathfrak{L}\{\mathbf{\Omega}_\beta(0;\lambda)\} = z^{-\beta-1}e^{\lambda/z} \tag{35}$$

when $\alpha = 0$.

It will often be convenient to speak in terms of the *generalized function* $\Omega_\beta(\alpha;\lambda\colon x)$ generating the distribution $\mathbf{\Omega}_\beta(\alpha;\lambda)$. In this regard, several particular cases will be of importance and we list them here:

$$ \Omega_\beta(0;-\lambda\colon x) = h(x)(x/\lambda)^{\beta/2}J_\beta(2\lambda^{\frac{1}{2}}x^{\frac{1}{2}}), \tag{36}$$

$$ \Omega_0(\beta;-\lambda\colon x) = h(x)(\lambda x)^{-\beta/2}J_\beta(2\lambda^{\frac{1}{2}}x^{\frac{1}{2}}), \tag{37}$$

$$ \lambda^{\frac{1}{2}}\Omega_{\beta+\frac{1}{2}}(\tfrac{1}{2};-\lambda\colon x) = h(x)(x/\lambda)^{\beta/2}\mathbf{H}_\beta(2\lambda^{\frac{1}{2}}x^{\frac{1}{2}}), \tag{38}$$

$$ \lambda^{\frac{1}{2}}\Omega_{\frac{1}{2}}(\beta + \tfrac{1}{2};-\lambda\colon x) = h(x)(\lambda x)^{-\beta/2}\mathbf{H}_\beta(2\lambda^{\frac{1}{2}}x^{\frac{1}{2}}). \tag{39}$$

In these formulas, J_β is the Bessel function[8]

$$ J_\beta(z) = \sum_{m=0}^{\infty}\frac{(-)^m(z/2)^{2m+\beta}}{m!\,\Gamma(m + \beta + 1)}, \tag{40}$$

and $\mathbf{H}_\beta$ is the Struve function[8]

$$ \mathbf{H}_\beta(z) = \sum_{m=0}^{\infty}\frac{(-)^m(z/2)^{2m+\beta+1}}{\Gamma(m + \frac{3}{2})\Gamma(m + \beta + \frac{3}{2})}. \tag{41}$$

The boldface $\mathbf{H}$ is standard notation for the Struve function and should not be confused with the boldface type for distributions.

One of the chief services to mathematical physics rendered by the theory of distributions is the provision of a precise analytical method for removing the troublesome restrictions which abound in classical analysis. Ordinary functions are given extended ranges of validity and difficulties with regard to convergence of integrals disappear. We turn our attention in particular to an integral which is essentially the Sonine integral with a convenient change of integration variable. Once the Sonine integral is interpreted as a distribution, explicit expressions for the Green's function $\Delta_{n,l}$ are easily obtained.

In the notation of generalized functions we write

$$ \mathfrak{I} = \int_0^\infty \Omega_\beta(0;x - a\colon u)\Omega_\nu(0;\lambda - u\colon a)\,du, \tag{42}$$

where the real parameter a is taken to be positive. Using the inverse Laplace transform [cf. (35)] in place of the second function under the integral sign, we have

$$ \mathfrak{I} = \frac{1}{2\pi i}\int_0^\infty\int_{c-i\infty}^{c+i\infty}\Omega_\beta(0;x - a\colon u)z^{-\nu-1} \times \exp\left(za + \frac{\lambda - u}{z}\right)dz\,du \tag{43}$$

with $c > 0$. Upon interchanging the order of integration, one recognizes the integral over u as the Laplace transform (35) with z replaced by $1/z$, that is,

$$ \int_0^\infty \Omega_\beta(0;x - a\colon u)e^{-u/z}\,du = z^{\beta+1}e^{z(x-a)}. \tag{44}$$

What remains is

$$ \mathfrak{I} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} z^{\beta-\nu}\exp\left(zx + \frac{\lambda}{z}\right)dz = \Omega_{\nu-\beta-1}(0;\lambda\colon x); \tag{45}$$

thus, with β and ν unrestricted,

$$ \int_0^\infty \Omega_\beta(0;x - a\colon u)\Omega_\nu(0;\lambda - u\colon a)\,du = \Omega_{\nu-\beta-1}(0;\lambda\colon x). \tag{46}$$

The classical condition for convergence is $\mathrm{Re}\ \nu > \mathrm{Re}\ \beta > -1$; however, within the framework of distribution theory, (46) is valid for all β and ν, and the integral is to be regarded as a distribution. The

connection with the Sonine integral (10) is easily seen with the aid of (36).

4. DISCUSSION OF THE GREEN'S DISTRIBUTION

Making use of (36), we may write Eq. (9) in the form

$$\Delta_{n,l} = \frac{\epsilon(t)}{2^n\pi^{(n-1)/2}\Gamma(l)} \int_0^\infty \Omega_{n/2-1}(0; -r^2/4: u) \times \Omega_{l-\frac{1}{2}}(0; -\mu^2 - u: t^2/4)\, du, \tag{47}$$

which becomes, according to (46),

$$\Delta_{n,l}(x) = \frac{\epsilon(t)\Omega_{l-(n+1)/2}(0; -\mu^2: s^2/4)}{2^n\pi^{(n-1)/2}\Gamma(l)}. \tag{48}$$

The last expression is equivalent to (11) except the restriction on n and has now been removed.

The corresponding result for the iterated d'Alembert equation

$$\Box^l \varphi(x) = 0 \tag{49}$$

is obtained by letting $\mu \to 0$ in (48). The homogeneous Green's function $D_{n,l}$ for (49) is thus

$$D_{n,l}(x) = \frac{\epsilon(t)\mathfrak{H}_{(1-n)/2+l}(s^2/4)}{2^n\pi^{(n-1)/2}\Gamma(l)}. \tag{50}$$

The Green's functions $\Delta_{n,l}$ and $D_{n,l}$ are now regarded as tempered distributions.

Several recurrence relations for $\Delta_{n,l}$ are easily obtained. Recalling (27) we have immediately

$$\Delta_{n,l-m} = \frac{4^m\Gamma(l)}{\Gamma(l-m)}\left(\frac{d}{ds^2}\right)^m \Delta_{n,l}, \tag{51}$$

$$\Delta_{n+2m,l} = (1/\pi^m)(d/ds^2)^m\, \Delta_{n,l}, \tag{52}$$

where m is an integer. Further, by means of the equation

$$(d/d\lambda)^m \mathbf{\Omega}_\beta(0; \lambda) = \mathbf{\Omega}_{\beta+m}(0; \lambda), \tag{53}$$

one obtains

$$\Delta_{n,l+m} = \frac{(-)^m\Gamma(l)}{\Gamma(l+m)}\left(\frac{d}{d\mu^2}\right)^m \Delta_{n,l} \tag{54}$$

$$\Delta_{n-2m,l} = (-4\pi)^m(d/d\mu^2)^m\, \Delta_{n,l}. \tag{55}$$

A straightforward calculation (cf. Appendix) shows that

$$\Delta_{n-m,l} = \int_{-\infty}^{\infty} \Delta_{n,l}\, dx_1 \cdots dx_m, \tag{56}$$

which is an expression of Hadamard's[2] "method of descent." These recurrence formulas indicate that all of the Green's functions $\Delta_{n,l}$ are derivable from $\Delta_{0,1}$ as expected.

From (50) it is evident that $\Delta_{n,l}$ has no singularities on the light cone when $(1-n)/2 + l \geq 1$. Remembering that l and n are integers, one may write this condition in the form $2l > n$ to infer that *no singularities appear on the light cone when the order of the differential equation is greater than the number of space dimensions.*

When the order is less than, or equal to, the number of dimensions, Eq. (30) can be applied to express $\Delta_{n,l}$ in a form which displays its singularities on the light cone explicitly. The profound difference that exists between spaces with an even number of dimensions and spaces with an odd number of dimensions is of course reflected in the nature of these singularities. When $2l \leq n$, the singularities appear as follows:

$$\Delta_{2m+1,l} = \frac{\epsilon(t)(-\mu^2)^{m-l+1}}{2^{2m+1}\pi^m\Gamma(l)}\left\{\Omega_0(m-l+1; -\mu^2: s^2/4) + \sum_{q=0}^{m-l}\frac{\mathfrak{H}_{-q}(s^2/4)}{(-\mu^2)^{q+1}(m-l-q)!}\right\}, \tag{57}$$

$$\Delta_{2m,l} = \frac{\epsilon(t)(-\mu^2)^{m-l+1}}{2^{2m}\pi^{m-\frac{1}{2}}\Gamma(l)}\left\{\Omega_{\frac{1}{2}}(m-l+1; -\mu^2: s^2/4) + \sum_{q=0}^{m-l}\frac{\mathfrak{H}_{\frac{1}{2}-q}(s^2/4)}{(-\mu^2)^{q+1}(m-l-q)!}\right\}. \tag{58}$$

Using Eqs. (37) and (39) along with Eq. (19) we write the above equations in the form

$$\Delta_{2m+1,l} = \frac{\epsilon(t)(-\mu^2)^{m-l+1}}{2^{2m+1}\pi^m\Gamma(l)}\left\{\frac{2^{m-l+1}h(s^2)J_{m-l+1}(\mu s)}{(\mu s)^{m-l+1}} + \sum_{q=0}^{m-l}\frac{(-\mu^2/4)^{-q-1}}{(m-l-q)!}\,\delta^{(q)}(s^2)\right\}, \tag{59}$$

$$\Delta_{2m,l} = \frac{\epsilon(t)(-\mu^2)^{m-l+1}}{2^{2m+1}\pi^{m-\frac{1}{2}}\Gamma(l)}\left\{\frac{2^{m-l+\frac{3}{2}}h(s^2)\mathbf{H}_{m-l+\frac{1}{2}}(\mu s)}{\mu(\mu s)^{m-l+\frac{1}{2}}} + \sum_{q=0}^{m-l}\frac{(-\mu^2/4)^{-q-1}h(s^2)}{(m-l-q)!\,\Gamma(\frac{1}{2}-q)}\left(\frac{1}{s}\right)^{2q+1}\right\}, \tag{60}$$

where J is the Bessel function and $\mathbf{H}$ is the Struve function.

In each of these equations, the first term contains no singularities and represents a finite jump discontinuity across the light cone. The contrast between even- and odd-dimensional spaces is made evident in the second term. For spaces with an odd number of dimensions, the singular part of $\Delta_{n,l}$ consists of a finite linear combination of derivatives of the Dirac delta function $\delta(s^2)$, the highest derivative being of order $\frac{1}{2}(n-2l-1)$. On the other hand, the singular part of $\Delta_{n,l}$ for spaces with an even

number or dimensions consists of a polynomial in $1/s$ of degree $n - 2l + 1$.

5. GENERAL SOLUTION OF THE CAUCHY PROBLEM

In terms of the Green's function $\Delta_{n,1} = \Delta_n$ the solution of the initial value problem for the ordinary Klein-Gordon equation (1) is given by the well-known equation[7]

$$\varphi(x) = \int d\mathbf{x}'[\Delta_n(x - x')\ \partial_0'\varphi(x') - \varphi(x')\ \partial_0'\ \Delta_n(x - x')]_{t'=0} \tag{61}$$

where $\partial_0 \equiv \partial/\partial t$. That this is the solution follows from the initial conditions

$$\begin{aligned} \Delta_n(\mathbf{x}, 0) &= 0, \\ \partial_0\ \Delta_n(\mathbf{x}, 0) &= \delta(\mathbf{x}), \\ \partial_0^2\ \Delta_n(\mathbf{x}, 0) &= 0. \end{aligned} \tag{62}$$

The corresponding solution for the iterated Klein-Gordon equation (2) requires all the independent Δ-function solutions $\Delta_{n,p}$ with $p = 1, 2, \cdots, l$. The initial conditions satisfied by these Green's functions may be obtained from

$$\Delta_{n,p}(\mathbf{x}, t) = (2\pi)^{-n} \int_{-\infty}^{\infty} d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} G_p(\mathrm{k}, t), \tag{63}$$

where

$$G_p(\mathrm{k}, t) = \sum_{m=0}^{\infty} \frac{(-\omega^2)^m (p)_m}{m!\ \Gamma(2p + 2m)}\ t^{2p+2m-1} \tag{64}$$

represents Eq. (6). Simple calculation gives

$$\partial_0^j\ \Delta_{n,p}(\mathbf{x}, 0) = \begin{cases} 0 \text{ for } j = 0, 1, \cdots, (2p - 2); \\ \delta(\mathbf{x}) \text{ for } j = 2p - 1; \\ 0 \text{ for all even } j. \end{cases} \tag{65}$$

In addition, one obtains the important relation

$$\partial_0^{2p+2q-1}\ \Delta_{n,p}(\mathbf{x}, 0) = \frac{(p)_q}{q!}\ (\nabla^2 - \mu^2)^q\ \delta(\mathbf{x}) \tag{66}$$

where q is any non-negative integer. In view of these initial conditions, we may construct the field $\varphi(x)$ described by (2) as follows:

The general solution is written in the form

$$\begin{aligned} \varphi(x) = &\int d\mathbf{x}' \sum_{m=0}^{l-1} \sum_{p=m+1}^{l} A_{mp} \\ &\times [\partial_0^{2p-2m-1}\ \Delta_{n,p}(x - x')\ \partial_0'^{2m}\varphi(x')]_{t'=0} \\ &+ \int d\mathbf{x}' \sum_{m=0}^{l-1} \sum_{p=m+1}^{l} A_{mp} \\ &\times [\partial_0^{2p-2m-2}\ \Delta_{n,p}(x - x')\ \partial_0'^{2m+1}\varphi(x')]_{t'=0}. \end{aligned} \tag{67}$$

For each $m = 0, 1, \cdots, (l - 1)$, the $l - m$ constants A_{mp} are to be determined from the $l - m$ equations

$$\sum_{p=m+1}^{l} A_{mp}\ \partial_0^{2p+2j-1}\ \Delta_{n,p}(\mathbf{x}, 0) = \delta(\mathbf{x})\ \delta_{0j}, \tag{68}$$

where $j = 0, 1, \cdots, (l - m - 1)$ and δ_{0j} is the Kronecker delta, that is, $\delta_{0j} = 1$ for $j = 0$ and $\delta_{0j} = 0$ for $j \neq 0$. By virtue of (66), these equations for the constants become

$$\sum_{p=m+1}^{l} A_{mp}(p)_j = \delta_{0j}, \tag{69}$$

where $(p)_j$ is given by (22).

The solution of Eq. (69) is

$$A_{mp} = (-)^{p-m-1} \binom{p - 1}{m} \binom{l}{p}, \tag{70}$$

with $\binom{\alpha}{\beta}$ representing the binomial coefficient. To prove this, we substitute (70) into (69) with the result

$$\sum_{p=m+1}^{l} A_{mp}(p)_j = \frac{l!\ (m + 1)_j}{\Gamma(l - m)(m + 1)!}\ {}_2F_1(m - l + 1, m + j + 1; m + 2; 1), \tag{71}$$

where ${}_2F_1$ is Gauss' hypergeometric series. Using the identity[8]

$${}_2F_1(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c - a - b)}{\Gamma(c - a)\Gamma(c - b)}, \tag{72}$$

which is valid provided $c \neq 0, -1, -2, \cdots$ and $\mathrm{Re}\ (c - a - b) > 0$, we have

$$\sum_{p=m+1}^{l} A_{mp}(p)_j = \frac{\Gamma(l - m - j)(m + 1)_j}{\Gamma(l - m)\Gamma(1 - j)} = \delta_{0j} \tag{73}$$

since $j = 0, 1, \cdots, l - m - 1$.

To show that Eq. (67) represents the solution to Cauchy's problem we note that

$$[\partial_0^{2M}\varphi(x)]_{t=0} = \int d\mathbf{x}' \sum_{m=0}^{M} \sum_{p=m+1}^{l} A_{mp} \times [\partial_0^{2p+2(M-m)-1}\ \Delta_{n,p}(x - x')\ \partial_0'^{2m}\varphi(x')]_{\substack{t'=0 \\ t=0}} \tag{74}$$

where the upper limit to the sum over m is obtained using (65). The second integral in (67) makes no contribution because of (65). By virtue of (68) we obtain the required result.

$$[\partial_0^{2M}\varphi(x)]_{t=0} = \int d\mathbf{x}' \sum_{m=0}^{M} \delta_{mM}\ \delta(\mathbf{x} - \mathbf{x}') \times [\partial_0'^{2m}\varphi(x')]_{t'=0} = \partial_0^{2M}\varphi(\mathbf{x}, 0). \tag{75}$$

An exactly analogous proof is obtained for $[\partial_0^{2M+1}\varphi(x)]_{t=0}$, except in this case the first integral in (67) contributes nothing and the second integral gives the required result.

6. EXPLICIT SOLUTIONS FOR THE KLEIN-GORDON EQUATION

The general solution of the initial value problem for the Klein-Gordon equation will now be calculated explicitly by carrying out the integral operation indicated in Eq. (61), which is equivalent to Eq. (67) when $l = 1$. Noting that $\Delta_n(\mathbf{x}, t) = \Delta_n(-\mathbf{x}, t)$, the solution may be written in the form

$$\varphi(x) = \int \Delta_n(\mathbf{x}' - \mathbf{x}, t)\, \partial_0'\varphi(\mathbf{x}', 0)\, d\mathbf{x}' + \int \partial_0\, \Delta_n(\mathbf{x}' - \mathbf{x}, t)\varphi(\mathbf{x}', 0)\, d\mathbf{x}'. \tag{76}$$

Changing the variable of integration to $\mathbf{R} = \mathbf{x}' - \mathbf{x}$ and introducing n-dimensional spherical coordinates in $\mathbf{R}$ space, we note that the integral over the angles gives the arithmetic average $\bar{\varphi}(\mathbf{x}; \mathrm{R})$ of the initial field on a sphere of radius R centered about the fixed position $\mathbf{x}$. That is,

$$\bar{\varphi}(\mathbf{x}; \mathrm{R}) \equiv \sigma_n^{-1} \int \varphi(\mathbf{x} + \mathbf{R}, 0)\, d\sigma_n, \tag{77}$$

where σ_n is the solid angle given by (8). Finally, using $\partial_0\Delta_n = 2\pi t\Delta_{n+2}$, we may write (76) as

$$\varphi(x) = \sigma_n \int_0^\infty \Delta_n(R, t)\overline{\varphi_{,t}}(\mathbf{x}; \mathrm{R})\mathrm{R}^{n-1}\, d\mathrm{R} + 2\pi t\sigma_n \int_0^\infty \Delta_{n+2}(\mathrm{R}, t)\bar{\varphi}(\mathbf{x}; \mathrm{R})\mathrm{R}^{n-1}\, d\mathrm{R}. \tag{78}$$

It is at this stage of the analysis that the difference between an even and an odd number of space dimensions becomes significant. In order to obtain $\varphi(x)$ in an explicit form one must distinguish between n even and n odd because the singularities of Δ_n are so different in the two cases.

Odd Number of Dimensions, $n = 2m + 1$

In this case we use Eq. (59) with $l = 1$ in Eq. (78) to obtain

$$\begin{aligned}\varphi(x) = {} & \frac{(\pi)^{\frac{1}{2}}}{\Gamma(m + \frac{1}{2})} \frac{\epsilon(t)}{2} \sum_{q=0}^{m-1} \frac{(-\mu^2/4)^{m-q-1}}{\Gamma(m - q)} \left(\frac{d}{dt^2}\right)^q \\ & \times \{\bar{\varphi}_{,t}(\mathbf{x}; |t|)\, |t|^{2m-1}\} \\ & + \frac{(\pi)^{\frac{1}{2}}\, |t|}{\Gamma(m + \frac{1}{2})} \sum_{q=0}^{m} \frac{(-\mu^2/4)^{m-q}}{\Gamma(m - q + 1)} \left(\frac{d}{dt^2}\right)^q \\ & \times \{\bar{\varphi}(\mathbf{x}; |t|)\, |t|^{2m-1}\} \\ & + \frac{(\pi)^{\frac{1}{2}}\epsilon(t)}{\Gamma(m + \frac{1}{2})} \left(\frac{-\mu}{2}\right)^m \int_0^{|t|} \frac{\mathrm{R}^{2m}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{m/2}} \\ & \times J_m[\mu(t^2 - \mathrm{R}^2)^{\frac{1}{2}}]\overline{\varphi_{,t}}(\mathbf{x}; \mathrm{R}) \\ & + \frac{2(\pi)^{\frac{1}{2}}\, |t|}{\Gamma(m + \frac{1}{2})} \left(\frac{-\mu}{2}\right)^{m+1} \int_0^{|t|} \frac{\mathrm{R}^{2m}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{(m+1)/2}} \\ & \times J_{m+1}[\mu(t^2 - \mathrm{R}^2)^{\frac{1}{2}}]\bar{\varphi}(\mathbf{x}; \mathrm{R}). \end{aligned} \tag{79}$$

Even Number of Dimensions, $n = 2m$

We use Eq. (60) in Eq. (78), calculating the contribution from the singular part of Δ_n by means of Eq. (16). The result is

$$\begin{aligned}\varphi(x) = {} & \frac{\epsilon(t)}{\Gamma(m)} \sum_{q=0}^{m-1} \frac{(-\mu^2/4)^{m-q-1}}{\Gamma(m - q)} \int_0^{|t|} \frac{\mathrm{R}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{\frac{1}{2}}} \\ & \times \left(\frac{d}{d\mathrm{R}^2}\right)^q \{\overline{\varphi_{,t}}(\mathbf{x}; \mathrm{R})\mathrm{R}^{2m-2}\} \\ & + \frac{2\, |t|}{\Gamma(m)} \sum_{q=0}^{m} \frac{(-\mu^2/4)^{m-q}}{\Gamma(m - q + 1)} \int_0^{|t|} \frac{\mathrm{R}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{\frac{1}{2}}} \\ & \times \left(\frac{d}{d\mathrm{R}^2}\right)^q \{\bar{\varphi}(\mathbf{x}; \mathrm{R})\mathrm{R}^{2m-2}\} \\ & + \frac{(-)^m(\pi)^{\frac{1}{2}}\epsilon(t)}{\Gamma(m)} \left(\frac{\mu}{2}\right)^{m-\frac{1}{2}} \int_0^{|t|} \frac{\mathrm{R}^{2m-1}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{(m-\frac{1}{2})/2}} \\ & \times \mathbf{H}_{m-\frac{1}{2}}[\mu(t^2 - \mathrm{R}^2)^{\frac{1}{2}}]\overline{\varphi_{,t}}(\mathbf{x}; \mathrm{R}) \\ & + \frac{(-)^{m+1}2(\pi)^{\frac{1}{2}}\, |t|}{\Gamma(m)} \left(\frac{\mu}{2}\right)^{m+\frac{1}{2}} \int_0^{|t|} \frac{\mathrm{R}^{2m-1}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{(m+\frac{1}{2})/2}} \\ & \times \mathbf{H}_{m+\frac{1}{2}}[\mu(t^2 - \mathrm{R}^2)^{\frac{1}{2}}]\bar{\varphi}(\mathbf{x}; \mathrm{R}). \end{aligned} \tag{80}$$

The corresponding results for the d'Alembert equation

$$\square\, \varphi(x) = 0 \tag{81}$$

are of course obtained in the limit as μ goes to zero. The solution of the Cauchy problem for the wave equation (81) is thus (compare with Courant and Hilbert[1]):

$$\begin{aligned}\varphi(x) = {} & \frac{(\pi)^{\frac{1}{2}}\epsilon(t)}{2\Gamma(n/2)} \left(\frac{d}{dt^2}\right)^{(n-3)/2} \{\overline{\varphi_{,t}}(\mathbf{x}; |t|)\, |t|^{n-2}\} \\ & + \frac{(\pi)^{\frac{1}{2}}\, |t|}{\Gamma(n/2)} \left(\frac{d}{dt^2}\right)^{(n-1)/2} \{\bar{\varphi}(\mathbf{x}; |t|)\, |t|^{n-2}\} \end{aligned} \tag{82}$$

for odd $n \geq 3$, and

$$\begin{aligned}\varphi(x) = {} & \frac{\epsilon(t)}{\Gamma(n/2)} \int_0^{|t|} \frac{\mathrm{R}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{\frac{1}{2}}} \left(\frac{d}{d\mathrm{R}^2}\right)^{(n-2)/2} \\ & \times \{\overline{\varphi_{,t}}(\mathbf{x}; \mathrm{R})\mathrm{R}^{n-2}\} + \frac{2\, |t|}{\Gamma(n/2)} \\ & \times \int_0^{|t|} \frac{\mathrm{R}\, d\mathrm{R}}{(t^2 - \mathrm{R}^2)^{\frac{1}{2}}} \left(\frac{d}{d\mathrm{R}^2}\right)^{n/2} \{\bar{\varphi}(\mathbf{x}; \mathrm{R})\mathrm{R}^{n-2}\} \end{aligned} \tag{83}$$

for even $n \geq 2$.

As is well known, Huygen's principle for the d'Alembert equation holds only for spaces with an odd number of dimensions, while the effect of diffusion takes place in even-dimensional spaces.[2] Equation (50) indicates that the Green's function for the iterated d'Alembert operator has a δ-function type of singularity only when n is odd and $2l < n$. Thus Huygen's principle for Eq. (49) holds only when the order of the equation is less than the number of space dimensions and when the number of space dimensions is odd. Huygen's principle for Eq. (2) does not hold.

APPENDIX. THE METHOD OF DESCENT

We want to evaluate

$$I = \int_{-\infty}^{\infty} \Delta_{n,l}\, dx_1 \cdots dx_m, \tag{A1}$$

where $m \leq n$. Introducing spherical coordinates for the volume element

$$dx_1 \cdots dx_m = \rho^{m-1}\, d\rho\, d\sigma_m$$

and using Eq. (9) for $\Delta_{n,l}$ we obtain

$$I = \sigma_m \left(\frac{1}{2\pi}\right)^{(n-1)/2} \int_0^{\infty} G(t)\mathrm{k}^{n/2}\, d\mathrm{k} \times \int_0^{\infty} \frac{J_{n/2-1}(\mathrm{k}r)}{r^{n/2-1}}\, \rho^{m-1}\, d\rho, \tag{A2}$$

where

$$G(t) = \frac{(t/\omega)^{l-\frac{1}{2}}}{2^l \Gamma(l)} J_{l-\frac{1}{2}}(\omega t). \tag{A3}$$

The integral over ρ in Eq. (A2) has the form of another Sonine integral when we set $r^2 = \rho^2 + \mathrm{R}^2$, namely,[14]

$$\int_0^{\infty} \frac{J_\nu[a(t^2+z^2)^{\frac{1}{2}}]}{(t^2+z^2)^{\nu/2}}\, t^{2\mu+1}\, dt = \frac{2^\mu \Gamma(\mu+1)}{a^{\mu+1} z^{\nu-\mu-1}} J_{\nu-\mu-1}(az), \tag{A4}$$

for $a \geq 0$. This result is obtained from the Sonine formula in Eq. (10) by letting $b \to 0$. The integral over ρ thus has the value

$$\frac{2^{m/2-1}\Gamma(m/2)}{\mathrm{k}^{m/2}\mathrm{R}^{(n-m-2)/2}} J_{(n-m)/2-1}(\mathrm{kR}).$$

[14] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, New York, 1922).

Remembering Eq. (8) for σ_m we finally have

$$I = \left(\frac{1}{2\pi}\right)^{(n-m-1)/2} \times \int_0^{\infty} \frac{J_{(n-m)/2-1}(\mathrm{kR})}{\mathrm{R}^{(n-m-2)/2}} G(t)\mathrm{k}^{(n-m)/2}\, d\mathrm{k}, \tag{A5}$$

which is equivalent to $\Delta_{n-m,l}$ as seen from Eq. (9). We thus have

$$\Delta_{n-m,l} = \int_{-\infty}^{\infty} \Delta_{n,l}\, dx_1 \cdots dx_m \tag{A6}$$

giving the method of descent.

Note added in proof. Equation (70) permits one to write the general solution (67) in the form

$$\varphi(x) = \int_{t'=0} d\mathbf{x}'\, \Delta_{n,l}(x - x') X' \varphi(x')$$

where the differential operator X is defined by

$$X \equiv (\overrightarrow{\partial_0} - \overleftarrow{\partial_0}) \sum_{p=1}^{l} \binom{l}{p} (\overleftarrow{\Box} + \mu^2)^{l-p} (\overrightarrow{\partial_0^2} - \overleftarrow{\partial_0^2})^{p-1},$$

the arrows indicating the directions in which the differentiations are to be carried out. We observe that X may be written

$$(\overrightarrow{\partial_0^2} - \overleftarrow{\partial_0^2})X = (\overrightarrow{\partial_0} - \overleftarrow{\partial_0}) \times [(\overleftarrow{\Box} + \mu^2 + \overrightarrow{\partial_0^2} - \overleftarrow{\partial_0^2})^l - (\overleftarrow{\Box} + \mu^2)^l].$$

The invariant form of the general solution is

$$\varphi(x) = \int_\sigma d\sigma_\beta(x')\, \Delta_{n,l}(x - x') X'_\beta\, \varphi(x'),$$

where σ is an arbitrary spacelike surface and

$$(\overrightarrow{\Box} - \overleftarrow{\Box})X_\beta = (\overrightarrow{\partial_\beta} - \overleftarrow{\partial_\beta})[(\overrightarrow{\Box} + \mu^2)^l - (\overleftarrow{\Box} + \mu^2)^l].$$

These results may be extended to include arbitrary polynomials in $\Box$; such a generalization will be published in a future paper.

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Simple Realizations of the Infinitesimal Generators of the Proper Orthochronous Inhomogeneous Lorentz Group for Mass Zero*

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A realization of the infinitesimal generators for the mass-zero case of the proper orthochronous inhomogeneous Lorentz group is given explicitly for both continuous and discrete spin cases in terms of a uniform notation. The realization for the discrete spin case is unitarily equivalent to that given by Shirokov.

For the sake of completeness the infinitesimal generators for the case of nonzero mass, derived by Foldy, are also given. Hence the present paper contains realizations for all irreducible unitary representations of the inhomogeneous Lorentz group of physical interest.

Since the irreducible representations of the two-dimensional Euclidean group play an important role in the massless case, simple realizations of the irreducible representations of the generators of this group are also given.

1. COMMUTATION RULES FOR THE INFINITESIMAL GENERATORS. INVARIANTS CHARACTERIZING THE REPRESENTATION

THE first to find and classify all physically interesting unitary ray representations of the proper orthochronous inhomogeneous Lorentz group was Wigner.[1] His approach was global in character and his treatment was a generalization of that used for finding representations of finite groups.

Bargmann and Wigner[2] gave explicit realizations for all physically interesting, Hermitian, irreducible representations of the infinitesimal generators of the group. For the discrete-spin representations of both nonzero and zero mass, the realizations were given in terms of Dirac-like wave equations. The realizations of the massless, so-called "continuous-spin" representations were given in terms of more complicated systems of equations.

Foldy[3] gave particularly simple realizations of the generators for the case of finite mass. The objective of the present paper is to present analogous realizations for all zero-mass representations.[4,5]

For the sake of completeness we shall also present Foldy's realizations for the case of finite mass. Hence the present paper will contain simple realizations for all cases of current physical interest.

Since the two-dimensional Euclidean group plays a particularly important role in the massless case, we shall give all irreducible representations of this group as well.

There are 10 infinitesimal generators of the proper, orthochronous Lorentz group. Those which correspond to time and space translations are the Hamiltonian and momentum operators, respectively, which we denote by H and P_i. The operators which correspond to rotations about the space axes are denoted by J_i. Rotations involving one-space axis and the time axis are denoted by $\mathcal{J}_i$. The subscript i takes on the values 1, 2, 3 corresponding to the three-space axes.

The commutation rules satisfied by the generators are

$$[H, P_i] = 0 \tag{1.1}$$
$$[P_i, P_j] = 0$$
$$[J_i, P_j] = 0$$
$$[J_i, H] = 0 \tag{1.2}$$
$$[J_i, \mathcal{J}_i] = 0$$
$$[\mathcal{J}_i, H] = iP_i \tag{1.3}$$
$$[\mathcal{J}_i, P_j] = i\,\delta_{ij}$$
$$[J_1, J_2] = iJ_3$$

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[1] E. P. Wigner, Ann. Math. **40**, 149 (1939).

[2] V. Bargmann and E. P. Wigner, Proc. Natl. Acad. Sci. U. S. **34**, 211 (1948).

[3] L. L. Foldy, Phys. Rev. **102**, 568–581 (1956).

[4] For the discrete spin case, our realization is unitarily equivalent to the realization of Shirokov.[5] The advantage of our realization is that it has a similar structure to the realizations of the other massless cases and, for that matter, of the case of finite mass.

[5] Iu. M. Shirokov, Soviet Physics—JETP **6**, 919 (1958).

$$[J_2, J_3] = iJ_1 \tag{1.4}$$
$$[J_3, J_1] = iJ_2$$
$$[\mathcal{J}_1, \mathcal{J}_2] = -iJ_3$$
$$[\mathcal{J}_2, \mathcal{J}_3] = -iJ_1 \tag{1.5}$$
$$[\mathcal{J}_3, \mathcal{J}_1] = -iJ_2$$
$$[J_1, P_2] = [P_1, J_2] = iP_3$$
$$[J_2, P_3] = [P_2, J_3] = iP_1 \tag{1.6}$$
$$[J_3, P_1] = [P_3, J_1] = iP_2$$
$$[J_1, \mathcal{J}_2] = [\mathcal{J}_1, J_2] = i\mathcal{J}_3$$
$$[J_2, \mathcal{J}_3] = [\mathcal{J}_2, J_3] = i\mathcal{J}_1 \tag{1.7}$$
$$[J_3, \mathcal{J}_1] = [\mathcal{J}_3, J_1] = i\mathcal{J}_2.$$

It can be shown that any operator which commutes with each operator of an irreducible set of Hermitian operators must be a scalar operator. In the present case the generators are to form such an irreducible set. Four operators which commute with this set and hence are scalar operators are particularly important. They label completely all cases of possible physical interest, except the mass-zero, discrete-spin case. These four operators, which are called invariants or Casimir operators are defined as follows:

$$\begin{aligned} C_0 &= H/|H| \\ C_1 &= \sum_{i=1}^{3} P_i^2 - H^2 = \mathbf{P}\cdot\mathbf{P} - H^2 \\ C_2 &= \sum_{i=1}^{3} w_i^2 - \sum_i (P_i J_i)^2 \\ &= \mathbf{w}\cdot\mathbf{w} - (\mathbf{P}\cdot\mathbf{J})^2, \end{aligned} \tag{1.8}$$

where

$$\begin{aligned} \mathbf{w} &= -[H\mathbf{J} + (\mathbf{P}\times\mathcal{J})] \\ C_3 &= e^{2\pi i J_1} = e^{2\pi i J_2} = e^{2\pi i J_3}, \end{aligned}$$

where here $\mathcal{J}$ is the 3-vector $(\mathcal{J}_1\mathcal{J}_2\mathcal{J}_3)$.

The invariant C_0, which gives the sign of the spectrum of the Hamiltonian, can take on the value $+1$ or -1. In what follows we shall consider representations only for the case of positive energy spectrum because for free particles the energy must be positive.

The invariant $C_1 = -m^2$ gives the negative of the square of the mass of the particle. The mass m is taken to positive or zero to be of physical interest.

The range of values of the invariant C_2 depends upon C_1, that is, upon whether m is zero or not. If m is not zero, C_2 will always have the following form

$$C_2 = m^2 s(s+1), \tag{1.9}$$

where s is any non-negative integer or half-integer and corresponds to the spin.

If $m = 0$, then C_2 can have the value zero or any positive value. We write

$$\begin{aligned} C_2 &= \Xi \\ 0 &\leq \Xi < \infty . \end{aligned} \tag{1.10}$$

In the case $C_2 = 0$, which is called the mass-zero, discrete-spin case, there is another scalar operator $(\mathbf{P}\cdot\mathbf{J})/H = S$. The real scalar S can take on any positive or negative integer or half-integer value.

The invariant C_3 can have only the values $+1$ or -1. If the value is $+1$, the representation is said to be single valued; if the value is -1, the representation is called double valued. In the non-zero mass case the value of C_3 is determined by C_2 or equivalently s. If s is an integer, the representation is single valued; if s is a half integer, the representation is double valued. In the zero-mass case the value of C_3 (that is, the single or double valuedness of the representation) must be prescribed.

2. THE GENERATORS AND REPRESENTATIONS OF THE EUCLIDEAN GROUP

The Euclidean group has three generators which we shall denote by T_2, T_3, and S. They satisfy the commutation rules

$$\begin{aligned} [T_2, S] &= -iT_3 \\ [T_3, S] &= iT_2 \\ [T_2, T_3] &= 0. \end{aligned} \tag{2.1}$$

The invariants which completely specify the representation are

$$\begin{aligned} T_2^2 + T_3^2 &= r^2 \\ e^{2\pi i S} &= e^{2\pi i \phi}, \end{aligned} \tag{2.2}$$

where ϕ is any real number and r is any non-negative number. The case for $r > 0$ and $r = 0$ lead to different irreducible representations.

a. The Case $r > 0$

In this case the scalar ϕ can take on any value $0 \leq \phi < 1$ for inequivalent representations. The generators are represented by infinite Hermitian matrices which we shall denote by the same letters as the abstract generators.

$$\begin{aligned} T_2 &= (T_{2n,n'}) \\ T_3 &= (T_{3n,n'}) \\ S &= (S_{n,n'}) \\ n, n' &= \text{any integer}, \end{aligned} \tag{2.3}$$

where the matrix elements are

$$\begin{aligned} T_{2n,n'} &= \tfrac{1}{2}ir[\delta_{n,n'+1} - \delta_{n,n'-1}] \\ T_{3n,n'} &= \tfrac{1}{2}r[\delta_{n,n'+1} + \delta_{n,n'-1}] \\ S_{n,n'} &= \delta_{n,n'}(n + \phi). \end{aligned} \tag{2.4}$$

The carrier space is the infinite dimensional vector space, i.e., each vector A in the space is represented by a column vector (a_n) where n assumes all integral values from $-\infty$ to $+\infty$. The square of the vector A is

$$\sum_{n=-\infty}^{+\infty} |a_n|^2.$$

b. The Case $r = 0$

In this case the matrices representing T_2 and T_3 are zero. The matrix representing S is one dimensional, i.e., S is any real scalar. The carrier space is one dimensional with the one-dimensional Hermitian inner product $|a|^2$.

3. REPRESENTATIONS OF THE INHOMOGENEOUS LORENTZ GROUP FOR THE MASSLESS CASE

Throughout this paper we take the positive energy representation. Hence,

$$\begin{aligned} C_0 &= 1 \\ C_1 &= 0. \end{aligned}$$

a. The Case for which $C_2 = \Xi > 0$

The carrier space is a complex separable Hilbert space which we proceed to describe.

It consists of complex functions $\psi(\mathbf{p}, n)$ where the vector p denotes collectively three variables p_1, p_2, p_3. The variable n is an integer which takes on all positive and negative values. The square of the length of the vector is given by

$$\sum_n \int \psi^*(\mathbf{p}, n)\psi(\mathbf{p}, n)\frac{d\mathbf{p}}{p},$$

where

$$p = |\mathbf{p}|.$$

The form of the inner product assures us that the generators given below are Hermitian.

The generators are defined on a dense subspace of the Hilbert space which consists of functions $\psi(\mathbf{p}, n)$ which are twice-differentiable with respect to the variables p_i and which vanish identically when $\mathbf{p}$ lies in a volume consisting of a right circular cylinder about the negative p_1 axis and a sphere about the origin. This volume may be arbitrarily small.

The operators P_1, P_2, P_3 acting on functions of this subspace consist of multiplication by p_1, p_2, p_3, respectively. The operator H consists of multiplication by p.

The Hermitian operators J_i and $\mathcal{J}_i$ are described in the following way:

$$\begin{aligned} J_1 &= -i(\mathbf{p} \times \nabla)_1 + S \\ J_2 &= -i(\mathbf{p} \times \nabla)_2 + \frac{p_2}{p + p_1} S \\ J_3 &= -i(\mathbf{p} \times \nabla)_3 + \frac{p_3}{p + p_1} S \end{aligned} \tag{3.1}$$

$$\begin{aligned} \mathcal{J}_1 &= ip\nabla_1 + \frac{p_2}{p} T_2 + \frac{p_3}{p} T_3 \\ \mathcal{J}_2 &= ip\nabla_2 + \frac{p_3}{p + p_1} S + \left[\frac{p_2^2}{p^2(p + p_1)} - \frac{1}{p}\right] T_2 \\ &\quad + \frac{p_2 p_3}{p^2(p + p_1)} T_3 \\ \mathcal{J}_3 &= ip\nabla_3 - \frac{p_2}{p + p_1} S + \frac{p_2 p_3}{p^2(p + p_1)} T_2 \\ &\quad + \left[\frac{p_3^2}{p^2(p + p_1)} - \frac{1}{p}\right] T_3. \end{aligned} \tag{3.2}$$

In Eqs. (3.1) and (3.2) the gradient operator is the gradient with respect to $\mathbf{p}$. The operators S, T_2, and T_3 are the matrices which are the irreducible representations of the two-dimensional Euclidean group given by (2.3) and (2.4) (with $r = \sqrt{\Xi}$) and act on the variable n of the functions in the carrier space. However, in the present case the number ϕ is determined by the invariant C_3, i.e., by the single or double valuedness of the representation. If the representation is single valued, $C_3 = 1$ and we must take $\phi = 0$. If the representation is double-valued, $C_3 = -1$ and $\phi = \frac{1}{2}$.

These representations are called "continuous-spin" representations for the massless case.

b. The Case for Which $C_2 = 0$

In the case $C_2 = 0$, the representation has the same form as for the previous case. The functions which comprise the Hilbert space, however, do not depend

on the variable n and there is no summation over this variable in the definition of inner product. Furthermore, the matrices $T_2 = T_3 = 0$. The matrix S is replaced by a positive or negative integer for the single-valued representations and is replaced by a positive or negative half-integer for the double-valued representations. Each choice of S leads to a different representation. These representations are called discrete-spin representations of the massless case.

4. REPRESENTATIONS FOR THE CASE OF PARTICLES OF FINITE MASS[6]

The carrier space is a space consisting of functions $\psi(\mathbf{p}, i)$ where i is a discrete variable which takes on $2s + 1$ values running from $i = -s$ to $i = s$ in steps of 1. (The quantity s is the spin described in part 1.) The square of the length of the vector is defined by

$$\sum_{i=-s}^{+s} \int \psi^*(\mathbf{p}, i)\psi(\mathbf{p}, i) \frac{d\mathbf{p}}{\omega(p)}$$

where

$$\omega(p) = (p^2 + m^2)^{\frac{1}{2}}. \tag{4.1}$$

The operators P_1, P_2, P_3 consist of multiplication by p_1, p_2, p_3, respectively. The operator H consists of multiplication by $\omega(p)$.

The operators J_i and $\mathcal{J}_i$ are given by

$$\begin{aligned} J_i &= -i(\mathbf{p} \times \nabla)_i + S_i \\ \mathcal{J}_i &= i\omega(p)\nabla_i + (\mathbf{p} \times \mathbf{S})_i/[\omega(p) + m] \,. \end{aligned} \tag{4.2}$$

The operators S_i are just the irreducible Hermitian spin matrices corresponding to the spin s and operate on the discrete variable i of the functions in the Hilbert space.

It should be mentioned that Chang[7] has given another form for the infinitesimal generators for the present case, which is based on the representations of the group given in reference 1.

[6] These generators were given in the x representation in reference 3 and in the momentum representation in reference 4. The latter is the one used above.

[7] T. S. Chang, Acta. Math. Sinica, 3, 59 (1953).

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Properties of the Irreducible Angular Momentum Tensors*

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The angular momentum operators define a set of irreducible tensors which are unique except for a normalization constant. The normalization is conveniently defined in terms of statistical tensors which describe oriented states. The properties of the tensors discussed here include: (1) the trace of products of components of such tensors, (2) symmetry properties of the traces, and (3) the expansion of products of components of these tensors into a sum of irreducible tensors. The corresponding expansion of commutators and anticommutators of these components is also discussed briefly.

I. INTRODUCTION

In many problems of solid-state physics, for example, paramagnetic resonance or nuclear orientation, the irreducible tensors in the space of the angular momentum operators play a central role. If we consider a physical system for which the angular momentum is well defined then the tensors in question depend only on the angular momentum operators j_x, j_y, j_z. The statement that the tensors are irreducible means that, to within a normalization constant, the tensors are uniquely defined by the tensor rank L and the projection quantum number M. The tensor of rank L, by definition transforms under the $2L + 1$ dimensional representation of the rotation group when a 3-space rotation of the coordinate axes is carried out. Thus, if R is the rotation operator[1]

$$RT_L^M R^{-1} = \sum_{M'} D^L_{M'M} T_L^{M'}, \tag{1}$$

where the arguments of the D matrices are the Euler angles.

It is convenient to define the normalization of the T_L^M in terms of the statistical tensors introduced by Fano.[2] For this purpose it is sufficient to consider the axially symmetric case wherein the statistical tensor G_L for a state with angular momentum j is

$$G_L = \sum_m p_m (-)^{j-m} C(jjL; m, -m). \tag{2}$$

In (2) p_m is the population (diagonal element of the density matrix) for the substate m, and the C coefficient is a vector addition coefficient.[1] Then T_L^0 is fixed by

$$G_L = \mathrm{Tr}\, T_L^0 \rho \tag{3}$$

wherein ρ is the density matrix given in terms of the spin Hamiltonian H by

$$\rho = \exp(-H/kT)/\mathrm{Tr} \exp(-H/kT).$$

Then, as has been shown elsewhere,[3]

$$T_L^0 = A_L(j)(\mathbf{j}\cdot\nabla)^L \mathcal{Y}_L^0(\mathbf{r}) \tag{4}$$

with

$$A_L(j) = \frac{2^L}{L!}\left[\frac{4\pi(2j-L)!}{(2j+L+1)!}\right]^{\frac{1}{2}} \tag{4a}$$

and $\mathcal{Y}_L^0(\mathbf{r})$ is the axially symmetric solid harmonic of degree L. It follows at once that

$$T_L^M = A_L(\mathbf{j})(\mathbf{j}\cdot\nabla)^L \mathcal{Y}_L^M(\mathbf{r}). \tag{4b}$$

Obviously, the vector $\mathbf{r}$ is, in a sense, a dummy symbol since, with the ∇ operator in $\mathbf{r}$ space, the T_L^M does not depend on these variables. Equation (4b) is thereby a convenient representation of the T_L^M from which these operators can readily be written in terms of the components of $\mathbf{j}$. The form (4b) also makes it obvious that T_L^M is an irreducible tensor component for rank L.

We proceed to discuss some of the properties of the tensors T_L^M with the end in view of providing a better understanding of them and of facilitating calculations in which they are involved. We mention that a table of the T_L^M for $L \leq 4$ has been given in the literature.[4]

II. TRACE OF PRODUCTS OF IRREDUCIBLE TENSOR COMPONENTS

The evaluation of the partition function and derived quantities, including the statistical tensors,

* Work partially supported by U. S. Atomic Energy Commission.

[1] M. E. Rose, *Elementary Theory of Angular Momentum*, (John Wiley & Sons, Inc., New York 1957).

[2] U. Fano, National Bureau of Standards Report No. 1214 (unpublished).

[3] M. E. Rose, Phys. Rev. 108, 362 (1957).

[4] E. Ambler, J. C. Eisenstein, and J. F. Schooley, J. Math. Phys. (to be published). See also, G. F. Koster and H. Statz, Phys. Rev. 113, 445 (1959).

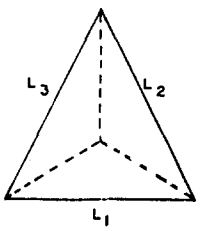

FIG. 1. Tetrahedron for $n = 3$. The unlabeled (dotted) lines are j in each case.

can be done in a practical manner whenever an expansion of the density matrix ρ in inverse powers of kT is justified. Since the spin Hamiltonian H can always be written in terms of contractions of various T_L^M with tensors of corresponding rank in the space of other variables (for example, magnetic field, electric field gradient, spin of interacting systems) one is led to the evaluation of traces of products of $T_{L_i}^{M_i}$. The evaluation of these traces when the tensors are expressed in Cartesian form has been discussed by Ambler *et al.*[4] The methods given here extend and supplement their results.

We define

$$Z_n = \mathrm{Tr}\, T_{L_n}^{M_n} T_{S_{n-1}}^{M_{n-1}} \cdots T_{L_1}^{M_1}. \tag{5}$$

From the Wigner-Eckart theorem[1]

$$(j'm' \,|T_L^M|\, jm) = C(jLj';\, mM)(j' \,||T_L||\, j)$$

and $m' = M + m$. From the fact that the commutator $(\mathbf{j}^2,\, T_L^M) = 0$, we see that $j = j'$ and from (4) it is seen that the reduced matrix element is[3]

$$(j \,||T_L||\, j) \equiv a_L(j) = [(2L + 1)/(2j + 1)]^{\frac{1}{2}}.$$

Thus,

$$T_L^M \psi_i^m = a_L(j) C(jLj;\, mM) \psi_i^{m+M}. \tag{6}$$

Using this result we find

$$Z_n = \prod_1^n a_{L_i}(j) S,$$

where

$$S = \sum_m C(jL_1j;\, mM_1) C(jL_2j;\, m + \mu_1,\, M_2) \cdots C(jL_nj;\, m + \mu_{n-1},\, M_n), \tag{7a}$$

and

$$\mu_k = \sum_1^k M_i\,.$$

The sum over m in (7a) can always be effected by $n - 2$ Racah recouplings. In all cases it should be emphasized that the trace of any T_L^M vanishes except when $L = 0$ and $T_0^0 = a_0(j) = (2j + 1)^{-\frac{1}{2}}$.

For $n = 1, 2$ the results are trivial. Specific results follow:

$$Z_1 = (2j + 1)^{\frac{1}{2}}\, \delta_{L_1 0}\, \delta_{M_1 0} \tag{8a}$$

$$Z_2 = (-)^{M_1}\, \delta_{L_1 L_2}\, \delta_{\mu_2 0}. \tag{8b}$$

For $n = 3$ one Racah recoupling gives

$$Z_3 = [(2L_1 + 1)(2L_2 + 1)]^{\frac{1}{2}} (-)^{M_3} C(L_1 L_2 L_3;\, M_1 M_2) \times W(jL_1jL_2;\, jL_3)\, \delta_{\mu_3 0}\,. \tag{8c}$$

A recurrence formula for $Z_3(M_1M_2)$ is[1]

$$\begin{aligned}[L_3(L_3 + 1) - L_1(L_1 + 1) &- L_2(L_2 + 1) - 2M_1M_2]Z_3(M_1M_2) \\ &= [(L_1 - M_1 + 1)(L_1 + M_1)(L_2 + M_2 + 1) \\ &\times (L_2 - M_2)]^{\frac{1}{2}} Z_3(M_1 - 1, M_2 + 1) \\ &+ [(L_1 + M_1 + 1)(L_1 - M_1)(L_2 - M_2 + 1) \\ &\times (L_2 + M_2)]^{\frac{1}{2}} Z_3(M_1 + 1, M_2 - 1),\end{aligned}$$

where $Z_3(M_1M_2) = Z_3$ as given in (8c).

For $n = 4$ two Racah recouplings give

$$Z_4 = [(2L_1 + 1)(2L_2 + 1)(2L_3 + 1)(2L_4 + 1)]^{\frac{1}{2}} \times (-)^{M_1 + M_3} \sum_s C(L_1L_2s;\, M_1M_2) C(L_3L_4s;\, M_3M_4) \times W(jL_1jL_2;\, js) W(jL_3jL_4;\, js)\, \delta_{\mu_4 0}. \tag{8d}$$

The limits on s are

$$\max(|L_1 - L_2|,\, |L_3 - L_4|) \leq s \leq \min(2j,\, L_1 + L_2,\, L_3 + L_4).$$

No further simplification can be made in this result and evaluation of Z_4 can be effected by use of numerical tables.[5] Clearly the Z_n cannot be expressed solely in terms of $3n$-j symbols because the latter are invariants independent of magnetic quantum numbers. However, it would be desirable to effect the summation in (8d). That this cannot be done in terms of familiar constructs is apparent from an examination of the topological diagrams corresponding to the various Z_n. Thus, for $n = 3$, to consider a simple example first, there is a triangular relation between the three L_i, symbolized by $\Delta(L_1L_2L_3)$, and also between each L_i and 2 vectors each equal to j. This gives the familiar tetrahedron characteristic of the Racah coefficient in (8c), see Fig. 1. While this case is fairly trivial the $n = 4$ problem is not. For $n = 4$ the triangular

[5] Rotenberg, Bivins, Metropolis, and Worten, *Table of 3j and 6j Symbols*, (MIT Press, Cambridge, Massachusetts, 1959).

relations are $\Delta(L_1L_2s)$, $\Delta(L_3L_4s)$ which show that L_1, L_2, L_3, and L_4 form a closed 4-sided figure as must be true. Also, $\Delta(jjL_i)$ applied for each L_i and $\Delta(jjs)$ appears as well. The diagram for $n = 4$, shown in Fig. 2, is two tetrahedra with a common edge s. Since the common edge is not one of the vectors in the originally defined vector addition,[6] it is clear that a summation over the auxiliary angular momentum vector s must appear in the result.

For larger values of n the results follow an easily discernible pattern although the expressions for Z_n become more and more complicated as n increases. Thus,

$$\begin{aligned} Z_5 = {} & [(2L_1 + 1)(2L_2 + 1)(2L_3 + 1)(2L_4 + 1)]^{\frac{1}{2}} \\ & \times (-)^{M_5} \sum_{s_1 s_2} [(2s_1 + 1)(2s_2 + 1)]^{\frac{1}{2}} \\ & \times C(L_1L_2s_1; M_1M_2)C(L_3L_4s_2; M_3M_4) \\ & \times C(s_1s_2L_5; M_1 + M_2, M_3 + M_4) \\ & \times W(jL_1jL_2; js_1)W(jL_3jL_4; js_2) \\ & \times W(js_1js_2; jL_5)\ \delta_{\mu_5 0}. \end{aligned} \tag{8e}$$

The $n = 5$ diagram consists of 3 tetrahedra with 2 common edges, s_1 and s_2, constructed so that the five L_i form a pentagon as required. One form of this is shown in Fig. 3. In general, the diagram for Z_n consists of $n - 2$ tetrahedra with $n - 3$ common edges with the n vectors L_i forming a polygon of n sides. The number of summations appearing in the expression for Z_n is always $n - 3$, it being understood that $n \geq 3$. These summations are over the auxiliary angular momenta which always appear in the topological figures as inside, and hence common, edges. The topological diagrams for any case are readily constructed from these rules. It is now seen that for $n > 3$ the Z_n are not familiar recoupling coefficients.

Since the quantities occurring in Z_n, for $n \geq 4$,

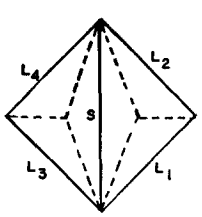

FIG. 2. Two tetrahedra with common edge describing $n = 4$. See also caption to Fig. 1. The labeling of the L values can be changed by cyclic permutation.

[6] These are the L_i and j.

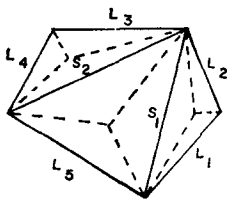

FIG. 3. Three tetrahedra with two common edges, s_1 and s_2, describing $n = 5$. See also caption to Fig. 1. The labeling of the L values can be changed by cyclic permutation.

constitute new constructs in the field of Racah algebra they should be interesting to study in their own right. Some of their properties emerge from a study of the symmetries of Z_n.

The most obvious symmetry property is that Z_n is unchanged by any cyclic permutation of the indices 1 to n.[7] Another symmetry property follows from consideration of the trace of the Hermitian conjugate operators. Thus, from the fact that $\mathbf{j}\cdot\nabla$ is Hermitian[8] it follows that

$$T_L^{M*} = (-)^M T_L^{-M}. \tag{9}$$

We make the notation more specific by writing $Z_n(M_i)$ for Z_n. Then

$$Z_n(M_i)^* = (-)^{\mu_n}\tilde{Z}_n(-M_i), \tag{10}$$

where the tilde means that the index order n, $n - 1, \cdots 1$ is to be changed into $1, 2, \cdots n$. The asterisk on Z_n means complex conjugate. From (7a) it is seen that

$$Z_n(-M_i) = (-)^{\Sigma L_i} Z_n(M_i). \tag{11}$$

The sum in the exponent is over all L_i. Also, the Z_n are manifestly real. Hence,

$$\tilde{Z}_n = (-)^{\Sigma L_i} Z_n. \tag{12}$$

That is, reversing the order of the indices (in both L and M) multiplies Z_n by a phase ± 1. Other symmetry rules are obviously obtained by combining this result with the invariance of the trace under cyclic permutations. Simultaneous inversion of the index order and changing the sign of all the M_i leaves Z_n unchanged. No other nontrivial symmetry relations exist unless it is assumed that some or all of the $T_{L_i}^{M_i}$ commute or anticommute. In this connection it may be remembered that two tensor components commute if for both of them $M_i = 0$.

[7] The lack of symmetry in (8e) is only apparent as may be seen by applying the Biedenharn-Elliott sum rule after performing a Racah recoupling to eliminate s_1 of s_2, see reference 1, Eq. (6.15).

[8] The operators j and ∇ operate in different spaces. We are concerned here only with the space in which j operates.

If all $M_i = 0$ it follows from (11) that $\sum L_i$ is even or that $Z_n = 0$. Obviously, Z_n is then invariant under all permutations of the L_i.

As an application of the foregoing consider a spin **j** coupled to a spin **s** by the invariant interaction

$$H = K \sum_M (-)^M T_L^M(\mathbf{j}) T_L^{-M}(\mathbf{s})$$

where K is a constant, $T_L^M(\mathbf{s})$ is constructed in exactly the same way as $T_L^M(\mathbf{j})$. The evaluation of a trace of an operator in **j** space, say, $T_1^{M'}(\mathbf{j})$, will involve evaluation of a sum of terms of the form

$$\zeta_n = K^n \operatorname{Tr} T_1^{M'}(\mathbf{j}) H^n$$

For simplicity we have assumed that the total Hamiltonian contains terms which commute with H. The trace operation will now involve a summation over all states of the compound system of the two angular momenta, **j** and **s**. For example, if **j** and **s** represent nuclear and electronic spins the trace involves summation over nuclear and electronic states. The terms with $n = 0$ and 1 vanish. Therefore, we consider

$$\zeta_2 = K^2 \operatorname{Tr} \sum_{M_1 M_2} T_1^{M'}(\mathbf{j}) (-)^{M_1+M_2} T_L^{M_1}(\mathbf{j}) T_L^{M_2}(\mathbf{j}) \times T_L^{-M_1}(\mathbf{s}) T_L^{-M_2}(\mathbf{s}).$$

The trace in **s** space gives $(-)^{M_1} \delta_{M_1+M_2,0}$ so that the preceding expression reduces to

$$\zeta_2 = K^2 \operatorname{Tr} \sum_{M1} T_1^{M'} (-)^{M_1} T_L^{M_1} T_L^{-M_1}$$

and the argument **j** has been dropped. This trace vanishes unless $M' = 0$ and in that case (8c) gives the result

$$\zeta_2 = -\frac{K^2}{2} M_1 \left[\frac{3}{j(j+1)(2j+1)}\right]^{\frac{1}{2}}$$

for it. The term we have evaluated contributes to the $1/T^2$ part of the nuclear polarization induced by the interaction H. It is interesting that this result is independent of L.

III. EXPANSION OF PRODUCTS OF IRREDUCIBLE TENSORS COMPONENTS

It is clear that the product of two irreducible tensors $T_{L_1}^{M_1}$ and $T_{L_2}^{M_2}$ can be expanded into irreducible tensors T_λ^M, with $M = M_1 + M_2$. The value of Z_2 is clearly related to the coefficient of T_0^0 in this expansion. Similarly, Z_n is related to the coefficient of T_0^0 in the expansion of the product of the n tensor components appearing in (5). In particular, if

$$\prod T_{L_i}^{M_i} = \sum_\lambda C_\lambda T_\lambda^{\mu_\lambda},$$

where the product on the left is ordered as in (5), then

$$Z_n = C_0 Z_1 = C_0 (2j+1)^{\frac{1}{2}}. \tag{13}$$

It is of interest to determine the complete expansion of a product of two tensors components since from this the expansion of a product of an arbitrary number of tensors components can be obtained by a step-wise procedure.[9] The expansion of the product of the components of two tensors can be written in the form

$$T_{L_2}^{M_2} T_{L_1}^{M_1} = \sum_\lambda C(L_1 L_2 \lambda; M_1 M_2) b_\lambda(L_1 L_2) T_\lambda^{\mu_\lambda}, \tag{14}$$

where the b_λ serve to adjust the normalization. It is these quantities we wish to determine. To do this we first give b_0. This is obtained from Z_2, and from (8b) it follows that[10]

$$b_0(L_1 L_2) = [(2L_1+1)/(2j+1)]^{\frac{1}{2}} (-)^{L_1} \delta_{L_1 L_2}. \tag{15}$$

To evaluate b_λ we use Z_3 and carry out the expansion of the ordered product of the three tensor components $T_{L_i}^{M_i}$, $i = 1, 2, 3$. Thus,

$$T_{L_3}^{M_3} T_{L_2}^{M_2} T_{L_1}^{M_1} = \sum_\lambda C(L_1 L_2 \lambda; M_1 M_2) b_\lambda(L_1 L_2) \times \sum_{\lambda'} C(\lambda L_3 \lambda'; \mu_2 M_3) \times b_{\lambda'}(\lambda L_3) T_{\lambda'}^{\mu_{\lambda'}}.$$

Taking the trace we have Z_3 on the left and on the right $\lambda' = \mu_3 = 0$. Using

$$C(\lambda L_3 0; \mu_2 M_3) = (2L_3+1)^{-\frac{1}{2}} (-)^{\lambda-\mu_3} \delta_{\lambda L_3} \delta_{\mu_3 0},$$

and (15) we find

$$b_\lambda(L_1 L_2) = [(2L_1+1)(2L_2+1)]^{\frac{1}{2}} W(jL_1 jL_2; j\lambda). \tag{16}$$

This result could also be derived by evaluating the nondiagonal matrix element of (14) using (6). If (16) is substituted in the ensuing equation the standard formula of the Racah recoupling emerges.[1]

From the symmetry properties of the Racah coefficient it follows from (16) that

$$b_\lambda(L_1 L_2) = b_\lambda(L_2 L_1),$$

even though $T_{L_2}^{M_2}$ and $T_{L_1}^{M_1}$, in general, will not commute. Then it is seen that

$$T_{L_2}^{M_2} T_{L_1}^{M_1} \pm T_{L_1}^{M_1} T_{L_2}^{M_2} = \sum_\lambda C(L_1 L_2 \lambda; M_1 M_2) b_\lambda(L_1 L_2) \epsilon_\lambda T_\lambda^{\mu_\lambda}, \tag{17}$$

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[9] The range of λ values is, of course,
$$\min \Sigma_i \delta_i L_i \leq \lambda \leq \Sigma_i L_i,$$
where $\delta_i = \pm 1$ incoherently.

[10] From (15) we obtain the useful result that the scalar $\Sigma_M (-)^M T_L^M T_L^{-M} = [a_L(j)]^2 = (2L+1)/(2j+1)$.

where

$$\epsilon_\lambda = 1 \pm (-)^{L_1+L_2+\lambda}. \tag{17'}$$

It follows then that the commutator contains only those λ for which $L_1 + L_2 + \lambda$ is odd and the anticommutator contains only those λ for which $L_1 + L_2 + \lambda$ is even. A trivial example is $T^{M_2}_{L_2} \sim j_1 \sim (j_x + ij_y)$ and $T^{M_1}_{L_1} \sim j_z = j_0$. Then $L_1 = L_2 = 1$ and $M_2 = 1$, $M_1 = 0$. The commutator $j_1 j_0 - j_0 j_1$ is known[1] to be proportional to j_1. Hence, only $\lambda = 1$, $\mu_2 = 1$ appears in (17) with the lower sign, which agrees with the rule given. Again, the anticommutator $j_1 j_0 + j_0 j_1$ is proportional to T^1_2. Thus, only $\lambda = 2$, $\mu_2 = 1$ appears in (17) in this case. The fact that $\lambda = 0$ does not occur in the anticommutator is trivial since in the example considered $\mu_2 \neq 0$. If $\mu_2 = 0$, as in the case $j_1 j_{-1} + j_{-1} j_1 = j_z^2 - \mathbf{j}^2$, the trace does not vanish. In general,

$$\mathrm{Tr}\,(T^{M_2}_{L_2}, T^{M_1}_{L_1})_+ = 2(-)^{M_1}\,\delta_{\mu_2 0}\,\delta_{L_1 L_2}, \tag{18}$$

which is obvious from (8b).

The rule given above is also consistent with the fact that the trace of a commutator is always zero. Hence, $\lambda = 0$ cannot occur in (17) with the lower sign even when $L_1 = L_2$. The relations (17) are generalizations of the commutation rules for the angular momentum operators; for $L_1 = L_2 = 1$ the commutator in (17) involves $\lambda = 1$ only and we obtain

$$(j_{M_2}, j_{M_1})_- = \sqrt{2}\, C(111; M_1 M_2) j_{M_1+M_2} \tag{19}$$

which are the well-known commutators[1] of the spherical components of $\mathbf{j}$.

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The Quantum-Mechanical Scattering Problem*†

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The purpose of this paper is threefold: to provide a mathematically rigorous formulation of the quantum-mechanical scattering problem from the time-independent point of view as has been done by Jauch from the time-dependent point of view, to establish a union between the two formulations, and to investigate the necessity of the asymptotic condition which occurs as a postulate in the time-dependent formulation. The formulation of the problem depends only on the "total" and "free" Hamiltonian operators. Under the conditions necessary for the time-dependent formulation, the wave operators defined by the asymptotic limits provide a unique solution of this problem. The possibility that solutions can exist when the asymptotic conditions are not valid is investigated by defining wave operators by an integral representation. The conditions sufficient for these to provide a unique solution are shown to be possibly weaker than the asymptotic conditions; there may be a class of Hamiltonian operators for which such solutions exist but for which the asymptotic limits do not. An explicit characterization of such a set of Hamiltonian operators is not achieved, but this question of the necessity of the asymptotic condition has been reduced to a specific mathematical problem. It is hoped that this paper will find a reader who is able to carry the mathematical investigation further.

I. INTRODUCTION

THE development of descriptions of scattering by quantum-mechanical theories has been marked by a shift from a time-independent to a time-dependent point of view as these theories have evolved from elementary wave mechanics to quantum field theory. In wave mechanics one solves the Schrödinger equation to find the wave functions which represent the stationary state of the Hamiltonian which describes the interacting system. The boundary conditions corresponding, for example, to an incident beam and outgoing scattered particles are readily applied, and the flux of particle probability current calculated from the resulting solution yields the scattering cross section. But the formulation of such boundary conditions becomes increasingly more difficult as the problems considered become more complicated than those involving the scattering of a fixed number of particles by potentials which are functions of their positions. Hence it has been advantageous to adopt a time-dependent formalism in which one considers time-dependent state vectors. Taking the limit of these (in the interaction picture) for infinitely positive and negative times serves as a substitute for applying the boundary conditions of incoming and outgoing scattered waves. This formalism has been an important factor in the development of the present form of quantum field theory in which the description of scattering depends on an asymptotic condition requiring the existence of limits of the field operators for infinitely past and future times. One would like to know to what extent such an asymptotic condition postulate is necessary, if it could be replaced by a weaker condition which is physically understandable but still gives the correct description of scattering, and if such a postulate could be understood just as well within the stationary state picture of scattering as within the time-dependent picture.

In this paper we will study the relation between the time-dependent and time-independent formalisms of scattering and the necessity of the asymptotic condition for a quantum mechanical system described by the "total" and "free" Hamiltonian operators. The asymptotic condition to which we refer is that of strong convergence as a parameter becomes infinite. This is considerably simpler than the asymptotic condition used in quantum field theory both from a physical and mathematical point of view. In general, our treatment will correspond to the usual formulation of nonrelativistic quantum mechanics. By thus limiting our study to a relatively simple mathematical structure we will be able to maintain complete mathematical rigor; we can use the mathematics of functional analysis to ensure that all the quantities we use are well defined and that our results are rigorously derived. We will not, for example, use such nonexisting quantities as eigenvectors of operators which have a purely con-

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tinuous spectrum. But before we begin the rigorous treatment it will be helpful to consider a brief nonrigorous outline of the two types of scattering formalism.

According to the time-independent approach[1,2] one finds the eigenstates ψ of the total Hamiltonian, $H = H_0 + V$, with eigenvalues E in the continuous spectrum, by considering the interaction V as a perturbation with eigenstates ϕ of the "free" Hamiltonian H_0 with identical eigenvalues E as the unperturbed states. From

$$(H_0 + V)\psi = E\psi, \qquad H_0\phi = E\phi$$

we get

$$(E - H_0)\psi = (E - H_0)\phi + V\psi.$$

The two solutions of this equation

$$\psi^{(\pm)} = \phi + \lim_{\epsilon\to 0^+} \frac{1}{E - H_0 \pm i\epsilon} V\psi^{(\pm)} \tag{1.1}$$

or, after iteration,

$$\psi^{(\pm)} = \phi + \lim_{\epsilon\to 0^+} \frac{1}{E - H_0 \pm i\epsilon} V\phi + \lim_{\epsilon\to 0^+} \frac{1}{E - H_0 \pm i\epsilon} V \lim_{\epsilon\to 0^+} \frac{1}{E - H_0 \pm i\epsilon} V\phi + \cdots \tag{1.2}$$

are identified as containing the "plane-wave" state ϕ plus "outgoing" and "incoming" scattered waves, respectively.

The scattering amplitude is then constructed as follows: If $\psi_n^{(+)}$ is a certain "outgoing wave" solution which reduces to the "free" state ϕ_n as the interaction vanishes, we want to known the probability amplitude $(\psi_m^{(-)}, \psi_n^{(+)})$ for observing, in this state, scattered particles as they would be measured in the "incoming-wave" state $\psi_m^{(-)}$ which reduces to the "free" solution ϕ_m. If we define wave operators $\Omega_\pm$ by

$$\psi^{(\pm)} = \Omega_\pm\phi \tag{1.3}$$

and a scattering operator S by

$$S = \Omega_-^+\Omega_+, \tag{1.4}$$

then the scattering amplitude has the form

$$(\psi_m^{(-)}, \psi_n^{(+)}) = (\Omega_-\phi_m, \Omega_+\phi_n) = (\phi_m, S\phi_n). \tag{1.5}$$

From this point of view the time development of the system is not to be considered: The system is described as being in a stationary state of the total Hamiltonian which differs from a stationary state of the unperturbed Hamiltonian only by the presence of "outgoing" scattered "waves." The scattering amplitude gives the probability for observing a stationary state of the total Hamiltonian which differs from a stationary state of the "free" Hamiltonian only by the presence of "incoming" scattered waves. We note here that the eigenstates of the unperturbed Hamiltonian need not in general describe free particles. Indeed it is common practice to use Coulomb wave functions, for example, to describe the unperturbed states.[3]

The central position of the time-dependent approach in the formalism of field theory[4] has resulted in much attention (see Sec. 2) being given to this method of describing scattering.[5-8] The system is described by a time-dependent state vector in the interaction representation. If these vectors at different times t, t_0 are related by the unitary transformation $U(t, t_0)$ then it follows from the Schrödinger equation that

$$i(\partial/\partial t)U(t, t_0) = V(t)U(t, t_0), \tag{1.6}$$

where

$$V(t) = e^{iH_0t}Ve^{-iH_0t}$$

with the boundary conditions

$$U(t_0, t_0) = 1$$

and

$$U(t, t_0) = U^+(t_0, t), \quad U(t_1, t)U(t, t_0) = U(t_1, t_0).$$

An explicit form for this operator is

$$U(t, t_0) = e^{iH_0t}e^{-iH(t-t_0)}e^{-iH_0t}. \tag{1.7}$$

In the distant past the scattering system is thought to consist of widely separated parts so that the interaction potential V is ineffective and the system can be represented by an eigenstate, say, ϕ_n, of the free Hamiltonian H_0. During the time interval

[1] P. A. M. Dirac, *Principles of Quantum Mechanics* (Clarendon Press, Oxford, England, 1958), Chap. 8, Fourth Ed.

[2] C. Møller, Kgl. Danske Videnskab Selskab, Mat.-fys. Medd. **23**, No. 1 (1945).

[3] For a more complete review of the time-independent method and its relation to the time-dependent approach see S. T. Ma, Phys. Rev. **87**, 652 (1952).

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[5] B. Lippman and J. Schwinger, Phys. Rev. **79**, 469 (1950).

[6] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).

[7] H. S. Snyder, Phys, Rev. **83**, 1154 (1951).

[8] J. M. Jauch and F. Rohrlich, *Theory of Photons and Electrons*, (Addison Wesley Publishing Company, Reading, Massachusetts, 1955), Chap. 7, provides a review of both the time-dependent and time-independent methods.

$-\infty < t < \infty$ the interaction causes the state of the system to change according to the transformation U. In the remote future the system separates again into noninteracting parts so that its state vector approaches an eigenstate of the free Hamiltonian. The scattering amplitude is taken to be the probability amplitude for observing, as $t \to +\infty$, the eigenstate ϕ_m of H_0, for the case that the system was initially (as $t \to -\infty$) described by the eigenstate ϕ_n. If we let

$$S = \lim_{\substack{t\to\infty,\\ t_0\to-\infty}} U(t, t_0) \tag{1.8}$$

then the scattering amplitude is

$$(\phi_m, S\phi_n).$$

The limits in Eq. (1.8) play a critical role in this formulation. Suppose that ψ represents the state of the scattering system at $t = 0$. Then at any other time the state of the system is represented by $e^{-iHt}\psi$. Now we have stated that as $t \to \pm\infty$ we wish this to behave as if the interaction were ineffective. That is we require the existence of vectors ϕ_{in} and ϕ_{out} such that

$$\begin{aligned} e^{-iHt}\psi &\to e^{-iH_0t}\phi_{\text{in}} \quad \text{as} \quad t \to -\infty \\ e^{-iHt}\psi &\to e^{-iH_0t}\phi_{\text{out}} \quad \text{as} \quad t \to +\infty . \end{aligned} \tag{1.9}$$

This is equivalent to[9]

$$e^{iHt}e^{-iH_0t}\phi_{\text{in,out}} \to \psi \quad \text{as} \quad t \to \mp\infty . \tag{1.10}$$

But any eigenstate of the free Hamiltonian with the eigenvalue belonging to the continuum is elegible to be an initial (in) or final (out) state. So if we assume, as is usually done, that H_0 has no bound states, then the "in" and "out" vectors span the whole space and the

$$\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t} = U(0, \mp\infty) \tag{1.11}$$

exists, and so does the scattering operator

$$\begin{aligned} S = U(\infty, -\infty) &= U(\infty, 0)U(0, -\infty) \\ &= U^+(0, \infty)U(0, -\infty). \end{aligned} \tag{1.12}$$

Comparing the above with Eqs. (1.3) and (1.4) and the preceding discussion shows that the connection between the two methods can be established by the identification

$$\Omega_{\mp} = U(0, \mp\infty). \tag{1.13}$$

The importance and validity of the asymptotic condition, Eq. (1.9) or (1.11), have been given much consideration.[10,11] Various devices such as an exponential cutoff of the interaction in time[5] or the averaging of the preparation of the initial state[6] have been used to ensure the existence of the limits. We only wish to note that the latter method leads to the formulas

$$\begin{aligned} U(0, -\infty) &= \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t}e^{iHt}e^{-iH_0t}\, dt \\ U(0, +\infty) &= \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}\, dt. \end{aligned} \tag{1.14}$$

It has been observed[3,5,6,10,12] that the time-dependent formulation, even with these methods of forcing the asymptotic condition, should give the same results as the time-independent formulation, as indicated by Eq. (1.13).

In the next section we will continue the review of the time-dependent formulation of scattering by outlining the mathematically rigorous treatment given by Jauch,[13] and the mathematical investigations of the conditions under which the asymptotic limits exist and render this treatment applicable.

It is to be emphasized that while much attention has been given to the rigorous formulation of the problem from the time-dependent point of view, there has been no mathematically satisfactory formulation of scattering theory according to the stationary-state approach. In Sec. 3 we will give a treatment of the problem which reflects the time-independent point of view, setting up a rigorous mathematical problem whose solutions define the wave operators of Eq. (1.3). This formulation is not limited by any dependence on configuration space methods.

In the following section we show how this problem is closely related to the time-dependent treatment given by Jauch and that, under the asymptotic conditions required in this treatment, the wave operators given by Jauch also provide a unique solution of the stationary state problem.

Since the asymptotic conditions do not enter the stationary-state problem, there is the possibility that solutions may be found even when the asymptotic limits do not exist. In Sec. 5 we explore this possibility by developing an integral representation

[9] The convergence in (1.9) and (1.10) is strong convergence; hence
$\lim_{t\to\mp\infty} ||\exp(-iHt)\psi - \exp(-iH_0t)\phi|| = ||\psi - \exp(iHt)\exp(-iH_0t)\phi||$
establishes the equivalence of (1.9) and (1.10).

[10] M. N. Hack, Phys. Rev. **96**, 196 (1954).
[11] H. E. Moses, Nuovo cimento **1**, 103 (1955).
[12] F. Coester, M. Hammernesh, and K. Tanaka, Phys. Rev. **96**, 1142 (1954).
[13] J. M. Jauch, Helv. Phys. Acta **31**, 127 (1958).

for the wave operators which, in the case that the asymptotic limits exist, have been shown by Jauch to equal the wave operators of the time-dependent formulation. We show that these wave operators provide a unique solution to the stationary-state problem whenever they exist and are partially isometric operators connecting the continuum subspaces of the free and total Hamiltonians.

In the following section we investigate the conditions under which these wave operators (when they exist) have the partially isometric property necessary and sufficient for a solution of the scattering problem. No necessary and sufficient conditions are given. We do show in a direct way how the conditions which have most often been used to prove the existence of the asymptotic limits can be used to prove the isometric property of these wave operators. We also show that the requirements that these wave operators have the isometric property are not stronger, and possibly weaker, than the asymptotic conditions necessary for the time-dependent formulation. Consequently there may be a class of Hamiltonians for which a solution of the scattering problem exists, but for which the asymptotic conditions are not valid. We have not been able to find any explicit characterization of such a set of Hamiltonian operators. But this question of the necessity of the asymptotic condition has been reduced to a specific mathematical problem. It is hoped that this paper will find a reader who is able to carry the mathematical investigation further.

2. TIME-DEPENDENT FORMULATION OF SCATTERING

We consider the description of a quantum-mechanical system in terms of operators on a (separable) Hilbert space $\mathfrak{H}$. In particular the "free" and "total" Hamiltonians are represented by linear, self-adjoint operators H_0 and H, respectively. Let $\mathfrak{K}_0$ and $\mathfrak{K}$ be the subspaces of $\mathfrak{H}$ spanned by the eigenvectors of H_0 and H, respectively, and let $\mathfrak{M}_0 = \mathfrak{K}_{0\perp}$ and $\mathfrak{M} = \mathfrak{K}_\perp$ be their orthogonal complements or the continuum subspaces[14] of H_0 and H, respectively. Let P_0 and P be the projections on $\mathfrak{M}_0$ and $\mathfrak{M}$, respectively.

In order to define the operators necessary for a description of scattering, Jauch[13] imposed the following two conditions on the Hamiltonians (we give these as slightly generalized by Kuroda[15]). For any $\phi \in \mathfrak{H}$ the strong limits

$$\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t}P_0\phi = \Omega_\mp\phi \tag{I}$$

exist. This defines the wave operators $\Omega_\mp$. Let $\mathfrak{R}^\mp$ be the ranges of the wave operators. The second requirement is that

$$\mathfrak{R}^+ = \mathfrak{R}^- = \mathfrak{M}. \tag{II}$$

The first requirement is the asymptotic condition. The second is characteristic of single-channel scattering; it ensures that the continuum states of H are the possible states of the scattering system at $t = 0$ and the continuum states of H_0 are the "in" and "out" states. The scattering operator may then be defined by

$$S = \Omega_-^+\Omega_+ . \tag{2.1}$$

It has then been shown[13,15] that these operators have all the properties needed for the description of scattering. It will be useful to state some of these here: The wave operators are partially isometric operators[16] mapping $\mathfrak{M}_0$ to $\mathfrak{M}$. That is,

$$\Omega_\mp\mathfrak{M}_0 = \mathfrak{M}$$

$$||\Omega_\mp\phi|| = ||\phi|| \quad \text{for} \quad \phi \in \mathfrak{M}_0$$

$$\Omega_\mp\phi = 0 \quad \text{for} \quad \phi \in \mathfrak{K}_0 = \mathfrak{M}_0^\perp$$

or equivalently,

$$\Omega_\mp^+\Omega_\mp = P_0 \tag{2.2}$$

$$\Omega_\mp\Omega_\mp^+ = P. \tag{2.3}$$

If $\mathfrak{M}_0 = \mathfrak{H}$ (H_0 has no bound states) then $\Omega_\mp$ are isometric; $\Omega_\mp^+\Omega_\mp = 1$. If also $\mathfrak{M} = \mathfrak{H}$ (H has no bound states) then $\Omega_\mp$ are unitary; $\Omega_\mp\Omega_\mp^+ = 1$ also. The scattering operator S is a partially isometric operator which is unitary in $\mathfrak{M}_0$

$$S^+S = SS^+ = P_0 \tag{2.4}$$

and commutes with the part of H_0 in $\mathfrak{M}_0$

$$SH_0P_0 = H_0P_0S. \tag{2.5}$$

The wave operators have the intertwining property

$$e^{iHt}\Omega_\mp = \Omega_\mp e^{-iH_0t} \quad \text{for all real} \quad t, \tag{2.6}$$

and the part of H in $\mathfrak{M}$ is unitarily equivalent to the part of H_0 in $\mathfrak{M}_0$

$$\begin{aligned} HP\Omega_\mp &= \Omega_\mp H_0P_0 \\ \Omega_\mp^+HP &= H_0P_0\Omega_\mp^+. \end{aligned} \tag{2.7}$$

[14] See, e.g., M. H. Stone, "Linear Transformations in Hilbert Space," American Math. Soc. Colloquium Publ. 15, Theorem 5.13.

[15] S. T. Kurtoda, Nuovo cimento **12**, 431 (1959).

[16] F. J. Murray and J. von Neumann, Ann. Math. **37**, 116 (1936), Sec. 4.3.

The wave operators have the integral representations

$$\begin{aligned}
\Omega_+ &= \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \, dt \\
\Omega_+^+ &= \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} e^{-iHt} \, dt \\
\Omega_- &= \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \, dt \\
\Omega_-^+ &= \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} e^{-iHt} \, dt.
\end{aligned} \tag{2.8}$$

We can form the operators

$$\Omega_\pm(t) = e^{iH_0 t} \Omega_\pm e^{-iH_0 t}.$$

By Eqs. (2.6), (I), (2.1), and (2.2) these have the properties that

$$\lim_{t\to\mp\infty} \Omega_\pm(t) = P_0$$

$$\lim_{t\to\infty} \Omega_+(t) = S, \qquad \lim_{t\to-\infty} \Omega_-(t) = S^+$$

$$i(\partial/\partial t)\Omega_\pm(t) = V(t)\Omega_\pm(t),$$

which, comparing with the discussion of Eqs. (1.6)–(1.8) allows us to make the identification

$$\Omega_\pm(t) = U(t, \mp\infty)$$

in agreement with Eqs. (1.11), (1.12), and (1.13).

These considerations provide a rigorous mathematical treatment of the scattering problem, from the time-dependent approach, whenever conditions (I) and (II) are valid. There have been several investigations[15,17–21] which provide conditions under which the asymptotic limits (I) exist. These have, for the most part, used the common result that when we can define $V = H - H_0$ with a domain $\mathfrak{D}(V)$ dense in $\mathfrak{M}_0$, and when there is a subset $\mathfrak{D}$ of $\mathfrak{M}_0$ such that the linear manifold determined by $\mathfrak{D}$ is dense in $\mathfrak{M}_0$ and $e^{-iH_0 t}\mathfrak{D} \subset \mathfrak{D}(V)$, it is sufficient for the existence of the limits (I) that for any $\phi \in \mathfrak{D}$

$$\int_{-\infty}^{\infty} ||Ve^{-iH_0 t}\phi|| \, dt < \infty. \tag{2.9}$$

Roughly speaking, it has been shown that for integral operators V this is true if V falls off at infinity faster than r^{-1}.

In order that condition (II) be valid, Kuroda[15] has shown that it is necessary and sufficient that the (strong) limits

$$\lim_{t\to\mp\infty} e^{iH_0 t} e^{-iHt} P\phi \tag{2.10}$$

also exist. Sufficient conditions for the existence of these limits have been found.[22] They provide a generalization of earlier investigated sufficient conditions[23,24] which required the trace of $|V|$ to be finite. We note that under these conditions Kuroda also proves the (strong) continuity of the wave operators and the scattering operator with respect to V (or with respect to H).

3. FORMULATION OF THE SCATTERING PROBLEM

We now want to provide a rigorous formulation of the scattering problem from the stationary-state point of view. Let, H, H_0, P, P_0 be defined as in the previous section on the separable Hilbert space $\mathfrak{H}$ with the subspaces $\mathfrak{M}$, $\mathfrak{M}_0$, etc. We want linear operators $\Omega_\pm$ [see Eq. (1.3)] which map the continuum states $\phi \in \mathfrak{M}_0$ of the "free" Hamiltonian to continuum states $\psi^{(\pm)} \in \mathfrak{M}$ of the total Hamiltonian. That is, we require for the solution of the scattering problem two linear operators $\Omega_\pm$ defined everywhere on $\mathfrak{M}_0$ such that if we let

$$\psi^{(\pm)} = \Omega_\pm \phi, \qquad \phi \in \mathfrak{M}_0 \tag{3.1}$$

then

$$\psi^{(\pm)} \in \mathfrak{M}$$

or

$$\Omega_\pm \mathfrak{M}_0 \in \mathfrak{M}.$$

Furthermore we want to be able to obtain all the "stationary states" $\psi^{(\pm)}$ of the scattering system by this operator (this means, as in the time-dependent case, that we have "single-channel" scattering), and we want any continuum state of the total Hamiltonian to be such a state. Therefore we require that $\Omega_\pm$ provide a one-to-one mapping of $\mathfrak{M}_0$ onto $\mathfrak{M}$ (one-to-one correspondence between the perturbed and unperturbed states)

$$\Omega_\pm \mathfrak{M}_0 = \mathfrak{M}; \tag{3.2}$$

since we are not interested in the eigenstates (bound states) of H_0, it is convenient to let $\Omega_\pm$ map these to zero, $\Omega_\pm \mathfrak{K}_0 = 0$; then

$$\Omega_\pm \mathfrak{H} \equiv \mathfrak{R}^\pm = \mathfrak{M}. \tag{3.3}$$

If $\phi \in \mathfrak{M}_0$ is normalized then we want $\psi^{(\pm)} \in \mathfrak{M}$ to

[17] J. M. Cook, J. Math. and Phys. **36**, 82 (1957).
[18] M. N. Hack, Nuovo cimento **9**, 731 (1958).
[19] J. M. Jauch and I. I. Zinnes, Nuovo cimento **11**, 553 (1959).
[20] T. A. Green and O. E. Lanford, III, J. Math. Phys. **1**, 139 (1960).
[21] T. Ikeba, Arch. Ratt. Mech. Anal. **5**, 1 (1960).
[22] S. T. Kuroda, J. Math. Soc. Japan (a) **11**, 247 (1959); (b) **12**, 243 (1960).
[23] M. Rosenblum, Pacific J. Math. **7**, 997 (1957).
[24] T. Kato, J. Math. Soc. Japan, **9**, 239 (1957); Proc. Japan Acad. **33**, 260 (1957).

also be normalized. Hence we require

$$||\Omega_\pm\phi|| = ||\phi|| \quad \text{for} \quad \phi \in \mathfrak{M}_0. \tag{3.4}$$

Therefore $\Omega_\pm$ must be partially isometric operators[16] from $\mathfrak{M}_0$ to $\mathfrak{M}$, or equivalently they must satisfy the equations

$$\begin{aligned} \Omega_\pm^+\Omega_\pm &= P_0 \\ \Omega_\pm\Omega_\pm^+ &= P. \end{aligned} \tag{3.5}$$

(Then $\Omega_\pm^+$ will be a partially isometric operator from $\mathfrak{M}$ to $\mathfrak{M}_0$.)

Now we require that

$$H\Omega_\pm P_0 = \Omega_\pm H_0 P_0.$$

Since $\Omega_\pm\phi = 0$ for $\phi \in \mathfrak{M}_{0\perp}$ and $\mathfrak{M}_0$ reduces H_0,[14] this is equivalent to

$$H\Omega_\pm = \Omega_\pm H_0. \tag{3.6}$$

By taking the adjoint of this, it follows that

$$\Omega_\pm^+ H = H_0\Omega_\pm^+. \tag{3.7}$$

Now we can observe, if we allow ourselves the luxury of using (nonexisting) eigenvectors of H_0 and H with eigenvalues in the continuous spectrum, that the requirement (3.6) is equivalent to the requirement of the nonrigorous formulation that: ϕ is an eigenvector of H_0 with eigenvalue E in the continuous spectrum if and only if $\psi^{(\pm)} = \Omega_\pm\phi$ are eigenvectors of H with the same eigenvalue. Let (3.6) be valid. Then if $H_0\phi = E\phi$ we have

$$H\psi^{(\pm)} = H\Omega_\pm\phi = \Omega_\pm H_0\phi = \Omega_\pm E\phi = E\psi^{(\pm)}$$

and if $H\psi^{(\pm)} = E\psi^{(\pm)}$, then

$$H_0\phi = H_0\Omega_\pm^+\psi^{(\pm)} = \Omega_\pm^+ H\psi^{(\pm)} = \Omega_\pm^+ E\psi^{(\pm)} = E\phi.$$

Conversely if $H_0\phi = E\phi$ and $H\Omega_\pm\phi = E\Omega_\pm\phi$, then

$$H\Omega_\pm\phi = E\Omega_\pm\phi = \Omega_\pm E\phi = \Omega_\pm H_0\phi.$$

But since such eigenvectors ϕ span $\mathfrak{M}_0$ this implies (3.6).

Now if we are going to be mathematically rigorous we can not use eigenstates corresponding to eigenvalues in continuous spectrum of the Hamiltonian. But we can retain some of their fundamental physical interpretations. In particular if ϕ and $\psi^{(\pm)} = \Omega_\pm\phi$ are eigenvectors with eigenvalue E of H_0 and H, respectively, which represent, at $t = 0$, the states of physical systems described by these Hamiltonians, then at any time t these states will be represented by

$$\phi(t) = e^{-iH_0t}\phi = e^{-iEt}\phi$$

and

$$\psi^{(\pm)}(t) = e^{-iHt}\psi^{(\pm)} = e^{-iEt}\psi^{(\pm)},$$

i.e., they are stationary states and since they have the same energy eigenvalue they have the same time dependence. But even in the rigorous case where the states are not represented by eigenvectors we have that

$$\psi^{(\pm)}(t) = e^{-iHt}\psi^{(\pm)} = e^{-iHt}\Omega_\pm\phi = \Omega_\pm e^{-iH_0t}\phi = \Omega_\pm\phi(t)$$

so that the perturbed and unperturbed states have essenentially the same time dependence.

Here we have used the fact that (3.6) is equivalent to

$$e^{-iHt}\Omega_\pm = \Omega_\pm e^{-iH_0t} \tag{3.8}$$

for all real t. This can be proved as follows. We introduce the two families of projection operators F_λ, E_λ, $-\infty < \lambda < \infty$ which provide a spectral representation of the operators H and H_0, respectively. That is, if $\phi, \psi \in \mathfrak{H}$ we have that

$$(\phi, H\psi) = \int_{-\infty}^{\infty} \lambda\, d(\phi, F_\lambda\psi)$$

and

$$(\phi, H_0\psi) = \int_{-\infty}^{\infty} \lambda\, d(\phi, E_\lambda\psi).$$

Let $H\Omega_\pm = \Omega_\pm H_0$. This means that if ϕ belongs to the domain of H_0, then $\Omega_\pm\phi$ belongs to the domain of H and

$$H\Omega_\pm\phi = \Omega_\pm H_0\phi$$

and conversely, if $\Omega_\pm\phi$ belongs to the domain of H, then ϕ belongs to the domain of H_0 and the above equality is valid. By induction we can prove that

$$H^n\Omega_\pm = \Omega_\pm H_0^n$$

for any positive integer n. For if this is true, we have that ϕ belongs to the domain of H_0^n if and only if ϕ belongs to the domain of $H^n\Omega_\pm$, in which case

$$H^n\Omega_\pm\phi = \Omega_\pm H_0^n\phi.$$

If, in addition, $H^n\Omega_\pm\phi$ belongs to the domain of H, or equivalently if ϕ belongs to the domain of $H^{n+1}\Omega_\pm$, then $\Omega_\pm H_0^n\phi$ belongs to the domain of H and

$$H^{n+1}\Omega_\pm\phi = H\Omega_\pm H_0^n\phi.$$

But if $\Omega_\pm H_0^n\phi$ belongs to the domain of H, then $H_0^n\phi$ belongs to the domain of H_0, or equivalently, ϕ belongs to the domain of H_0^{n+1}, and

$$H^{n+1}\Omega_\pm\phi = H\Omega_\pm H_0^n\phi = \Omega_\pm H_0^{n+1}\phi.$$

By reversing the argument, one can show that if ϕ belongs to the domain of H_0^{n+1}, then $\Omega_\pm\phi$ belongs to the domain of H^{n+1} with the above equality again being valid. Hence

$$H^{n+1}\Omega_\pm = \Omega_\pm H_0^{n+1},$$

which completes the proof of the induction procedure. From this we obtain that

$$P(H)\Omega_{\pm} = \Omega_{\pm}P(H_0)$$

where $P(x)$ is any polynomial in x. This can be extended to obtain[25]

$$e_\lambda(H)\Omega_{\pm} = \Omega_{\pm}e_\lambda(H_0) \quad \text{for all real} \quad \lambda,$$

where $e_\lambda(x) = 1$ for $x \leq \lambda$, and $e_\lambda(x) = 0$ for $x > \lambda$: or equivalently we have that

$$F_\lambda\Omega_{\pm} = \Omega_{\pm}E_\lambda.$$

For any ϕ, ψ belonging to $\mathfrak{H}$ it follows that

$$\int_{-\infty}^{\infty} e^{-i\lambda t}\, d(\psi, F_\lambda\Omega_{\pm}\phi) = \int_{-\infty}^{\infty} e^{-i\lambda t}\, d(\psi, \Omega_{\pm}E_\lambda\phi)$$

for all real t, which is the precise statement of the desired result that

$$e^{-iHt}\Omega_{\pm} = \Omega_{\pm}e^{-iH_0t}$$

for all real t. Conversely, if the above equality is valid for all real t, the uniqueness of the Fourier transform implies that for any ψ, ϕ belonging to $\mathfrak{H}$

$$(\psi, F_\lambda\Omega_{\pm}\phi) = (\psi, \Omega_{\pm}E_\lambda\phi)$$

for all real λ. From this it follows that ϕ belongs to the domain of H_0 if and only if $\Omega_{\pm}\phi$ belong to the domain of H, in which case

$$(\psi, H\Omega_{\pm}\phi) = \int_{-\infty}^{\infty} \lambda\, d(\psi, F_\lambda\Omega_{\pm}\phi)$$

$$= \int_{-\infty}^{\infty} \lambda\, d(\psi, \Omega_{\pm}E_\lambda\phi) = (\psi, \Omega_{\pm}H_0\phi),$$

or equivalently

$$H\Omega_{\pm} = \Omega_{\pm}H_0.$$

While we can not have states with an exact value of the energy in the continuous spectrum, we can have states with an arbitrarily small spread in the energy about some mean value E. An example of such states can be constructed as follows. If H is a self-adjoint operator, it can be approximated by $H - A$, where A is completely continuous and symmetric, such that $H - A$ has a pure point spectrum but the limit points of the spectrum of H and of the spectrum of $H - A$ are the same.[26] Since A is completely continuous there exists a set of basis vectors ϕ_k in $\mathfrak{H}$ such that for any $\psi \in \mathfrak{H}$

$$A\psi = \sum_k \mu_k(\phi_k, \psi)\phi_k$$

$$(\phi_k, \phi_i) = \delta_{ij}$$

where μ_k are the eigenvalues of A. Then

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

$$= \sum_{kj} \mu_k\mu_j(\phi_k, \psi)(\phi_j, \psi)^*(\phi_j, \phi_k)$$

$$= \sum_k \mu_k^2\, |(\psi, \phi_k)|^2.$$

If ψ has unit norm, we have

$$|(\psi, \phi_k)|^2 \leq ||\psi||^2\, ||\phi_k||^2 = 1$$

so that

$$||A\psi||^2 \leq \sum_k \mu_k^2.$$

Now in our approximation of H by $H - A$ we can choose A so that $\sum_k \mu_k^2$ is arbitrarily small.[26] Since the limit points of the spectra of H and $H - A$ are the same, given any point in the continuous spectrum of H, there is a point E arbitrarily close to it which is an eigenvalue of $H - A$. Thus there exists a vector ϕ with unit norm such that

$$(H - A)\phi = E\phi$$

or

$$(H - E)\phi = A\phi.$$

Such state vectors can be seen to have arbitrarily small dispersion of the energy. For

$$(\phi, (H - E)^2\phi) = ((H - E)\phi, (H - E)\phi)$$

$$= (A\phi, A\phi) = ||A\phi||^2$$

$$\leq \sum_k \mu_k^2$$

can be chosen to be arbitrarily small.

The time dependence of these states can be made to approximate, over some finite interval, that of a stationary state. The mean value and second moment of the energy will be preserved in time and they will be the same for the perturbed and unperturbed states

$$(\psi^{(\pm)}, H\psi^{(\pm)}) = (\Omega_{\pm}\phi, H\Omega_{\pm}\phi)$$

$$= (\Omega_{\pm}\phi, \Omega_{\pm}H_0\phi) = (\phi, H_0\phi)$$

$$(\psi^{(\pm)}, H^2\psi^{(\pm)}) = (H\Omega_{\pm}\phi, H\Omega_{\pm}\phi) = (\Omega_{\pm}H_0\phi, \Omega_{\pm}H_0\phi)$$

$$= (H_0\phi, H_0\phi) = (\phi, H_0^2\phi).$$

Another requirement which is a standard part of perturbation theory is that the perturbed states reduce to the unperturbed states, $\psi^{(\pm)} \to \phi$, as the interaction vanishes, $H \to H_0$. We could require

[25] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1955), pp. 141–145.

[26] Riesz and Sz. Nagy, *Functional Analysis* (Ungar Publishing Company, New York, 1955), p. 367.

that $\Omega_\pm$ be strongly continuous[27] as a function of H and of H_0, and that

$$\Omega_\pm \to P_0 \quad \text{if} \quad H \to H_0. \tag{3.9}$$

In the particular case that the common domain $\mathfrak{D}(H) \cap \mathfrak{D}(H_0)$ of H and H_0 is dense in $\mathfrak{H}$ and the operator V defined by $H = H_0 + gV$ is bounded, this would imply that $\Omega_\pm$ are strongly continuous functions of g and $\Omega_\pm \to P_0$ as $g \to 0$. However, we will see that the wave operators can be uniquely determined without their satisfying this condition. It may even be desirable for some problems that they do not.[28] Hence we will not include this condition in our formulation.

Finally we need a condition which ensures us that $\Omega_\pm\phi$ correspond to the solutions with purely "outgoing" or "incoming" scattered "waves". Now Coester, Hammermesh, and Tanka[12] have shown that if we find the wave operators using perturbation theory with eigenfunctions of the Hamiltonian [Eqs. (1.1) and (1.3)] then $\Omega_\pm$ are equal to the operators $U(0, \mp\infty)$ as given by Gell-Mann and Goldberger[6] [Eqs. (1.4)]. In other words, by (3.6) we have that

$$\begin{aligned}
&\lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} \Omega_+ e^{-iH_0 t}\, dt \\
&\quad = \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} e^{-iHt}\, dt \Omega_+ = \Omega_+^+ \Omega_+ \\
&\lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} \Omega_- e^{-iH_0 t}\, dt \\
&\quad = \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} e^{-iHt}\, dt \Omega_- = \Omega_-^+ \Omega_-.
\end{aligned} \tag{3.10}$$

Since we have required that $\Omega_\pm$ satisfy Eqs. (3.15), we will select the solutions with "outgoing" and "incoming" scattered waves by imposing the conditions that

$$\begin{aligned}
&\lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} \Omega_+ e^{-iH_0 t}\, dt = P_0 \\
&\lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} \Omega_- e^{-iH_0 t}\, dt = P_0.
\end{aligned} \tag{3.11}$$

These are a weakening of the conditions of Jauch and Rohrlich[8] that

$$\lim_{t\to\mp\infty} P_0 e^{iH_0 t} \Omega_\pm e^{-iH_0 t} = P_0. \tag{3.12}$$

(Note that this would imply asymptotic conditions.) Conditions (3.11) can be obtained from (3.12) by noting that whenever the limits exist the integrals also exist and are equal to the limits. There are surely other conditions, possibly weaker, which give unique solutions $\Omega_\pm$, but Eqs. (3.11) will be convenient for our purposes. We can now summarize the conditions of Eqs. (3.5), (3.6), and (3.11) in the form of a definition of the scattering problem.

Definition: Linear operators $\Omega_\pm$ on $\mathfrak{H}$ are solutions of the scattering problem associated with the self-adjoint operators H_0 and H if they satisfy the following conditions:

(α) $\Omega_\pm$ are partially isometric operators from $\mathfrak{M}_0$ to $\mathfrak{M}$, that is

$$\Omega_\pm^+ \Omega_\pm = P_0, \qquad \Omega_\pm \Omega_\pm^+ = P.$$

(β) $e^{-iHt}\Omega_\pm = \Omega_\pm e^{-iH_0 t}$ for all real t (or equivalently $H\Omega_\pm = \Omega_\pm H_0$).

(γ)
$$\begin{aligned}
&\lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} \Omega_+ e^{-iH_0 t}\, dt = P_0 \\
&\lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} \Omega_- e^{-iH_0 t}\, dt = P_0.
\end{aligned}$$

The scattering operator is then defined by $S = \Omega_-^+ \Omega_+$ and the scattering amplitude found as in Eq. (1.5). [See discussion preceding and following Eq. (1.5)].

In this form the scattering problem does not depend in any way on a configuration space representation of the Hilbert space and hence its applicability is not limited to situations where configuration space methods are useful. It is obvious from conditions (α) and (β) that a necessary condition in order that a solution of the scattering problem exist is that the continuum parts of H and H_0 be unitarily equivalent.

4. ASYMPTOTIC LIMITS AS A SOLUTION

We now turn our attention to finding solutions of the problem formulated in the preceding section. We first notice that whenever the asymptotic conditions of the time-dependent formulation are valid the solutions obtained from this treatment are also solutions of the time-independent problem.

Theorem 1: If conditions (I) and (II) of the time-dependent treatment of scattering are valid, the operators $\Omega_\pm$ defined by the limits (I) provide a unique solution of the scattering problem.

[27] By a strongly continuous function $f(A)$ of an operator A we mean a function which is continuous from the strong operator topology to the strong operator topology, i.e., if $A_n \to A$ strongly, then $f(A_n) \to f(A)$ strongly (see Riesz and Sz. Nagy, reference 26, pp. 150, 298).

[28] That solutions which are not continuous functions of the interaction may be important in theories of elementary particles has been pointed out by R. E. Marshak and S. Okubo, Nuovo cimento 19, 1226 (1961).

Proof: The Eqs. (2.2) and (2.3) are equivalent to condition (α), and Eqs. (2.6) and (2.7) are equivalent to condition (β). We can use the integral representations of Eq. (2.8) for the wave operators $\Omega_\pm$. In the next section (see proof of Theorem 3) we will prove that if these satisfy (α) and (β) then they also satisfy (γ). We will also show there that this solution is unique. Thus we have dispensed with the proof of Theorem 1.

Note that if we consider $\Omega_\pm$ as a solution of the time-independent problem, the parameter t used in defining the limits (I) need not be interpreted as a time variable.

A result of Theorem 1 is that all the investigations which have provided sufficient conditions for the validity of conditions (I) and (II) also provide sufficient conditions for the existence of a solution of the time-independent problem.

5. INTEGRAL REPRESENTATIONS AS A SOLUTION

Since the asymptotic condition does not appear in our formulation of the scattering problem, we are led to consider the possibility that solutions of this problem exist even when the asymptotic limits fail to exist. As a means of pursuing this possibility we will develop in this section a solution which consists of wave operators in the integral form [Eq. (2.8)] which we have already used. To this end we first prove the following:

Theorem 2: Let H_0 and H be self-adjoint operators on $\mathfrak{H}$ and let $\phi, \psi \in \mathfrak{H}$. In the equations

$$\Omega_+\phi = \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \phi \, dt \tag{5.1}$$

$$\Omega_-\phi = \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \phi \, dt. \tag{5.2}$$

The integrals exist as Bochner integrals[29] and when the limits exist they define linear operators $\Omega_\pm$. The adjoints of these operators are equal to the limits of the (Bochner) integrals

$$\Omega_+^+\phi = \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} e^{-iHt} \phi \, dt \tag{5.3}$$

$$\Omega_-^+\phi = \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} e^{-iHt} \phi \, dt \tag{5.4}$$

whenever the limits exist. The integrals in these equations also always exist. The operators $\Omega_\pm$ are bounded by unity,

$$||\Omega_\pm\phi|| \leq ||\phi||$$

for all $\phi \in \mathfrak{H}$, and they have the intertwining property that

$$e^{-iHt}\Omega_\pm = \Omega_\pm e^{-iH_0 t} \tag{5.5}$$

for all real t, or equivalently that

$$H\Omega_\pm = \Omega_\pm H_0.$$

In the case that the conditions (I) and (II) of the time-dependent formulation are valid, the limits of the integrals in (5.1) and (5.2) exist and define operators identical to those defined by the asymptotic limits of (I).

Proof: Since the function

$$\epsilon e^{-\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \phi$$

is strongly measurable, and

$$\int_0^\infty ||\epsilon e^{-\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \phi|| \, dt = \int_0^\infty \epsilon e^{-\epsilon t} \, dt \, ||P_0\phi|| = ||P_0\phi|| < \infty ,$$

the integral

$$\int_0^\infty \epsilon e^{-\epsilon t} e^{iHt} e^{-iH_0 t} P_0 \phi \, dt$$

exists as a Bochner integral for any $\phi \in \mathfrak{H}$.[29] In a similar manner one can show the existence of the integrals in (5.1), (5.3), and (5.4). Since both integration and passage to the limit are linear operations, the operators $\Omega_\pm$ defined by the limits are linear. When all the limits exist we have that, for any $\psi, \phi \in \mathfrak{H}$,

$$\begin{aligned}(\psi, \Omega_-\phi) &= \lim_{\epsilon\to 0^+} \int_0^\infty \epsilon e^{-\epsilon t} (\psi, e^{iHt} e^{-iH_0 t} P_0 \phi) \, dt \\ &= \lim_{\epsilon\to 0^+} \int_0^\infty \epsilon e^{-\epsilon t} (P_0 e^{iH_0 t} e^{-iHt} \psi, \phi) \, dt \\ &= \left(\lim_{\epsilon\to 0^+} \int_0^\infty \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} e^{-iHt} \psi \, dt, \phi \right),\end{aligned}$$

which establishes the validity of Eq. (5.4). A similar argument establishes Eq. (5.3). To obtain the boundedness of these operators we write

$$\begin{aligned}||\Omega_-\phi|| &\leq \int_0^\infty \epsilon e^{-\epsilon t} \, ||e^{iHt} e^{-iH_0 t} P_0 \phi|| \, dt \\ &= \int_0^\infty \epsilon e^{-\epsilon t} \, dt \, ||P_0\phi|| = ||P_0\phi|| \leq ||\phi||\end{aligned} \tag{5.6}$$

since this is independent of ϵ. A similar inequality proves the boundedness of Ω_+. Jauch[13] (see first theorem of Sec. 5) has proved Eq. (5.5) so we will not repeat the proof here. Also Jauch has proved

[29] For the theory of Bochner integrals as used here see, e.g., E. Hille, "Functional Analysis and Semi-groups," American Math. Soc., Colloquium Publ. 31, (1948), pp. 40–48.

that in the case that conditions (I) and (II) of the time-dependent formulation are valid the wave operators defined by the limits (I) have the integral representations of Eqs. (5.1) and (5.2). Hence the proof of Theorem 2 is complete.

We can now see that, when the limits exist to define the wave operators and their adjoints by Eqs. (5.1)–(5.4) of the proceeding theorem, these operators have most of the properties necessary and sufficient for a unique solution of the scattering problem.

Theorem 3: Let the limits of the integrals of Eqs. (5.1)–(5.4) exist and let $\Omega_\pm$ be the operators defined by these equations. If they are partially isometric from $\mathfrak{M}_0$ to $\mathfrak{M}$, that is, if

$$\Omega_\pm^\dagger \Omega_\pm = P_0, \qquad \Omega_\pm \Omega_\pm^\dagger = P \tag{5.7}$$

then the wave operators $\Omega_\pm$ provide a unique solution of the scattering problem.

Proof: Equation (5.7) is condition (α). From Theorem 2 we have that condition (β) is satisfied. To prove (γ) we use Eqs. (5.7), (5.3), (5.4), and (5.5) to write

$$\begin{aligned} P_0 = \Omega_+^\dagger \Omega_+ &= \lim_{\epsilon \to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} e^{-iHt}\, dt \Omega_+ \\ &= \lim_{\epsilon \to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} \Omega_+ e^{-iH_0 t}\, dt \\ P_0 = \Omega_-^\dagger \Omega_- &= \lim_{\epsilon \to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} e^{-iHt}\, dt \Omega_- \\ &= \lim_{\epsilon \to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} \Omega_- e^{-iH_0 t}\, dt. \end{aligned}$$

Finally we must show that the solution is unique. Let $\omega_\pm$ satisfy conditions (α), (β), and (γ). Using (γ) then (β) we get that

$$\begin{aligned} P_0 &= \lim_{\epsilon \to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} \omega_+ e^{-iH_0 t}\, dt \\ &= \lim_{\epsilon \to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} P_0 e^{iH_0 t} e^{-iHt}\, dt \omega_+ = \Omega_+^\dagger \omega_+ \\ P_0 &= \lim_{\epsilon \to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} \omega_- e^{-iH_0 t}\, dt \\ &= \lim_{\epsilon \to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} P_0 e^{iH_0 t} e^{-iHt}\, dt \omega_- = \Omega_-^\dagger \omega_-. \end{aligned}$$

Taking the adjoints of these equations gives

$$\omega_+^\dagger \Omega_+ = P_0, \qquad \omega_-^\dagger \Omega_- = P_0.$$

But because of (α), $\omega_\pm$ are partially isometric operators from $\mathfrak{M}_0$ to $\mathfrak{M}$. Hence[16] $\omega_\pm^\dagger = \Omega_\pm^\dagger$ or $\omega_\pm = \Omega_\pm$ which shows that $\Omega_\pm$ are the unique solutions and completes the proof of Theorem 3.

From the above theorems we can see that the three conditions contained in our formulation of the scattering problem are sufficient to determine a unique solution. We also see that such unique solutions exist if either the asymptotic conditions of the time-dependent formulation are valid, or if the limits of the integrals in Eqs. (5.1)–(5.4) exist and define operators satisfying Eqs. (5.7). But from the point of view of perturbation theory, we might want the wave operators to be continuous functions of the Hamiltonian operators, as was mentioned in the preceding section. Therefore, it is interesting to inquire as to what further conditions might be needed if this is to be the case. The integral representation form of the wave operators gives us a method of investigating this problem.

Stated more precisely, the problem is this: Given any "free" Hamiltonian operator H_0 there is a set of Hamiltonian operators H such that the wave operators exist as the limits of the integrals of Eqs. (5.1) and (5.2) and their adjoints are the limits of the integrals of Eqs. (5.3) and (5.4) and these operators satisfy Eqs. (5.7) and hence provide a unique solution of the scattering problem. In particular this is true when the asymptotic conditions (I) and (II) are valid. We want to know if there are further conditions satisfied by a subset of these operators H which ensures that the corresponding wave operators are continuous functions of the operators H of this subset. A similar problem can be stated by interchanging the roles of H_0 and H. A partial answer to this question is given by the following:

Lemma: If for a set of Hamiltonian operators the limits of the integrals of Eqs. (5.1)–(5.4) exist and define wave operators satisfying Eqs. (5.7), a sufficient condition on this set of Hamiltonian operators in order that the wave operators be strongly continuous[27] functions of the Hamiltonian operators is that the limits of the integrals in equations (5.1) and (5.2) exist uniformly with respect to the Hamiltonian operators. This is true for the case that the asymptotic limits (I) exist uniformly with respect to the Hamiltonian operators.

Proof: Let H and H' be two Hamiltonian operators belonging to the set under consideration, and let $\Omega_\pm$ and $\Omega_\pm'$ be the respective wave operators defined by Eqs. (5.1) and (5.2). For any $\alpha > 0$ and any ϕ we need to show that

$$||\Omega'_{\pm}\phi - \Omega_{\pm}\phi|| < \alpha$$

when H' is sufficiently close to H in the strong operator topology. Since the wave operators are uniformly bounded, we need only to show that this is true for a dense set of vectors ϕ. We first note that

$$\begin{aligned}||\Omega'_{-}\phi - \Omega_{-}\phi|| \leq{}& \left|\left|\Omega'_{-}\phi - \int_0^\infty \epsilon e^{-\epsilon t}e^{iH't}e^{-iH_0t}P_0\phi\, dt\right|\right| \\ &+ \left|\left|\int_0^\infty \epsilon e^{-\epsilon t}e^{iH't}e^{-iH_0t}P_0\phi\, dt \right.\right. \\ &\left.\left. - \int_0^\infty \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi\, dt\right|\right| \\ &+ \left|\left|\int_0^\infty \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi\, dt - \Omega_{-}\phi\right|\right|.\end{aligned}$$

Since the convergence of the integral in Eq. (5.2) is assumed to be uniform in the Hamiltonian operators, we can find an $\epsilon > 0$ such that the first and last terms on the right-hand side of the above inequality are less than or equal to $\alpha/3$. Therefore we need only to show that for this ϵ the middle term is also less than or equal to $\alpha/3$ for H' sufficiently near to H. In other words, we need only to establish the continuity of

$$\int_0^\infty \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi\, dt$$

as a function of H. Let

$$\begin{aligned}x(t) &= \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi \\ x_n(t) &= x(t) \quad \text{if} \quad t \leq n \\ x_n(t) &= 0 \quad \text{if} \quad t > n;\end{aligned}$$

let $x'(t)$, $x'_n(t)$ be defined similarly with H replaced by H'. We wish to show that

$$\left|\left|\int_0^\infty x'(t)\, dt - \int_0^\infty x(t)\, dt\right|\right| \leq \frac{\alpha}{3}$$

Now

$$\begin{aligned}&\left|\left|\int_0^\infty x'(t)\, dt - \int_0^\infty x(t)\, dt\right|\right| \\ &\qquad \leq \left|\left|\int_0^\infty (x'(t) - x'_n(t))\, dt\right|\right| \\ &\qquad + \left|\left|\int_0^\infty x'_n(t)\, dt - \int_0^\infty x_n(t)\, dt\right|\right| \\ &\qquad + \left|\left|\int_0^\infty (x(t) - x_n(t))\, dt\right|\right|\end{aligned}$$

and

$$\begin{aligned}\left|\left|\int_0^\infty (x(t) - x_n(t))\, dt\right|\right| &= \left|\left|\int_n^\infty \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi\, dt\right|\right| \\ &\leq \int_n^\infty \epsilon e^{-\epsilon t}\, dt\, ||P_0\phi|| \\ &= e^{-\epsilon n}\, ||P_0\phi||\end{aligned}$$

which is independent of H so that also

$$\left|\left|\int_0^\infty (x'(t) - x'_n(t))\, dt\right|\right| \leq e^{-\epsilon n}\, ||P_0\phi||,$$

so if we pick n such that

$$e^{-\epsilon n}\, ||P_0\phi|| \leq \alpha/9,$$

we need only show that

$$\begin{aligned}&\left|\left|\int_0^\infty x'_n(t)\, dt - \int_0^\infty x_n(t)\, dt\right|\right| \\ &\qquad = \left|\left|\int_0^n \epsilon e^{-\epsilon t}e^{iH't}e^{-iH_0t}P_0\phi\, dt \right.\right. \\ &\qquad\quad \left.\left. - \int_0^n \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi\, dt\right|\right| \\ &\qquad \leq \alpha/9;\end{aligned}$$

that is, we need only establish the continuity of

$$\int_0^n \epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi\, dt$$

in H. But this follows (see Hille[29] Theorem 3.6.6) if $\epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi$ is a strongly continuous function of H, since it is bounded uniformly in H and in $t \in (0, n)$,

$$\begin{aligned}||\epsilon e^{-\epsilon t}e^{iH't}e^{-iH_0t}P_0\phi|| &= \epsilon e^{-\epsilon t}\, ||P_0\phi|| \\ &= ||\epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi|| \leq \epsilon\, ||P_0\phi||.\end{aligned}$$

A similar argument follows for the case of Ω_+.

We can establish the strong continuity of $\epsilon e^{-\epsilon t}e^{iHt}e^{-iH_0t}P_0\phi$ as a function of H if we can show that e^{iHt} is a strongly continuous function of the self-adjoint operator H. We can do this as follows: Let H_n, $n = 1, 2, 3, \cdots$, be a sequence of self-adjoint operators converging strongly to H. This means that the domain $\mathfrak{D}$ of H is within the domain of each H_n and for any vector ϕ belonging to $\mathfrak{D}$

$$||H_n\phi - H\phi|| \to 0$$

as $n \to \infty$. It can be shown that e^{iH_nt} converges strongly to e^{iHt} for all real t if the resolvent operators $(H_n - z)^{-1}$ converge strongly to the resolvent operator $(H - z)^{-1}$ for all nonreal z.[30] Now these

[30] See Kuroda, reference 22(a), proof of Eq. (4.4).

resolvent operators are bounded uniformly in H_n and H by $|\mathrm{Im}\ z|^{-1}$ (see Riesz and Nagy[26], p. 321) so they will converge to the desired limit whenever

$$||(H_n - z)^{-1}\phi - (H - z)^{-1}\phi|| \to 0$$

for a dense set of vectors ϕ. But

$$\begin{aligned}
&||(H_n - z)^{-1}\phi - (H - z)^{-1}\phi|| \\
&\quad = ||(H_n - z)^{-1}(H - z)(H - z)^{-1}\phi \\
&\qquad - (H_n - z)^{-1}(H_n - z)(H - z)^{-1}\phi|| \\
&\quad = ||(H_n - z)^{-1}(H - H_n)(H - z)^{-1}\phi|| \\
&\quad \leq |\mathrm{Im}\ z|^{-1}\ ||(H - H_n)(H - z)^{-1}\phi|| \to 0
\end{aligned}$$

for all ϕ such that $(H - z)^{-1}\phi$ belongs to $\mathfrak{D}$. But such vectors ϕ form a dense set since in fact $(H - z)^{-1}\mathfrak{H} = \mathfrak{D}$.

A similar argument establishes the continuity of Ω_- as functions of H_0. This completes the proof of the first statement of the lemma.

From the proof given by Jauch[13] of the convergence of the integral representation of the wave operators in the case that conditions (I) and (II) are valid, one can easily see that the limits of the integrals of Eqs. (5.1) and (5.2) exist uniformly with respect to the Hamiltonian operators whenever the asymptotic limits of condition (I) exist uniformly with respect to the Hamiltonian operators. This proves the second statement of the lemma.

6. CONDITIONS SUFFICIENT FOR A SOLUTION

As we have seen in the preceding section, sufficient conditions for the existence of a unique solution of the scattering problem are that the limits of the integrals of Eqs. (5.1)–(5.4) exist and that they define wave operators which satisfy Eqs. (5.7) [which are equivalent to condition (α) of the scattering problem]. In particular, this is true whenever conditions (I) and (II) of the time-dependent formulation are valid. But the problem of greatest interest would be to find if there exists a set of Hamiltonian operators for which conditions (I) and (II) are not valid, while the conditions sufficient for the existence of the integral representation solution are still satisfied. This would permit solutions which could not be treated from the time-dependent point of view, and would carry the mathematical analysis of the conditions sufficient for a solution beyond the problem of the existence of the asymptotic limits. We are unable to present any explicit characterization of such a set of Hamiltonian operators or show that such a set exists. But we can make some remarks which will clarify the problem, and we can make an argument which makes it appear quite plausible that such a set of Hamiltonian operators does exist.

First we show that if the limits of the integrals of Eqs. (5.1)–(5.4) exist and define wave operators which satisfy the first of Eqs. (5.7),

$$\Omega_-^+\Omega_- = P_0 \tag{6.1}$$

then these wave operators are partially isometric with the initial set $\mathfrak{M}_0$. This follows from the boundedness property of the wave operators and their adjoints that

$$||\Omega_-\phi|| \leq ||\phi||$$
$$||\Omega_-^+\phi|| \leq ||\phi||$$

for any $\phi \in \mathfrak{H}$. Let $\phi \in \mathfrak{M}_0$. Then

$$\Omega_-^+\Omega_-\phi = P_0\phi = \phi$$

and

$$||\phi|| = ||\Omega_-^+\Omega_-\phi|| \leq ||\Omega_-\phi|| \leq ||\phi||,$$

which implies that

$$||\Omega_-\phi|| = ||\phi||.$$

If $\phi \in \mathfrak{M}_{0\perp}$ then $P_0\phi = 0$, and

$$\Omega_-\phi = 0.$$

Hence Ω_- are partially isometric with the domain $\mathfrak{M}_0$.

The conditions sufficient for a unique solution of the scattering problem by the integral representation wave operators have thus been reduced to: the limits of the integrals in Eqs. (5.1)–(5.4) exist; the wave operators thus defined satisfy the first of Eqs. (5.7); the ranges of the wave operators coincide with $\mathfrak{M}$.

It is easy to show directly that the wave operators satisfy the first of Eqs. (5.7) under the conditions which have been used[15,17,19,21] most often to prove the existence of the asymptotic limits (I) of the time-dependent formulation.

Theorem 4: Let H and H_0 be self-adjoint operators with $V = H - H_0$ defined in the common domain $\mathfrak{D}(V) = \mathfrak{D}(H) \cap \mathfrak{D}(H_0)$ of H and H_0. Let the limits of the integrals in Eqs. (5.1)–(5.4) exist and define the wave operators Ω_-. A sufficient condition for

$$\Omega_-^+\Omega_- = P_0$$

is that there exist a set $\mathfrak{D}_0$ dense in $\mathfrak{M}_0$ such that for any $\phi \in \mathfrak{D}_0 \cap \mathfrak{M}_0$

$$e^{-iH_0t}\phi \in \mathfrak{D}(V)$$

for every real t, and

$$\int_{-\infty}^{\infty} ||Ve^{-iH_0t}\phi||\, dt < \infty .$$

[This statement corresponds to the sufficiency of these conditions for the existence of the asymptotic limits (I) of the time-dependent formulation.]

Proof: Let $\phi \in \mathfrak{D}_0 \cap \mathfrak{M}_0$. Then

$$\begin{aligned}\Omega_-^+\Omega_-\phi &= \lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\, dt \lim_{\eta\to 0^+} \\ &\times \int_0^\infty \eta e^{-\eta s}\, ds P_0 e^{iH_0t}e^{-iHt}e^{iHs}e^{-iH_0s}P_0\phi \\ &= \lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\, dt \lim_{\eta\to 0^+} \\ &\times \int_0^\infty \eta e^{-\eta s}\, ds P_0 e^{iH_0t}e^{iH(s-t)}e^{-iH_0(s-t)}e^{-iH_0t}P_0\phi .\end{aligned}$$

If we substitute (see Rosenblum,[23] Theorem 3.3)

$$e^{iH(s-t)}e^{-iH_0(s-t)} = 1 + i\int_0^{s-t} e^{iHx}Ve^{-iH_0x}\, dx$$

which is possible because

$$e^{-iH_0x}e^{-iH_0t}P_0\phi \in \mathfrak{D}(V),$$

we get that

$$\begin{aligned}\Omega_-^+\Omega_-\phi = P_0\phi &+ i\lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\, dt \lim_{\eta\to 0^+}\int_0^\infty \eta e^{-\eta s}\, ds \\ &\times \int_0^{s-t} dx P_0 e^{iH_0t}e^{iHx}Ve^{-iH_0(x+t)}P_0\phi .\end{aligned}$$

But the norm of the second term is less than or equal to

$$\begin{aligned}&\lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\, dt \lim_{\eta\to 0^+}\int_0^\infty \eta e^{-\eta s}\, ds \\ &\times \int_0^{s-t} dx\, ||Ve^{-iH_0(x+t)}P_0\phi|| \\ &\le \lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\, dt \lim_{\eta\to 0^+}\int_0^\infty \eta e^{-\eta s}\, ds \\ &\times \int_t^s dy\, ||Ve^{-iH_0y}\phi|| \\ &= \lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\, dt \int_t^0 dy\, ||Ve^{-iH_0y}\phi|| \\ &+ \lim_{\eta\to 0^+}\int_0^\infty \eta e^{-\eta s}\, ds \int_0^s dy\, ||Ve^{-iH_0y}\phi|| = 0\end{aligned}$$

whenever the limits exist. The limits clearly will exist when

$$\int_{-\infty}^{\infty} ||Ve^{-iH_0t}\phi||\, dt < \infty .$$

Hence $\Omega_-^+\Omega_-\phi = P_0\phi$ if $\phi \in \mathfrak{D}_0 \cap \mathfrak{M}_0$. Since $\mathfrak{D}_0$ is dense in $\mathfrak{M}_0$ and $\Omega_-^+\Omega_-$ is a bounded operator, this can be extended to any $\phi \in \mathfrak{M}_0$. A similar argument shows that $\Omega_+^+\Omega_+ = P_0$ and completes the proof of the theorem.

As we have already mentioned, our main interest is in comparing the conditions sufficient for a unique solution by the integral representation wave operators with the conditions (I) and (II) of the time-dependent formulation. For this purposes we recall [see Eq. (2.10)] that the latter conditions are equivalent to the existence of the limits

$$\lim_{t\to\pm\infty} e^{iHt}e^{-iH_0t}P_0\phi \qquad \text{(I)}$$

and

$$\lim_{t\to\pm\infty} e^{iH_0t}e^{-iHt}P\phi \qquad \text{(II}'\text{)}$$

for all $\phi \in \mathfrak{H}$. Now we know that whenever the limits (I) and (II′) exist the limits of the integrals of Eqs. (5.1)–(5.4) exist and are equal to the respective limits (I) and (II′). But it may be possible for the limits of the integrals of Eqs. (5.1)–(5.4) to exist when (I) and (II′) do not. Consider the analogous problem where instead of vector-valued functions of t we work with complex-valued functions of t. In this case we can make the following statements: If $f(t)$ is a complex-valued function of the real variable t, if $|f(t)|$ is bounded uniformly in t, and if $e^{-\epsilon t}f(t)$ is integrable for any $\epsilon > 0$, then if

$$\lim_{t\to\infty} f(t) \qquad (6.2)$$

exists, the limit

$$\lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}f(t)\, dt \qquad (6.3)$$

also exists and the limits (6.2) and (6.3) are identical. However, if we add to such a function another function which oscillates as $t \to \infty$, the limit (6.3) remains unchanged but the limit (6.2) does not exist. Now it could be possible that the analogous statements are valid for the vector valued functions occurring in the Eqs. (5.1)–(5.4) and in the limits (I) and (II′) and that the integral representations exist when the asymptotic limits do not.

Similarly there is a possibility that the other conditions on the integral representation wave operators, which are needed to insure that they provide a unique solution, can be satisfied when the limits (I) and (II′) do not exist. Consider the Eq. (6.1). We write this in the form that

$$(\psi, (\Omega_\pm^+\Omega_\pm - P_0)\phi) = 0$$

for any $\psi, \phi \in \mathfrak{H}$. For the case of Ω_- we can write

this out explicitly as

$$\lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}\,dt \lim_{\eta\to 0^+}\int_0^\infty \eta e^{-\eta s}\,ds(P_0\psi, \times (e^{iH_0t}e^{-iHt}e^{iHs}e^{-iH_0s} - 1)P_0\phi) = 0 \qquad (6.4)$$

which could possibly be satisfied when the limits (I) and (II′) do not exist. In fact when the limits (I) do exist we have that

$$\lim_{t\to\infty}\lim_{s\to\infty}(P_0\psi, (e^{iH_0t}e^{-iHt}e^{iHs}e^{-iH_0s} - 1)P_0\phi) = \lim_{t\to\infty}\lim_{s\to\infty}(e^{iHt}e^{-iH_0t}P_0\psi, e^{iHs}e^{-iH_0s}P_0\phi) - \lim_{t\to\infty}(e^{iHt}e^{-iH_0t}P_0\psi, e^{iHt}e^{-iH_0t}P_0\phi) = 0 \qquad (6.5)$$

which is apparently stronger than Eq. (6.4) in that limits of the form (6.2) have replaced limits of the form (6.3). The validity of Eq. (6.5) is a consequence of the following properties of strongly converging sequences of vectors in a Hilbert space: Let f_n be a sequence of vectors converging strongly to the vector f, and let g_n be a sequence of vectors converging strongly to the vector g. Let the norm of each f_n equal the norm of f and let the norm of each g_n equal the norm of g. Then

$$\lim_{n\to\infty}\lim_{m\to\infty}(f_n, g_m) = \lim_{n\to\infty}(f_n, g_n) = (f, g).$$

We can prove this by writing that

$$|(f_n, g_m) - (f, g)| \le |(f_n - f, g)| + |(f_n, g - g_m)| \le ||f_n - f||\,||g|| + ||f||\,||g - g_m||$$

which goes to zero as $n, m \to \infty$, and by writing out a similar inequality with g_m replaced by g_n and letting $n \to \infty$.

The remaining condition on the integral representation wave operators in order that they provide a unique solution is that their ranges coincide with the continuum subspace $\mathfrak{M}$ of the total Hamiltonian operator. For any vector $\phi \in \mathfrak{M}_\perp$ we must have that

$$\Omega_\pm^+\phi = 0. \qquad (6.6)$$

For the case of Ω_- this has the explicit form

$$\lim_{\epsilon\to 0^+}\int_0^\infty \epsilon e^{-\epsilon t}P_0e^{iH_0t}e^{-iHt}\phi\,dt = 0. \qquad (6.7)$$

Jauch[13] has shown that Eq. (6.7) and the similar equation for Ω_+ are valid for the case that the operator H_0 has a purely continuous spectrum. One can easily see that Jauch's proof is also good for the case where H_0 also has a point spectrum since the reduction of H_0 by its continuum subspace allows us to consider only the continuum part of this operator. Hence the condition that the ranges of $\Omega_\pm$ coincide with $\mathfrak{M}$ reduces to the requirement that for any $\phi \in \mathfrak{M}$

$$\Omega_\pm^+\phi \neq 0. \qquad (6.8)$$

For the case of Ω_- this will have the form of Eq. (6.7) with the equals sign replaced by a not-equal sign. It could be possible for this to be valid when the limits (I) and (II′) do not exist. When the latter limits do exist, Eq. (6.8) will be true with the limits of the form (6.3) as in Eq. (6.7) replaced by limits of the form (6.2), resulting in an apparently stronger condition.

By way of summary we can make the following statements:

The conditions sufficient for the integral representation wave operators to be a unique solution of the scattering problem are that: the limits of the integrals of Eqs. (5.1)–(5.4) exist; the wave operators thus defined satisfy the first of Eqs. (5.7) [Eq. (6.1)]; the ranges of these wave operators coincide with $\mathfrak{M}$.

These conditions are satisfied in the case where the conditions (I) and (II) of the time-dependent formulation are valid. Then the wave operators defined by the asymptotic limits are identical to those defined by the integral representation. Hence we have a new physical interpretation of the asymptotic limits as a solution of the stationary-state scattering problem. There is no need to interpret the parameter t occurring in these limits as having anything to do with time.

It appears to be possible, because of the possibility that limits of the form (6.3) can exist when limits of the form (6.2) do not, that the conditions sufficient for a solution are weaker than the asymptotic conditions (I) and (II). The settlement of this question has been reduced to a definite mathematical problem. One should be able either to find Hamiltonian operators for which the conditions (I) and (II) are not valid while the conditions sufficient for the integral representation solution are valid, or to prove that the former conditions are implied by the latter.

We have not been able to do either of these and hence the questions as to whether such a set of Hamiltonian operators exists as well as whether it contains any Hamiltonians of physical interest remain as unsolved problems.

We can make some observations to roughly determine what the properties of such Hamiltonian

operators would be if they exist. If we can define a self-adjoint potential operator $V = H - H_0$, then there is a nesting set of classes, defined by increasingly restrictive conditions, to which such an operator can belong: the class of all bounded self-adjoint operators (finite norm of the operator); the subclass of the latter of completely continuous operators (spectrum consists of discrete points of finite multiplicity, except possibly for the point zero); the subclass of the latter of operators with finite Schmidt norm (finite sum of squares of eigenvalues); the subclass of the latter of operators with finite-trace norm (finite trace of absolute value or finite sum of absolute values of eigenvalues). Now in order to have a solution of the scattering problem the continuum part of H_0 must be unitarily equivalent to the continuum part of H, which means that these operators must have the same continuous spectrum. But there are potential operators V having finite Schmidt norm such that H_0 has a purely continuous spectrum while H has a pure point spectrum.[26] On the other hand, the existence of the asymptotic limits has been established for potential operators which form a slightly more general class than those having finite trace norms.[22] Hence we should expect that the class of Hamiltonians which we are looking for would, if they exist, roughly correspond to potential operators forming a class intermediate between those having finite Schmidt norms and those having finite trace norms.

7. ASYMPTOTIC OPERATORS

If we have wave operators which provide a solution to a scattering problem we can use them to define "asymptotic" operators as follows. Let A be one of a set of operators defined on the continuum subspace of H. Let

$$A_{\text{in}} = \Omega_-^\dagger A \Omega_-$$

$$A_{out} = \Omega_+^\dagger A \Omega_+.$$

These will have their range and domain in the continuum subspace $\mathfrak{M}_0$ of H_0. By multiplying the second equation on the left by Ω_+ and on the right by $\Omega_+^\dagger$, and then multiplying on the left by $\Omega_-^\dagger$ and on the right by Ω_-, we get that

$$\Omega_+ A_{\text{out}} \Omega_+^\dagger = PAP$$

$$\Omega_-^\dagger \Omega_+ A_{\text{out}} \Omega_+^\dagger \Omega_- = \Omega_-^\dagger A \Omega_-$$

or

$$S A_{\text{out}} S^+ = A_{\text{in}}.$$

If the set of operators A is such that the set of operators A_{in} and the set of operators A_{out} each generate an irreducible operator ring in $\mathfrak{M}_0$, then the latter equation determines S up to a phase factor. In this case, the operators A_{in} and A_{out} can be used to provide an alternative specification of the scattering operator. In the case that the wave operators are defined by asymptotic limits, Jauch has shown that the operators A_{in} and A_{out} are the weak limits of

$$e^{-iH_0 t} e^{iHt} A e^{-iHt} e^{iH_0 t}$$

as $t \to \mp\infty$, respectively. But our definition is more general than this and does not depend on the existence of the weak limit since the wave operators may be defined, for example, by the integral representation. When these limits do exist, the parameter t need not be interpreted as a time variable. An example of an "asymptotic" operator is the continuum part of the "free" Hamiltonian operator. From the equation

$$\Omega_\pm H_0 = H \Omega_\pm$$

we get that

$$P_0 H_0 = \Omega_\pm^\dagger H \Omega_\pm$$

so that

$$P_0 H_0 = H_{\text{in}} = H_{\text{out}},$$

which is consistent with the commutability of S and H_0.

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The Quantum-Mechanical Scattering Problem. II. Multi-Channel Scattering*†

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The study reported in an earlier paper of the single channel scattering problem is extended to include the multi-channel case.

1. INTRODUCTION

In an earlier paper[1] we were concerned with a mathematically rigorous formulation of the single-channel scattering problem. This essentially time-independent method was compared with the rigorous time-dependent formulation of scattering which had been given by Jauch[2] and it was shown that, under the conditions which are necessary for the time-dependent formulation, the wave operators that are defined by the asymptotic limits provide a unique solution of the problem. The definition of wave operators by an integral representation provided a method for investigating the possibility that solutions can exist even when the asymptotic conditions are not valid, and indeed it was shown that the conditions sufficient for such solutions are possibly weaker than the asymptotic conditions. In the present paper these considerations will be extended to the multi-channel scattering problem.

The distinguishing feature of the single-channel scattering problem is that every state of the scattering system can be related to a stationary state of a single "free" Hamiltonian. The latter state is considered either as an asymptotic limit of the state of the system in the distant past or remote future or as an unperturbed state, depending on whether one views the situation from the time-dependent or time-independent point of view. In either case the continuum states of the "free" Hamiltonian correspond to the possible measurements which can be made on the system. In the time-dependent formalism they provide the initial conditions at $t = -\infty$ and a basis with respect to which the final state is analyzed at $t = +\infty$. In the stationary state formalism they form the "free" stationary states from which the interacting stationary states containing either "outgoing" or "incoming" scattered "waves" are obtained by perturbation.

A description of multi-channel scattering demands a generalization due to the fact that the "free" states to which the scattering states are made to correspond, either as asymptotic limits or as unperturbed states, can not be thought of as stationary states of a single "free" Hamiltonian. One can produce and measure states of the scattering system corresponding to several different configurations of the system which in the absence of interaction would have dynamical properties described by several different "free" Hamiltonians. This type of situation has been described by Ekstein[3] and by Jauch.[4]

Each dynamically different "free" configuration defines a different channel of the scattering system. The "free" states of a configuration are represented by the continuum eigenvectors of a "free" Hamiltonian operator which is characteristic of that channel and which we call the channel Hamiltonian. Since we are not interested in distinguishing between channels which differ only in properties which have no effect on the dynamics of the scattering process, two channels are considered to be different if and only if they have different channel Hamiltonian operators.

Examples of dynamically different channels are those whose "free" configurations contain different numbers or kinds of particles.[3,4] We do not distinguish between elementary and composite particles. Each configuration containing bound states or composite fragments composed of any number of particles simply represents a different channel for each different binding energy or mass of the fragment, just as does each configuration of "free" "elementary" particles.

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[1] T. F. Jordan, (preceding paper) J. Math. Phys. **3**, 414 (1962). A more detailed discussion of some topics mentioned in the present paper as well as references to the literature of single channel scattering can be found in this reference.
[2] J. M. Jauch, Helv. Phys. Acta **31**, 127 (1958).
[3] H. Ekstein, Phys. Rev. **101**, 880 (1956).
[4] J. M. Jauch, Helv. Phys. Acta **31**, 661 (1958).

Let H_a be the channel Hamiltonian for channel a, H the Hamiltonian of the interacting scattering system, and define V_a by $H = H_a + V_a$. According to the time-independent point of view we wish to find eigenstates ψ of H with eigenvalue E in the continuous spectrum by considering V_a as a perturbation with the eigenstates ϕ_a of H_a with the same eigenvalue E as the unperturbed states. The two solutions

$$\psi_a^{(\pm)} = \phi_a + \lim_{\epsilon \to 0^+} \frac{1}{E - H_a \pm i\epsilon} V_a \psi_a^{(\pm)} \qquad (1.1)$$

are identified as the stationary states of the scattering system which contain "outgoing" or "incoming" scattered waves, respectively, and reduce to the unperturbed states ϕ_a as the interaction vanishes. The cross section for scattering from channel a to channel b is obtained from the probability amplitude[5]

$$(\psi_b^{(-)}, \psi_a^{(+)}).$$

If for each channel we define wave operators by

$$\psi_a^{(\pm)} = \Omega_\pm^a \phi_a,$$

the scattering amplitude has the form

$$(\psi_b^{(-)}, \psi_a^{(+)}) = (\phi_b, \Omega_-^{b+} \Omega_+^a \phi_a) = (\phi_b, S_{ba}\phi_a) \qquad (1.2)$$

with

$$S_{ba} = \Omega_-^{b+} \Omega_+^a.$$

We note that the scattering amplitude is a matrix element of an operator which is dependent in an essential manner on the channels involved. As has been emphasized by Ekstein,[3] it is not in general possible to define a single scattering operator S such that the scattering amplitude for any process, say for scattering from channel a to channel b, is given by the matrix element $(\phi_b, S\phi_a)$ of that operator. Such an operator could be defined by $S = \sum_{ab} \Omega_-^{b+} \Omega_+^a$ if it were true that $\Omega_\pm^b \phi_a = 0$ for $a \neq b$, but Ekstein[3] has shown that in general this will not be the case. Therefore, we are content to describe the scattering by a family of wave operators, two for each channel.

The time-dependent formulation of multi-channel scattering must be approached in a manner that is somewhat different from that which is customary for single-channel scattering. This is because the use of the interaction representation is made impossible by the nonexistence of a single "free" Hamiltonian of which all the asymptotic states are eigenstates. However Ekstein[3] has shown how these difficulties can be avoided and the scattering amplitude defined in terms of the asymptotic states.

In the distant past the system is thought of as existing in one of its possible "free" configurations, say in a state ϕ_a which is a stationary state of the "free" Hamiltonian H_a of channel a. In other words, as $t \to -\infty$ the channel interaction $V_a = H - H_a$ becomes ineffective. After evolving during the infinite time interval $-\infty < t < \infty$ under the influence of the Hamiltonian H, the state of the system approaches, as $t \to +\infty$, one of the possible "free" configurations. One can then compute the cross section from the probability amplitude for measuring, as $t \to +\infty$, a state ϕ_b which is an eigenstate of the "free" Hamiltonian H_b of channel b.

Just as in the single channel case, the asymptotic limits play a central role in the time-dependent description of multi-channel scattering. If ψ represents the state of the system at $t = 0$, then

$$e^{-iHt}\psi$$

represents the state of the system at time t. If this state is one which, as $t \to -\infty$, approaches a "free" configuration of channel a, then its time dependence should approach that of an eigenstate of the channel Hamiltonian H_a. In other words, there must exist a continuum eigenstate ϕ_{in}^a of H_a such that

$$e^{-iHt}\psi \to e^{-iH_at}\phi_{\text{in}}^a \quad \text{as} \quad t \to -\infty.$$

This is equivalent to

$$e^{iHt}e^{-iH_at}\phi_{\text{in}}^a \to \psi \quad \text{as} \quad t \to -\infty.$$

Hence for a set of continuum eigenstates ϕ^a of the channel Hamiltonian H_a the limits

$$\lim_{t \to -\infty} e^{iHt}e^{-iH_at}\phi^a = \Omega_+^a \phi^a \qquad (1.3)$$

exist and define the linear isometric operator Ω_+^a. Similarly if

$$e^{-iHt}\psi$$

is a state which, as $t \to +\infty$, approaches a "free" state of channel b, its time dependence must approach that of an eigenstate of the channel Hamiltonian H_b, so there must exist a continuum state ϕ_{out}^b of H_b such that

$$e^{-iHt}\psi \to e^{-iH_bt}\phi_{\text{out}}^b \quad \text{as} \quad t \to +\infty$$

or

$$e^{iHt}e^{-iH_bt}\phi_{\text{out}}^b \to \psi \quad \text{as} \quad t \to +\infty.$$

[5] See the discussion for the single-channel case in reference 1.

Hence for a set of continuum states ϕ^b of H_b, the limit

$$\lim_{t\to+\infty} e^{iHt}e^{-iH_bt}\phi^b = \Omega_-^b\phi^b \tag{1.4}$$

exists and defines the linear isometric operator Ω_-^b.

Suppose that the system is initially, as $t \to -\infty$, in the state

$$e^{-iH_at}\phi^a.$$

Then at $t = 0$ it is in the state

$$\psi_a^{(+)} = \Omega_+^a\phi^a.$$

The state which at $t = 0$ is

$$\psi_b^{(-)} = \Omega_-^b\phi^b$$

approaches, as $t \to +\infty$, the final "free" state

$$e^{-iH_bt}\phi^b.$$

Hence the scattering amplitude for scattering from the initial state ϕ^a of channel a to the final state ϕ^b of channel b is

$$(\psi_b^{(-)}, \psi_a^{(+)}) = (\phi^b, \Omega_-^{b^+}\Omega_+^a\phi^a)$$

which is to be compared with Eq. (1.2) of the stationary-state formalism.

Just as in the time-independent formulation, the scattering amplitude is a matrix element of an operator which is different for different channels, and it is in general impossible to define a single scattertng operator as in the single-channel case. According to the time-dependent interpretation this means that there is no operator which takes each initial state to a final state in the interaction picture. In both the time-dependent and stationary-state formulations the most immediate description of scattertng is provided by the two families of wave operators $\Omega_\pm^a$ which map the "free" stationary states ϕ^a of the channel Hamiltonian H_a onto the scattering states $\psi_a^{(\pm)}$. In terms of these, we can make some remarks which are of importance from either point of view.

Any continuum eigenstate ψ of the Hamiltonian H should describe a possible state of the interacting system, say at $t = 0$. If this state is the result of a mapping by a wave operator from a "free" state of some specific channel, then it should be orthogonal to all states similarly obtained from "free" states of other channels,

$$(\psi_b^{(+)}, \psi_a^{(+)}) = (\Omega_+^b\phi^b, \Omega_+^a\phi^a) = 0$$

$$(\psi_b^{(-)}, \psi_a^{(-)}) = (\Omega_-^b\phi^b, \Omega_-^a\phi^a) = 0 \quad \text{for} \quad a \neq b. \tag{1.5}$$

In other words, any state of the interacting system should be decomposable into states which, from the time-dependent point of view, approach as $t \to -\infty$ ($t \to +\infty$) asymptotic states of the different channels, or, from the stationary-state point of view reduce, with the switching off of the channel interaction and the resulting removal of "outgoing scattered waves" ("incoming scattered waves"), to unperturbed states of the different channels. But we should not in general expect that $(\psi_b^{(-)}, \psi_a^{(+)})$ vanishes for $a \neq b$ because this would mean that there is no scattering between different channels.

A simple example might help to clarify the basic ideas of this approach to the scattering problem. Suppose we have a system on which we can make measurements corresponding to just one of two configurations: In configuration (1.) there are three different free particles, n, p, and π; in configuration (2.) there are two particles, π and d, the latter being considered as a bound state of n and p. Let H_1 be the Hamiltonian operator describing the system (1.) of three free particles. The continuum eigenstates of H_1 (products of three plane-wave functions) span the whole Hilbert space and so we have a free Hamiltonian and a complete set of free states. If we know the Hamiltonian of the interacting system, we can calculate the scattering from a three-particle state to a three-particle state. In other words, these are sufficient for a description of scattering from channel (1.) to channel (1.). But in order to describe scattering processes involving channel (2.) we need states of two free particles, π and d, the d being a bound state and having a mass corresponding to the binding energy of n and p. The free Hamiltonian H_2 describing this system of two free particles is not the same as H_1 (see Jauch,[4] Sec. 3) and the free $\pi - d$ states are not in general eigenstates of H_1 (see Ekstein,[3] Sec. VII). Thus, while the introduction of a second free Hamiltonian H_2 is not necessary to generate a complete set of free states, it is necessary to define what we mean by a measurement of a state of the system corresponding to the free $\pi - d$ configuration.

In the next section we outline the mathematical structure of the multi-channel scattering problem which is contained in the properties of the Hamiltonian operators. The form of the following sections is similar to that of the discussion of the single-channel case. In Sec. 3 we briefly review the rigorous time-dependent formulation of multi-channel scattering which was given by Jauch.[4] In Sec. 4 we give a rigorous formulation of the scattering problem

which reflects the stationary state point of view. This will be entirely analogous to that given for the single channel case. In Sec. 5 we show that the wave operators defined by the asymptotic limits provide a solution of this problem whenever the conditions necessary for the time-dependent formulation are valid. The possibility that a solution can exist when the asymptotic conditions are not valid is investigated in the following two sections. Wave operators are defined by an integral representation just as in the single-channel case and the conditions sufficient for these to be a solution of the scattering problem are shown to be possibly weaker than the conditions necessary for the time-dependent formulation. Hence in general there may be a class of Hamiltonians for which a solution exists but for which the asymptotic conditions are not valid. However, just as in the single-channel case we do not present any explicit demonstration of such a set of Hamiltonian operators. The mathematical problems involved are completely similar to those encountered in the single-channel case. In the final section we make some remarks about the form of the Hamiltonian operators in nonrelativistic and relativistic theories.

2. STRUCTURE OF THE PROBLEM—HAMILTONIAN OPERATORS

The structure of the mathematical description of single-channel scattering is determined by two self-adjoint linear operators, H and H_0, on a separable Hilbert space $\mathfrak{K}$. The scattering problem can be formulated without imposing any further restrictions on these operators, but the existence of a solution depends on their satisfying certain conditions. In particular, a necessary condition for a solution to exist is that the continuum parts of these two operators be unitarily equivalent.

In the multi-channel case the structure of the problem is determined by a self-adjoint operator H representing the Hamiltonian of the interacting system and a family of self-adjoint operators H_a representing the channel Hamiltonians. These are assumed to be defined on a separable Hilbert space $\mathfrak{K}$. While we are able to formulate the scattering problem without imposing any further restrictions on these operators, as in the single channel case, the existence of solutions depends on their satisfying certain conditions which are rather characteristic of the problem. It is perhaps helpful then to state these at the outset.

First it is convenient to introduce notation which is used in all of the following sections: Let $\mathfrak{K}$ be the subspace of $\mathfrak{K}$ spanned by the eigenvectors of H, $\mathfrak{M} = \mathfrak{K}_\perp$ the continuum subspace of H or the orthogonal complement of $\mathfrak{K}$, and P the projection operator whose range is $\mathfrak{M}$, Similarly let $\mathfrak{K}_a$ be the subspace spanned by the eigenvectors of H_a, $\mathfrak{M}_a = \mathfrak{K}_{a\perp}$ the continuum subspace of H_a or the orthogonal complement of $\mathfrak{K}_a$, and P_a the projection operator whose range is $\mathfrak{M}_a$.

We will find that the following is a necessary condition for the existence of any solution of the scattering problem: $\mathfrak{M}$ can be decomposed in two ways into a direct sum of a finite or countably infinite number of subspaces, one corresponding to each channel and each reducing H. The part of H in a subspace corresponding to channel a is unitarily equivalent to the part of H_a in a subspace of $\mathfrak{M}_a$ which reduces H_a.

We have already indicated in the preceding section that we consider channel a to be identical with channel b if and only if $H_a = H_b$. According to Stone's theorem the latter is equivalent to

$$e^{-iH_at} = e^{-iH_bt}$$

for all real t. In addition, Jauch[4] assumed for the time-dependent formulation that

$$e^{-iH_at}\phi = e^{-iH_bt}\phi \quad \text{for all real} \quad t,$$

implies that $\phi = 0$ unless $a = b$. It was also assumed that all of the channel Hamiltonian operators commute

$$[e^{-iH_at}, e^{-iH_bs}]_- = 0$$

for all a, b, t, s. Although these seem to be stronger than is necessary, we have been unable to substitute a simple weaker set of conditions on the Hamiltonian operators sufficient for the existence of a solution of the scattertng problem.

3. TIME-DEPENDENT FORMULATION

The theory of multi-channel, as well as single-channel scattering, has been formulated in a mathematically rigorous way by Jauch[4] from the time-dependent point of view. We briefly review some of the essential features of this formulation. Our discussion is slightly generalized to include channel Hamiltonians which may have bound states.

In order to provide a rigorous time-dependent description of scattering for a system described by the Hamiltonian operator H and the family of channel Hamiltonian operators H_a, Jauch requires that these operators satisfy the following conditions: All of the channel Hamiltonian operators commute,

$$[e^{-iH_at}, e^{-iH_bs}]_- = 0 \tag{3.1}$$

for all a, b and real s, t, and

$$e^{-iH_a t}\phi = e^{-iH_b t}\phi \tag{3.2}$$

for all real t implies $\phi = 0$ unless $a = b$. For each channel a there exists a subspace $\mathfrak{D}_a$ of $\mathfrak{M}_a$ such that, if E_a is the projection with range $\mathfrak{D}_a$, the limits

$$\lim_{t\to\mp\infty} e^{iHt}e^{-iH_a t}E_a\phi = \Omega_\pm^a\phi \tag{3.3}$$

exist for any $\phi \in \mathfrak{H}$.[6] This defines the linear operators $\Omega_\pm^a$ which are partially isometric with the initial set $\mathfrak{D}_a$. Let $\mathfrak{R}_a^{(\pm)}$ be the subspaces which are the ranges of $\Omega_\pm^a$, let $\mathfrak{R}_+$ be the subspace spanned by all subspaces $\mathfrak{R}_a^{(+)}$, and let $\mathfrak{R}_-$ the subspace spanned by all the subspaces $\mathfrak{R}_a^{(-)}$. Then it is further required that

$$\mathfrak{R}_+ = \mathfrak{R}_- = \mathfrak{M}. \tag{3.4}$$

Under these conditions one can show that the operators $\Omega_\pm^a$ have all of the properties needed for a description of scattering. Each $\Omega_\pm^a$ is a partially isometric operator from $\mathfrak{D}_a$ to $\mathfrak{R}_a^{(\pm)}$. Let $F_\pm^a$ be the projection operators with ranges $\mathfrak{R}_a^{(\pm)}$. Then we have

$$\begin{aligned}\Omega_\pm^{a+}\Omega_\pm^a &= E_a\\ \Omega_\pm^a\Omega_\pm^{a+} &= F_\pm^a.\end{aligned} \tag{3.5}$$

By using the conditions (3.1) and (3.2) one can show that the ranges are orthogonal for different channels, or

$$F_+^aF_+^b = F_-^aF_-^b = 0 \tag{3.6}$$

for $a \neq b$. This and the separability of $\mathfrak{H}$ requires that the number of channels be finite or countably infinite. It also follows from Eqs. (3.6) and (3.4) that

$$P = \textstyle\sum_a F_+^a = \sum_a F_-^a, \tag{3.7}$$

and from equations (3.6) and (3.5) that

$$\Omega_+^{a+}\Omega_+^b = \Omega_-^{a+}\Omega_-^b = E_a\,\delta_{ab}. \tag{3.8}$$

One can also prove that the wave operators have the intertwining property

$$H\Omega_\pm^a = \Omega_\pm^a H_a \tag{3.9}$$

or more precisely,[7]

$$e^{iHt}\Omega_\pm^a = \Omega_\pm^a e^{iH_a t}$$

for all real t, from which it follows that each subspace $\mathfrak{R}_a^{(\pm)}$ reduces H and each subspace $\mathfrak{D}_a$ reduces H_a.

The conditions (3.1) and (3.2) are needed only for the proof of the orthogonality condition (3.6) and are stronger than is necessary. In fact Zinnes[8] has shown that for a special class of channel Hamiltonian operators, the orthogonality property (3.6) can still be proved if the condition (3.2) is replaced by the weaker one that $H_a \neq H_b$ for $a \neq b$. However the conditions (3.3) and (3.4) are quite essential for the time-dependent formulation. The former is the asymptotic condition that the states of the scattering system approach asymptotic "free" states in the distant past and remote future, and the latter is the requirement that any state of the scattering system be obtainable as a sum of states originating (or terminating) in the different channels. The mathematical investigation of the class of Hamiltonian operators for which these two conditions are satisfied has not been as extensive as for the corresponding single-channel problem, although many of the results of the latter can be made applicable here.

One can show that a necessary requirement for validity of all of these conditions is that the Hamiltonian operators have the structure described in the preceding section[9]: $\mathfrak{M}$ is decomposable into a direct sum of the subspaces $\mathfrak{R}_a^{(+)}$ and into the subspaces $\mathfrak{R}_a^{(-)}$ each of which reduces H. The part of H in $\mathfrak{R}_a^{(\pm)}$ is unitarily equivalent to the part of H_a in the subspace $\mathfrak{D}_a$ of $\mathfrak{M}_a$ which reduces H_a.

4. FORMULATION OF THE SCATTERING PROBLEM

We now develop a formulation of the multichannel scattering problem which reflects the stationary-state point of view. A solution of the scattering problem consists of two families of wave operators $\Omega_\pm^a$ which map sets of "unperturbed" states ϕ_a belonging to the continuum subspaces of the channel Hamiltonians H_a onto the scattering states

$$\psi_a^{(\pm)} = \Omega_\pm^a\phi_a. \tag{4.1}$$

The latter states belong to the continuum subspace of H and satisfy conditions which select the solutions containing "outgoing" or "incoming" scattered "waves," respectively.

For any channel a the set of "unperturbed"

[6] Actually Jauch showed that if $\lim_{t\to\mp\infty} e^{iHt}\,e^{-iH_a t}\,\phi$ exists for some $\phi \in \mathfrak{D}_a$, then there exists an infinite-dimensional subspace $\mathfrak{M}_a$ such that the limits (3.3) exist. We take $\mathfrak{D}_a$ to be the largest subspace of $\mathfrak{M}_a$ with this property. One can easily see that Jauch's proof extends to the case where H_a has bound states; since we assume that $\mathfrak{D}_a \subset \mathfrak{M}_a$ we need only consider the continuum part of H_a.

[7] See Sec. 3 of reference 1. A more direct logical procedure is to consider the equation $e^{iHt}\,\Omega_\pm^a = \Omega_\pm^a\,e^{iH_a t}$ to be the statement of the intertwining property and the equation $H\Omega_\pm^a = \Omega_\pm^a H_a$ to be implied by it, as was shown by Hack in Sec. 3 of reference 9.

[8] I. I. Zinnes, Nuovo cimento Suppl. **12**, 87 (1959).

[9] M. N. Hack, Nuovo cimento **13**, 231 (1959).

states ϕ_a should form a subspace $\mathfrak{D}_a$ of $\mathfrak{M}_a$ which reduces H_a. This has the physical interpretation that this set of states is invariant under the dynamical transformations generated by the "free" Hamiltonian H_a. In general we need not require that

$$\mathfrak{D}_a = \mathfrak{M}_a, \tag{4.2}$$

but in many problems it may be desirable for the physical interpretation to do so. Every vector of the continuum subspace $\mathfrak{M}$ of H should represent a possible state of the scattering system and it should be decomposable into vectors of the different channels. If $\mathfrak{R}_a^{(\pm)}$ are the ranges of $\Omega_\pm^a$ this means that $\mathfrak{M}$ must be the direct sum of subspaces $\mathfrak{R}_a^{(+)}$ and also the direct sum of the subspaces $\mathfrak{R}_a^{(-)}$. In order that the mapping (4.1) from "unperturbed" to interacting states preserves the normalization we must require that each $\Omega_\pm^a$ be a partially isometric operator from $\mathfrak{D}_a$ to $\mathfrak{R}_a^{(\pm)}$.

If E_a is the projection operator with range $\mathfrak{D}_a$, and $F_\pm^a$ are the projection operators with ranges $\mathfrak{R}_a^{(\pm)}$, the above conditions can be summarized in the form of the equations

$$\Omega_\pm^{a+}\Omega_\pm^a = E_a \tag{4.3}$$

$$\Omega_\pm^a\Omega_\pm^{a+} = F_\pm^a \tag{4.4}$$

$$\sum\nolimits_a F_+^a = \sum\nolimits_a F_-^a = P. \tag{4.5}$$

We also require that

$$e^{iHt}\Omega_\pm^a = \Omega_\pm^a e^{iH_a t} \tag{4.6}$$

for all real t. By an argument identical in form to the discussion of the single-channel case one can show that this condition is the rigorous statement of the requirement that ϕ_a is an eigenvector of H_a with eigenvalue E in the continuous spectrum if and only if $\psi_a^{(\pm)} = \Omega_\pm^a\phi_a$ are eigenvectors of H with the same eigenvalue also in the continuous spectrum of H. Also this means that the scattering and "unperturbed" states have essentially the same time dependence as well as the same mean value and second moment of the energy.

Also we could require that $\Omega_\pm^a$ be strongly continuous as functions of H and of H_a and that $\Omega_\pm^a = E_a$ if $H = H_a$. This would be a rigorous statement of the continuous reduction of the scattering states to the "unperturbed" states as the interaction vanishes. But we do not need this condition to specify a unique set of wave operators and it is not necessarily desirable that it be satisfied for every problem. Hence we do not include it in our formulation.

Finally we need a condition which selects the scattering solutions corresponding to "outgoing" and "incoming" scattered waves. It is advantageous to use a condition which is slightly different than that used for the single-channel case. Namely, we require that

$$\begin{aligned} &\lim_{\epsilon\to 0^+}\int_{-\infty}^{0} \epsilon e^{\epsilon t}e^{iH_a t}\Omega_+^{a+}e^{-iH_a t}E_a\,dt = E_a \\ &\lim_{\epsilon\to 0^+}\int_{0}^{\infty} \epsilon e^{-\epsilon t}e^{iH_a t}\Omega_-^{a+}e^{-iH_a t}E_a\,dt = E_a. \end{aligned} \tag{4.7}$$

This condition can be motivated by an argument which is entirely analogous to that used to arrive at the condition used in the single channel case [see the discussion preceding and following Eq. (3.10) of reference 1]. We could have used a condition of the form (4.7) to provide an alternative formulation of the single-channel problem. In fact such a formulation might provide a slight generalization. That this condition is needed for the multi-channel problem is due to the fact that in general we can not establish the existence of integral representations for the adjoints of the wave operators even in the case that the conditions of the time-dependent formulation are valid. As a result it is easier to work with the Eqs. (4.7) which already contain the adjoint operators, as becomes clearer in the following sections.

We can summarize all of the conditions of the scattering problem in the following:

Definition: A family of linear operators $\Omega_\pm^a$ on $\mathfrak{K}$ are solutions of the scattering problem defined by the self-adjoint operator H and family of self-adjoint operators H_a if they satisfy the following conditions:

(α) Each $\Omega_\pm^a$ is a partially isometric operator from $\mathfrak{D}_a \subset \mathfrak{M}_a$ to $\mathfrak{R}_a^{(\pm)} \subset \mathfrak{M}$. The subspace $\mathfrak{M}$ is the direct sum of the subspaces $\mathfrak{R}_a^{(+)}$ and is also the direct sum of the subspaces $\mathfrak{R}_a^{(-)}$.

(β) $e^{iHt}\,\Omega_\pm^a = \Omega_\pm^a\, e^{iH_a t}$ for all real t.

(γ)
$$\begin{aligned} &\lim_{\epsilon\to 0^+}\int_{-\infty}^{0} \epsilon e^{\epsilon t}e^{iH_a t}\Omega_+^{a+}e^{-iH_a t}E_a\,dt = E_a \\ &\lim_{\epsilon\to 0^+}\int_{0}^{\infty} \epsilon e^{-\epsilon t}e^{iH_a t}\Omega_-^{a+}e^{-iH_a t}E_a\,dt = E_a. \end{aligned}$$

Just as in the single-channel case, this formulation of the scattering problem does not depend on a configuration space representation of the Hilbert space and hence its applicability is not limited to situations where configuration space methods are useful.

From condition (β) it follows that

$$e^{iHt}\Omega_\pm^a\phi \in \mathfrak{R}_a^{(\pm)}$$

for any $\phi \in \mathfrak{K}$ and any real t, which implies that $\mathfrak{R}_a^{(*)}$ reduces H. It also follows that

$$e^{iH_a t}\Omega_{\pm}^{a+}\phi = \Omega_{\pm}^{a+}e^{iHt}\phi \in \mathfrak{D}_a$$

for any $\phi \in \mathfrak{K}$, which implies that $\mathfrak{D}_a$ reduces $\mathfrak{K}_a$. The part of H in $\mathfrak{R}_a^{(*)}$ is clearly unitarily equivalent to the part of H_a in $\mathfrak{D}_a$. Hence a necessary condition for the existence of a solution of the scattering problem is that the Hamiltonian operators have the structure mentioned in Sec. 2, namely: $\mathfrak{M}$ is the direct sum of the $\mathfrak{R}_a^{(+)}$ or of the $\mathfrak{R}_a^{(-)}$, each of which reduces H, and the part of H in $\mathfrak{R}_a^{(*)}$ is unitarily equivalent to the part of H_a in a subspace $\mathfrak{D}_a$ of $\mathfrak{M}_a$ which reduces H_a.

It should be observed that when the number of channels is set equal to one, this formulation of the multi-channel scattering problem does not reduce to the formulation of the single-channel scattering problem which was given in reference 1. In the first place we have chosen a different form for condition (γ), and secondly we have not assumed that the domain of the wave operators is the whole of the continuum subspace of the "free" Hamiltonian. It may even be that the multi-channel formulation provides, for the case of one channel, a nontrivial generalization of the single-channel formulation; there may be Hamiltonian operators for which the former allows solutions but the latter does not. If this is the case we would want to adopt the more general formualtion since the single-channel formulation was adopted for convenience in comparison with other treatments and not out of necessity.

5. ASYMPTOTIC LIMITS AS A SOLUTION

In investigating possible solutions of the scattering problem as formulated in the preceding section, we first observe that a solution exists whenever the conditions necessary for the time-dependent formulation are valid. Specifically if the limits (3.3) exist such that (3.4) is valid, and if Eq. (3.6) is satisfied [in particular the orthogonality condition is satisfied whenever the channel Hamiltonian operators satisfy (3.1) and (3.2)], then the wave operators defined by the limits (3.3) provide a solution of the scattering problem which is unique in the sense that there is no other solution with the same set of domains $\mathfrak{D}_a$ and ranges $\mathfrak{R}_a^{(*)}$ of the wave operators.

The necessary properties of the $\Omega_{\pm}^{a}$ have essentially already been proved. Equations (3.4)–(3.7) show that condition (α) is satisfied and Eq. (3.9) is identical to condition (β). Just as in the single-channel case (reference 1, Sec. 4) we can introduce the integral representations

$$\Omega_{+}^{a}\phi = \lim_{\epsilon\to 0^+}\int_{-\infty}^{0}\epsilon e^{\epsilon t}e^{iHt}e^{-iH_a t}E_a\phi\,dt$$

$$\Omega_{-}^{a}\phi = \lim_{\epsilon\to 0^+}\int_{0}^{\infty}\epsilon e^{-\epsilon t}e^{iHt}e^{-iH_a t}E_a\phi\,dt,$$

which have been shown by Jauch[2] to exist when the asymptotic limits exist. In the next section we see that these operators satisfy condition (γ) and provide a unique solution of the scattering problem. This is completely analogous to the single-channel case except for the changes introduced by the modified form of condition (γ). Just as in the single-channel case one need not interpret the parameter t occurring in the asymptotic limits as having anything to do with time. We may simply regard the resulting wave operators as being a solution of the stationary state problem.

6. INTEGRAL REPRESENTATIONS AS A SOLUTION

Just as in the single-channel case, no asymptotic condition appears in our formulation of the scattering problem and there is a possibility that a solution exists in cases where the asymptotic limits fail to exist. A means of investigating this possibility is provided by the integral representation definition of the wave operators

$$\Omega_{+}^{a}\phi = \lim_{\epsilon\to 0^+}\int_{-\infty}^{0}\epsilon e^{\epsilon t}e^{iHt}e^{-iH_a t}E_a\phi\,dt \tag{6.1}$$

$$\Omega_{-}^{a}\phi = \lim_{\epsilon\to 0^+}\int_{0}^{\infty}\epsilon e^{-\epsilon t}e^{iHt}e^{-iH_a t}E_a\phi\,dt. \tag{6.2}$$

The integrals in these equations will always exist as Bochner integrals and whenever the limits of the integrals exist they will define the linear wave operators $\Omega_{\pm}^{a}$. These operators will then be bounded by unity,

$$||\Omega_{\pm}^{a}\phi|| \leq ||\phi||$$

for any $\phi \in \mathfrak{K}$, and will have the intertwining property that

$$e^{iHt}\Omega_{\pm}^{a} = \Omega_{\pm}^{a}e^{iH_a t}$$

for all real t. In the case that the asymptotic limits (3.3) of the time-dependent formulation exist, the limits of the integrals in (6.1) and (6.2) will also exist and the wave operators defined by the two sets of limits will be identical if the domains $\mathfrak{D}_a$ are taken to be the same in each case. These statements can be proved as in the proof of Theorem 2 of reference 1.

The lemma of reference 1 also applies to the multi-channel case. The wave operators will be

strongly continuous functions of a set of Hamiltonian operators if they are defined by limits of the integrals of Eqs. (6.1) and (6.2) which converge uniformly with respect to the set of Hamiltonian operators. This will be true in particular when the wave operators are defined by asymptotic limits which converge uniformly with respect to the Hamiltonian operators.

Whenever the wave operators defined by Eqs. (6.1) and (6.2) exist and satisfy condition (α), they provide a solution of the scattering problem which is unique in the sense that there is no other solution having the same domain $\mathfrak{D}_a$ and ranges $\mathfrak{R}_a^{(*)}$ of the wave operators. The proof of this is similar to that of Theorem 3 of reference 1. The only differences are introduced by the different form of condition (γ). We have postulated that condition (α) holds, and we know that condition (β) also holds. To prove condition (γ) we write

$$E_a = \Omega_+^{a+}\Omega_+^a = \Omega_+^{a+} \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} e^{iHt} e^{-iH_a t} E_a \, dt$$

$$= \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} e^{iH_a t} \Omega_+^{a+} e^{-iH_a t} E_a \, dt$$

$$E_a = \Omega_-^{a+}\Omega_-^a = \Omega_-^{a+} \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} e^{iHt} e^{-iH_a t} E_a \, dt$$

$$= \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} e^{iH_a t} \Omega_-^{a+} e^{-iH_a t} E_a \, dt.$$

Let $\omega_\pm$ be operators satisfying conditions (α), (β), and (γ). Then

$$E_a = \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} e^{iH_a t} \omega_+^+ e^{-iH_a t} E_a \, dt$$

$$= \omega_+^+ \lim_{\epsilon\to 0^+} \int_{-\infty}^{0} \epsilon e^{\epsilon t} e^{iHt} e^{-iH_a t} E_a \, dt = \omega_+^+ \Omega_+^a$$

$$E_a = \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} e^{iH_a t} \omega_-^+ e^{-iH_a t} E_a \, dt$$

$$= \omega_-^+ \lim_{\epsilon\to 0^+} \int_{0}^{\infty} \epsilon e^{-\epsilon t} e^{iHt} e^{-iH_a t} E_a \, dt = \omega_-^+ \Omega_-^a$$

so that the uniqueness of the operators which satisfy both the above equations and condition (α) implies that

$$\omega_\pm^+ = \Omega_\pm^{a+}$$

or

$$\omega_\pm = \Omega_\pm^a.$$

This proves that the wave operators $\Omega_\pm^a$ defined by Eqs. (6.1) and (6.2) are unique solutions when they exist and satisfy condition (α).

Note that we have been able to develop a solution in terms of the integral representation wave operators without giving an integral representation for their adjoints. It was to this end that we modified the condition (γ). For in general we can not expect to be able to establish such a representation for the adjoints as we did in the single-channel case.

In the time-dependent formulation, the domain $\mathfrak{D}_a$ is determined to be the largest subspace of $\mathfrak{M}_a$ for which the limits (3.3) exist. Then of course the ranges $\mathfrak{R}_a^{(*)}$ are determined as the images of $\mathfrak{D}_a$ under the mappings $\Omega_\pm^a$. But in the definition of the wave operators by the integral representations (6.1) and (6.2) the domains $\mathfrak{D}_a$ are not specified. It is to be expected that the specification of $\mathfrak{D}_a$ will be a critical factor in establishing the validity of condition (α) for these wave operators. That is $\mathfrak{D}_a$ must be chosen in such a way that equations (4.3), (4.4), and (4.5) can be valid. Because of condition (β) it is necessary, as we have seen, that $\mathfrak{D}_a$ reduce H_a. Of course it is also necessary that the subspaces $\mathfrak{D}_a$ be such that the limits of the integrals of Eqs. (6.1) and (6.2) exist.

7. CONDITIONS SUFFICIENT FOR A SOLUTION

As we have seen in the preceding section, sufficient conditions for the existence of a unique solution of the scattering problem are that the limits of the integrals of Eqs. (6.1) and (6.2) exist and that they define wave operators which satisfy condition (α). In particular this is true whenever the conditions necessary for the time-dependent formulation are valid. But the problem of greatest interest would be to find if there exists a set of Hamiltonian operators for which the conditions of the time-dependent formulation are not valid while the conditions sufficient for the existence of the integral representation solution are still satisfied. This would permit solutions which could not be treated from the time-dependent point of view and would carry the mathematical analysis of the conditions sufficient for a solution beyond the problem of the existence of the asymptotic limits. We are unable to present any explicit characterization of such a set of Hamiltonian operators or show that such a set exists. But we can make some remarks which will clarify the problem, and we can make an argument which makes it appear quite plausible that such a set of Hamiltonian operators does exist. This is identical to the situation of the single-channel case.

Condition (α) can be written in the form of Eqs. (4.3), (4.4), and (4.5). The Eqs. (4.3) and (4.4), which state that $\Omega_\pm^a$ must be partially isometric operators from $\mathfrak{D}_a$ to $\mathfrak{R}_a^{(*)}$, together with the requirement that the two sets of ranges $\mathfrak{R}_a^{(*)}$ must each span

$\mathfrak{M}$ are analogous to condition (α) of the single-channel problem. But Eq. (4.5) implies the orthogonality condition

$$F_+^a F_+^b = F_-^a F_-^b = 0 \tag{7.1}$$

for $a \neq b$ which is characteristic of the multi-channel problem only.

One can show that if the limits of the integrals of Eqs. (6.1) and (6.2) exist, and if they define wave operators which satisfy Eqs. (4.3), then these wave operators are partially isometric with the initial set $\mathfrak{D}_a$. This follows from the boundedness property of the wave operators just as in the single-channel case. Hence if we let $\mathfrak{R}_a^{(\pm)}$ be the ranges of the wave operators $\Omega_\pm^a$ and if we let $F_\pm^a$ be the projections onto these subspaces, we have that Eqs. (4.4) are valid. In other words Eqs. (4.4) are a consequence of Eqs. (4.3) for the integral-representation wave operators.

The conditions sufficient for a unique solution of the scattering problem by the integral representation wave operators have thus been reduced to (1) The limits of the integrals in Eqs. (6.1) and (6.2) exist; (2) the wave operators thus defined satisfy Eqs. (4.3); and (3) the continuum subspace $\mathfrak{M}$ of H is the direct sum of the ranges $\mathfrak{R}_a^{(+)}$ of the Ω_+^a and is also the direct sum of the ranges $\mathfrak{R}_a^{(-)}$ of the Ω_-^a. The last condition implies the orthogonality property of the ranges and also implies that the two sets of ranges each span $\mathfrak{M}$.

The sufficient conditions for the existence of the asymptotic limits of the time-dependent formulation which have been developed for the single-channel case can in general be made to apply to the multi-channel case with only minor modifications. Similarly, in complete analogy to the single channel case, one can prove the following statement[10]: If $V_a = H - H_a$ is defined in the common domain $\mathfrak{D}(V_a) = \mathfrak{D}(H) \cap \mathfrak{D}(H_a)$ of H and H_a, a sufficient condition in order that

$$\Omega_\pm^{a+} \Omega_\pm^a = E_a,$$

is that there exists a subset $\mathfrak{C}_a$ of $\mathfrak{D}_a$ dense in $\mathfrak{D}_a$ such that, for any $\phi \in \mathfrak{C}_a$,

$$e^{-iH_a t}\phi \in \mathfrak{D}(V_a)$$

for any real t, and

$$\int_{-\infty}^{\infty} ||V_a e^{-iH_a t}\phi||\, dt < \infty. \tag{7.2}$$

As we have already mentioned, our main interest is comparing the conditions sufficient for a unique solution by the integral-representation wave operators with the conditions necessary for the time-dependent formulation. We know that when the asymptotic limits (3.3) exist the limits of the integrals of Eqs. (6.1) and (6.2) also exist and the two kinds of limits define identical wave operators as long as the domains $\mathfrak{D}_a$ are taken to be identical. Just as in the single-channel case one can argue that it may be possible for the limits of the integrals of Eqs. (6.1) and (6.2) to exist in cases where the asymptotic limits (3.3) do not exist analogously to the fact that limits of the form

$$\lim_{\epsilon \to 0^+} \int_0^\infty \epsilon e^{-\epsilon t} f(t)\, dt \tag{7.3}$$

can exist for functions for which the limits

$$\lim_{t \to \infty} f(t) \tag{7.4}$$

do not exist.

In a manner completely analogous to that of the single channel case, we can write our Eqs. (4.3) in an explicit form for the integral representation wave operators. In this form it appears to be possible for these equations to be valid when the asymptotic limits (3.3) do not exist. In fact we can show, just as in the single-channel case, that the existence of the latter limits implies an apparently stronger equation [see Eqs. (6.4) and (6.5) and the accompanying discussion of reference 1].

The remaining condition on the integral-representation wave operators in order that they provide a unique solution is that $\mathfrak{M}$ must be the direct sum of the ranges $\mathfrak{R}_a^{(+)}$ of Ω_+^a and also the direct sum of the ranges $\mathfrak{R}_a^{(-)}$ of Ω_-^a. This condition contains three parts: All of the ranges $\mathfrak{R}_a^{(\pm)}$ are contained in $\mathfrak{M}$; the set of ranges $\mathfrak{R}_a^{(+)}$ and the set of ranges $\mathfrak{R}_a^{(-)}$ each span $\mathfrak{M}$; the ranges have the orthogonality property that $\mathfrak{R}_a^{(+)}$ is orthogonal to $\mathfrak{R}_b^{(+)}$ and $\mathfrak{R}_a^{(-)}$ is orthogonal to $\mathfrak{R}_b^{(-)}$ for $a \neq b$.

The first part of this condition is always true for the integral-representation wave operators. One can prove this as follows: The adjoints of the wave operators have the integral representation

$$\Omega_+^{a+}\phi = \lim_{\epsilon \to 0^+} \int_{-\infty}^0 \epsilon e^{\epsilon t} E_a e^{iH_a t} e^{-iHt}\phi\, dt$$

$$\Omega_-^{a+}\phi = \lim_{\epsilon \to 0^+} \int_0^\infty \epsilon e^{-\epsilon t} E_a e^{iH_a t} e^{-iHt}\phi\, dt$$

whenever the limits of the integrals exist. This can be proved just as in Theorem 2 of reference 1. But Jauch[2] [see discussion following Eq. (6.7) of reference

[10] The proof is identical to that of Theorem 4, reference 1.

1] has shown that these limits do exist and are equal to zero when ϕ is an eigenvector of H. Hence we have that $\Omega_{\pm}^{a+}\phi = 0$ for all ϕ belonging to the orthogonal complement of the subspace $\mathfrak{M}$. This implies that the ranges $\mathfrak{R}_a^{(*)}$ of the $\Omega_{\pm}^{a}$ are subspaces of $\mathfrak{M}$.

The condition that the two sets of ranges each span $\mathfrak{M}$ can be stated as follows: For any $\psi \in \mathfrak{M}$ there exists a channel a such that

$$\Omega_{+}^{a+}\psi \neq 0$$

and a channel b such that

$$\Omega_{-}^{b+}\psi \neq 0;$$

or for any $\psi \in \mathfrak{M}$ there exists a channel a and a $\phi \in \mathfrak{D}_a$ such that

$$(\psi, \Omega_{+}^{a}\phi_a) \neq 0 \tag{7.5}$$

and there exists a channel b and a $\phi_b \in \mathfrak{D}_b$ such that

$$(\psi, \Omega_{-}^{b}\phi_b) \neq 0. \tag{7.6}$$

For the integral-representation definition of the wave operators, (7.6) has the explicit form

$$\lim_{\epsilon \to 0^+} \int_0^\infty \epsilon e^{-\epsilon t}(\psi, e^{iHt}e^{-iH_b t}E_b\phi_b)\, dt \neq 0, \tag{7.7}$$

and (7.5) for Ω_+ has a similar form. If the wave operators are defined by the asymptotic limits, then (7.6) has a form identical to (7.7) except that the limits of the form (7.3) are replaced by limits of the form (7.4) resulting in an apparently stronger condition. It appears to be possible for (7.5) and (7.6) to be valid when the asymptotic limits do not exist.

The orthogonality condition can be written as

$$(\Omega_{+}^{a}\phi, \Omega_{+}^{b}\psi) = (\Omega_{-}^{a}\phi, \Omega_{-}^{b}\psi) = 0$$

for $a \neq b$ and $\phi, \psi \in \mathfrak{K}$. For the case of Ω_- and the integral representation of the wave operators this has the explicit form

$$\lim_{\epsilon \to 0^+} \int_0^\infty \epsilon e^{-\epsilon t}\, dt \lim_{\eta \to 0^+} \int_0^\infty \eta e^{-\eta s}\, ds \times (e^{iHt}e^{-iH_a t}E_a\phi, e^{iH_s}e^{-iH_b s}E_b\psi) = 0 \tag{7.8}$$

for $a \neq b$ and $\phi, \psi \in \mathfrak{K}$. It appears to be possible that this is also valid for cases where the asymptotic limits do not exist. A similar equation results for the case of Ω_+. If the wave operators are defined by the asymptotic limits the orthogonality condition has the form of Eq. (7.8) except again the limits of the form (7.3) are replaced by limits of the form (7.4) resulting in an apparently stronger condition.

By the way of summary we can make the following statements in analogy to the single-channel case:

The conditions sufficient for the integral-representation wave operators to be a unique solution of the scattering problem are that: the limits of the integrals of Eqs. (6.1) and (6.2) exist; the wave operators thus defined satisfy Eqs. (4.3); the two sets of ranges of the wave operators each span $\mathfrak{M}$ and have the orthogonality property.

The conditions are satisfied in the case where the conditions of the time-dependent formulation are valid. Then the wave operators defined by the asymptotic limits are identical to those defined by the integral representation. Hence we have a new physical interpretation of the asymptotic limits as a solution of the stationary-state scattering problem. There is no need to interpret the parameter t occurring in these limits as having anything to do with time.

It appears to be possible, because of the possibility that limits of the form (7.3) can exist when limits of the form (7.4) do not, that the conditions sufficient for a solution are weaker than the asymptotic conditions. The settlement of this question has been reduced to a definite mathematical problem. One should be able either to find Hamiltonian operators for which the conditions of the time-dependent formulation are not valid while the conditions sufficient for the integral representation are valid, or to prove that the former conditions are implied by the latter.

We have been unable to do either of these and hence the questions as to whether such a set of Hamiltonian operators exists as well as to whether it contains any Hamiltonians of physical interest remain as unsolved problems.

8. REMARKS ON THE HAMILTONIAN OPERATOR FOR NONRELATIVISTIC AND RELATIVISTIC THEORIES

We have said very little about how the Hamiltonian operators are to be defined. Usually they will be defined in terms of a basic set of operators, for example the coordinate and momentum operators of the particles involved, to which a natural physical interpretation can be attached. The "free" Hamiltonians corresponding to the various channels determine the various kinds and numbers of particles whoes measurement can be described by the theory, and the relation of the "free" Hamiltonians to the "total" Hamiltonian determines the dynamics of the interaction or scattering process.

We have developed our formulation according to

the traditional framework of nonrelativistic quantum mechanics. However this framework is not necessarily restricted to nonrelativistic theories; whether the theory is relativistic or nonrelativistic depends on the form of the Hamiltonian operators.

The "free" Hamiltonian associated with a given channel must describe the dynamics associated with the unperturbed motion of the particles of that channel. For the purpose of illustrating our ideas suppose that for a given channel this unperturbed dynamics is that of N free particles. If we wish to give a nonrelativistic description of the scattering of those particles, then the channel Hamiltonian operator should have the form of the nonrelativistic expression for the energy of the N free particles, while if we want to give a relativistic description it should have the form of the relativistic expression for the energy of the free particles (see Jauch,[4] Sec. 3).

The "total" Hamiltonian operator must satisfy conditions which are required for a meaningful physical interpretation of the theory. Among these are the existence of operators which commute with the Hamiltonian operator and represent the total momentum and angular momentum of the system. In a nonrelativistic theory the conditions of Galilean invariance must be satisfied.[11] This means that the Hamiltonian, momentum, and angular momentum operators, together with the generators of Galilean transformations, must form a set of ten operators which have the correct commutation relations to be infinitesimal generators for a representation of the Galilean group. A relativistic theory must satisfy the conditions of Lorentz invariance, the main one of which is that the Hamiltonian, momentum and angular momentum operators, together with the generators of Lorentz transformations, form a set of 10 operators which have the correct commutation relations to be the infinitesimal generators for a representation of the inhomogeneous Lorentz group.[12]

Thus relativistic as well as nonrelativistic theories can fit into the framework which we have used, provided they contain "total" and "free" Hamiltonian operators. It is only these operators, their relationships, and the structure of the Hilbert space determined by their relationships that are fundamental to our formulation of the scattering problem.

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Theory of High-Energy Potential Scattering*†

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The exact amplitude for scattering of a Schrödinger or Dirac particle by a static potential is rewritten in a two-potential form by splitting the potential into two parts, one of which contributes only to exactly forward scattering. Replacement of the exact wave function by a modified plane wave gives a high-energy approximation that is shown to be equivalent to the Saxon-Schiff approximation in the Schrödinger case. Corrections to the approximation are obtained in principle from a simplified series expansion of the exact wave function having the modified plane wave as leading term. The approximate amplitude reduces at small scattering angles to a well-known result; at large angles, it reduces to Schiff's stationary-phase approximation in the Dirac case but not, as shown by the example of a Gaussian potential, in the Schrödinger case.

I. INTRODUCTION

ELASTIC scattering of a high-energy particle by a static potential can be calculated either by partial-wave analysis, if the potential has spherical symmetry; by the Born approximation, if the potential is sufficiently weak; or by a less familiar high-energy approximation, if the scattering angle is sufficiently small. The last of these methods was initiated by Molière,[1] but has been developed and expounded primarily by Glauber.[2] Briefly, it consists in approximating the unknown exact wave function by a plane wave modified in phase to take account of the shift in de Broglie wavelength while the particle is passing through the potential. Its virtue is its applicability to potentials so strong that the Born approximation is useless. Its weakness is the restriction to small angles: Although most of the scattering at high energies is nearly forward, the large-angle scattering is often crucial for the interpretation of an experiment.

An extension of the high-energy approximation to large angles was made by Schiff,[3] who summed the infinite Born series after approximating each term by the method of stationary phase. For both Schrödinger and Dirac particles, Schiff obtained a large-angle scattering amplitude that differs from the Born approximation by phase modification of both the initial and final plane waves. He also recovered by the same method the small-angle approximation (in which only the initial plane wave is modified in phase), but obtained no results for intermediate angles. This gap was remedied by Saxon and Schiff[4] in a paper dealing only with the Schrödinger equation. The exact scattering amplitude was recast in a form that reduces to the small-angle approximation if the exact wave function is replaced by a plane wave. The high-energy approximation consists in replacing it instead by a plane wave modified in phase. Beside providing a well-defined (although somewhat cumbersome) approximation for all angles, this new approach to the problem was used to rederive the simplified small-angle and large-angle formulas and to revise their estimated ranges of validity.

The present paper develops a two-potential formulation of the high-energy approximation for both the Schrödinger and Dirac equations. The scattering potential (assumed real, although this is not essential to the method) is split into two parts, one of which is chosen to be the potential occurring in the wave equation satisfied by a modified plane wave. Since this part contributes only to exactly forward scattering, the remaining part provides a compact rearrangement of the exact scattering amplitude for nonzero angles. The exact wave function is then replaced by a modified plane wave as a high-energy approximation.

Although an approximation of this kind for all angles has not been given previously in the Dirac case, our procedure is related to earlier work on the Schrödinger scattering problem in two ways.

* Based in part on a thesis presented by one of the authors (P. J. L.) in partial fulfillment of requirements for the Ph. D. degree at Iowa State University. The work was performed in the Ames Laboratory of the U. S. Atomic Energy Commission.

† Preliminary accounts have been given by B. C. Carlson and P. J. Lynch, Bull. Am. Phys. Soc. 5, 35 (1960) and by P. J. Lynch, thesis, Ames Laboratory Report IS-203 (unpublished).

‡ Now at Space Technology Laboratories, Los Angeles, California.

[1] G. Molière, Z. Naturforsch. **2A**, 133 (1947).

[2] R. J. Glauber, *Lectures in Theoretical Physics* (Interscience Publishers, Inc., New York, 1959), Vol. I, p. 315.

[3] L. I. Schiff, Phys. Rev. **103**, 443 (1956).

[4] D. S. Saxon and L. I. Schiff, Nuovo cimento **6**, 614 (1957).

Lippmann[5] proposed a two-potential formalism and used it to obtain an integral equation for the wave function, but his splitting of the potential is different from ours. Secondly, our form of the high-energy approximation will be shown in Sec. III to be equivalent to Saxon and Schiff's, although the conclusions that we draw from it are at variance with theirs. Specifically, for 180° scattering from a Gaussian potential, we shall find in Sec. V the Schiff large-angle formula multiplied by $\frac{1}{2}$, plus additional terms that are small in a wide range of parameters (not including the range of validity of the Born approximation). The discrepancy is attributed to the method by which Saxon and Schiff estimate the size of discarded terms. For large-angle Dirac scattering, on the other hand, we recover the Schiff large-angle formula with no factor $\frac{1}{2}$, its absence being due to the linearity of the Dirac Hamiltonian in space derivatives.

II. TWO-POTENTIAL FORM OF THE SCATTERING AMPLITUDE

The exact amplitude for scattering of a Schrödinger particle by a scalar potential will first be rearranged in a form that is characteristic of two-potential theory and has certain advantages at high energies. In order to simplify the derivation, the potential $V(\mathbf{r})$ will be assumed to vanish outside a bounded region. If the particle has energy $E = \hbar^2k^2/2m$, its wave function satisfies

$$[\nabla^2 + k^2 - U(\mathbf{r})]\psi(\mathbf{r}) = 0, \tag{2.1}$$

where $U(\mathbf{r}) = (2m/\hbar^2)V(\mathbf{r})$. Solutions having the asymptotic form of a plane wave plus outgoing or incoming spherical waves will be denoted by ψ^+ or ψ^-, respectively. The exact scattering amplitude f is given by the well-known expressions[6]

$$-4\pi f(\mathbf{k}_f, \mathbf{k}_0) = (\varphi_f, U\psi_0^+) \tag{2.2a}$$

$$= (\psi_f^-, U\varphi_0), \tag{2.2b}$$

where the plane waves φ satisfy

$$(\nabla^2 + k^2)\varphi(\mathbf{r}) = 0. \tag{2.3}$$

The subscripts on the wave functions specify whether the plane wave (or plane-wave part of the asymptotic form) has the initial wave vector $\mathbf{k}_0$ or the final wave vector $\mathbf{k}_f$. Each of these vectors has magnitude k and direction given by the unit vector $\hat{k}_0$ or $\hat{k}_f$. The momentum transfer $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_f$ has magnitude $q = 2k \sin(\theta/2)$, where θ is the scattering angle.

A high-energy approximation to ψ_0^+ is the modified plane wave[2]

$$\chi_0^+(\mathbf{r}) = \varphi_0(\mathbf{r}) \exp i\,\delta_0(\mathbf{r}), \tag{2.4}$$

where

$$\varphi_0(\mathbf{r}) = \exp i\mathbf{k}_0\cdot\mathbf{r}, \tag{2.5}$$

$$\delta_0(\mathbf{r}) = -(2k)^{-1}\int_0^\infty U(\mathbf{r} - \hat{k}_0 s)\,ds. \tag{2.6}$$

The phase modification δ_0 takes account, to first order in U/k^2, of the shift in de Broglie wavelength when the particle is inside the potential. By observing that

$$\hat{k}_0\cdot\nabla\,\delta_0(\mathbf{r}) = -(2k)^{-1}U(\mathbf{r}), \tag{2.7}$$

it is easily verified that the modified plane wave satisfies the differential equation

$$[\nabla^2 + k^2 - U_S(\mathbf{r})]\chi_0^+(\mathbf{r}) = 0, \tag{2.8}$$

where

$$U_S = U - U_L \tag{2.9}$$

$$U_L = -\exp(-i\,\delta_0)\nabla^2 \exp i\,\delta_0. \tag{2.10}$$

To express the scattering amplitude in terms of χ_0^+, we apply Green's theorem to $\chi_0^+ - \varphi_0$ and $(\psi_f^- - \varphi_f)^*$, the star denoting complex conjugation:

$$\begin{aligned}\int d\mathbf{r}[&(\psi_f^- - \varphi_f)^*\nabla^2(\chi_0^+ - \varphi_0) \\ &- (\chi_0^+ - \varphi_0)\nabla^2(\psi_f^- - \varphi_f)^*] \\ &= \int d\mathbf{S}\cdot[(\psi_f^- - \varphi_f)^*\nabla(\chi_0^+ - \varphi_0) \\ &- (\chi_0^+ - \varphi_0)\nabla(\psi_f^- - \varphi_f)^*].\end{aligned} \tag{2.11}$$

The right side is proportional to a transition current through the surface of a large sphere; we shall first show that this current vanishes as the radius of the sphere becomes infinite. The quantities $\delta_0(\mathbf{r})$ and $\chi_0^+(\mathbf{r}) - \varphi_0(\mathbf{r})$ vanish unless $\mathbf{r}$ lies either in the potential or in a semi-infinite cylinder such that a straight line proceeding from $\mathbf{r}$ in the direction $-\hat{k}_0$ pierces the potential. This second region will be called the forward cylinder with axis in the direction $\hat{k}_0$. Thus the surface integral reduces to an integral over the area of intersection of the forward cylinder with the sphere. As the radius of the sphere tends to infinity, this area remains

[5] B. A. Lippmann, Ann. Phys. 1, 113 (1957).
[6] B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950).

bounded because the potential vanishes outside a bounded region, but $(\psi_f^- - \varphi_f)^*$ and its gradient decrease as the reciprocal radius; hence the surface integral tends to zero.

If Eqs. (2.1), (2.3), and (2.8) are substituted in the volume integral in Eq. (2.11), we obtain (for real U)

$$((\psi_f^- - \varphi_f), U_S\chi_0^+) = (\psi_f^-, U(\chi_0^+ - \varphi_0)) \qquad (2.12)$$

By use of Eqs. (2.2b) and (2.9), this equation becomes

$$-4\pi f(\mathbf{k}_f, \mathbf{k}_0) = (\varphi_f, U_S\chi_0^+) + (\psi_f^-, U_L\chi_0^+). \qquad (2.13)$$

Equation (2.13) has a form characteristic of scattering by two potentials: the first term is the scattering by U_S alone and the second term is the scattering by U_L as modified by the presence of U_S. A similar division of the amplitude is familiar[7] in scattering problems where two physically distinct forces are acting, particularly when the scattering produced by one of them alone can be calculated exactly. In the present situation a single potential has been divided into two parts in a convenient but artificial way by introducing χ_0^+; the separate parts are not real, and they differ from zero throughout both the potential region and the forward cylinder. Because of these peculiarities, we shall have to discuss the existence of the separate terms of Eq. (2.13); also, we have felt it desirable to derive this equation by an elementary procedure for which the conditions of validity are more evident than for the operator method.[7] Our method can be used also when the two potentials both have finite range, for the surface integral in Eq. (2.11) then vanishes because of cancellation between the two terms in the integrand. With a different choice of outgoing or incoming spherical waves, the same procedure is convenient for deriving other identities between different forms of the scattering amplitude; for instance, replacement of $\chi_0^+ - \varphi_0$ by $\psi_0^+ - \varphi_0$ in Eq. (2.11) shows the equivalence of Eqs. (2.2a) and (2.2b).

As mentioned, both U_S and U_L are nonzero throughout the forward cylinder. This implies that each term of Eq. (2.13) is an integral that appears to oscillate rather than converge, although the sum of the two terms is well defined. For exactly forward or backward scattering, this appearance is illusory as each term can actually be shown to converge separately. At all other angles, it will be convenient to define the integrals separately by adding a small positive imaginary part to the component of momentum transfer along the direction $\hat{k}_0$. That is, if the z axis is chosen along this direction, we replace q_z by $q_z + i\epsilon$ and take the limit of each integral as ϵ goes to zero. The use of this Abelian definition of the integrals cannot change their sum, which is well defined in any case. One may like to think of the convergence factor $\exp(-\epsilon z)$ as a device for representing the attenuation of the geometrical shadow by diffraction effects.

Because χ_0^+ describes a particle whose direction of motion is unchanged as it passes through the potential, U_S may be expected to contribute only to exactly forward scattering, while U_L produces scattering through finite angles. The idea of splitting the potential into two parts of this kind has been discussed by Lippmann,[5] but his division of the potential is different and less explicit than the one given by Eqs. (2.9) and (2.10).

One's qualitative view of the contributions of U_S and U_L to the scattering process is confirmed by the following exact result:

$$(\varphi_f, U_S\chi_0^+) = \begin{cases} (\varphi_0, U\chi_0^+), & \theta = 0, \\ 0, & \theta > 0. \end{cases} \qquad (2.14)$$

Since the scattering amplitude is a continuous function of θ, this discontinuity in the first term of Eq. (2.13) must of course be accompanied by a compensating discontinuity in the second term. In order to prove Eq. (2.14), we consider first the matrix element

$$(\varphi_f, U_L\chi_0^+) = -\int d\mathbf{r}\, (\exp i\mathbf{q}\cdot\mathbf{r})\nabla^2 \exp i\,\delta_0(\mathbf{r}). \qquad (2.15)$$

When the scattering is forward, q vanishes and the volume integral can be rewritten as an integral over the surface of a large sphere:

$$(\varphi_0, U_L\chi_0^+) = -\int d\mathbf{S}\cdot\nabla \exp i\,\delta_0(\mathbf{r}) = 0, \quad \theta = 0. \qquad (2.16)$$

Because $\nabla \exp i\,\delta_0$ is nonzero only on the intersection of the sphere with the forward cylinder, only its component along the axis of the cylinder contributes to the integral when the sphere has infinite radius. However, this axial component is proportional to $U(\mathbf{r})$ by Eq. (2.7) and therefore vanishes at large distances.

For nonzero angles, it is convenient to integrate

[7] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953). A misprint in Eq. (4.4) is corrected by Lippmann.[5] See also M. Hack, Phys. Rev. **108**, 1636 (1957).

by parts with respect to z in Eq. (2.15):

$$(\varphi_f, U_L\chi_0^+) = i(q_z + i\epsilon)^{-1} \times \iint_{-\infty}^{\infty} dx\, dy \exp(iq_x x + iq_y y) \times [\exp(iq_z z - \epsilon z)\nabla^2 \exp i\,\delta_0(\mathbf{r})]_{z=-\infty}^{\infty} - (2k)^{-1}(q_z + i\epsilon)^{-1} \times \int d\mathbf{r} \exp(i\mathbf{q}\cdot\mathbf{r})\nabla^2(U \exp i\,\delta_0). \quad (2.17)$$

The boundary term vanishes because the convergence factor is zero at the upper limit and the factor $\nabla^2 \exp i\,\delta_0$ is zero at the lower limit. In the second term, the quantity ϵ may be set equal to zero (when $\theta > 0$), for the integration is limited to the potential region. The Laplacian operator can be transferred to the factor $\exp i\mathbf{q}\cdot\mathbf{r}$ by an application of Green's theorem, the surface integral vanishing because the potential is bounded in space. Since the quantity $q^2/2kq_z$ is unity, Eq. (2.17) becomes, in conjunction with Eq. (2.16),

$$(\varphi_f, U_L\chi_0^+) = \begin{cases} 0, & \theta = 0, \\ (\varphi_f, U\chi_0^+), & \theta > 0. \end{cases} \quad (2.18)$$

[A unified proof of both parts of Eq. (2.18) may be obtained by observing that the limit as $\epsilon \to 0$ of $(2k)^{-1}(q_z + i\epsilon)^{-1} q^2$ is 0 for $\theta = 0$ and 1 for $\theta > 0$.] Because $U = U_S + U_L$, Eq. (2.14) follows directly. Finally, we can rewrite Eq. (2.13) as

$$-4\pi f(\mathbf{k}_f, \mathbf{k}_0) = \begin{cases} (\varphi_0, U\chi_0^+) + (\psi_0^-, U_L\chi_0^+), & \theta = 0, \\ (\psi_f^-, U_L\chi_0^+), & \theta > 0. \end{cases} \quad (2.19)$$

Equation (2.19) is a rearrangement (without approximation) of the exact scattering amplitude, Eq. (2.2b), in a form that is expected to be useful at high energies. This expectation is supported by a comparison of the results of replacing ψ_f^- by the plane wave φ_f in the two expressions. Equation (2.2b) gives the Born approximation, while Eq. (2.19) becomes

$$-4\pi f(\mathbf{k}_f, \mathbf{k}_0) \approx (\varphi_f, U\chi_0^+) \quad (2.20)$$

by virtue of Eq. (2.18). The last equation is a well-known approximation for high-energy scattering valid at small angles.[2] The use of a better approximate wave function in Eq. (2.19) will be discussed in Sec. V.

III. DERIVATION OF THE SAXON-SCHIFF AMPLITUDE

Saxon and Schiff[4] have rewritten the exact scattering amplitude in another form that is useful for obtaining high-energy approximations. We shall now show that the two-potential form of the amplitude, Eq. (2.13), is closely related to the Saxon-Schiff form and incidentally provides a substantially simpler way of deriving it than that given originally by Saxon and Schiff. Secondly, we shall show the equivalence of the high-energy approximations obtained when ψ_f^- is replaced by a modified plane wave χ_f^- in these two forms of the amplitude.

The Saxon-Schiff amplitude is

$$-4\pi f(\mathbf{k}_f, \mathbf{k}_0) = (\varphi_f, U\chi_0^+) + \frac{i}{2k}\int d\mathbf{r}U(\mathbf{r})[\exp i\,\delta_0(\mathbf{r})]\nabla^2 \int_z^{\infty} dz'\varphi_0(\mathbf{r}')\psi_{sc}^*(\mathbf{r}'), \quad (3.1)$$

where $r' = (x, y, z')$ and

$$\psi_{sc}(\mathbf{r}) = \psi_f^-(\mathbf{r}) - \varphi_f(\mathbf{r}). \quad (3.2)$$

To obtain this result from Eq. (2.13), we first substitute $U_S = U - U_L$:

$$-4\pi f(\mathbf{k}_f, \mathbf{k}_0) = (\varphi_f, U\chi_0^+) - [\psi_{sc}, (\nabla^2 \exp i\,\delta_0)\varphi_0]. \quad (3.3)$$

With the z axis parallel to $\hat{k}_0$, integration by parts with respect to z and use of Eq. (2.7) change the second term of Eq. (3.3) to

$$-\iint dx\, dy[\nabla^2 \exp i\,\delta_0(\mathbf{r})] \times \int_z^{\infty} dz'\varphi_0(\mathbf{r}')\psi_{sc}^*(\mathbf{r}') \Big|_{z=-\infty}^{z=+\infty} - \frac{i}{2k}\int d\mathbf{r}\{\nabla^2[U(\mathbf{r}) \exp i\,\delta_0(\mathbf{r})]\} \times \int_z^{\infty} dz'\varphi_0(\mathbf{r}')\psi_{sc}^*(\mathbf{r}'). \quad (3.4)$$

Since the asymptotic form of ψ_{sc} is an incoming spherical wave, $\varphi_0(\mathbf{r}')\,\psi_{sc}^*(\mathbf{r}')$ varies as $(1/z')\exp(2ikz')$ at large positive z' for fixed x and y. Hence the integral over z' exists and tends to zero as $z \to +\infty$. Since $\nabla^2 \exp(i\,\delta_0)$ vanishes at large negative z, the first term of Eq. (3.4) clearly vanishes at both limits. Green's theorem applied to the second term now yields Eq. (3.1), the surface integral in Green's theorem having a vanishing integrand because U vanishes at large distances.

If ψ_f^- is replaced by a modified plane wave χ_f^-,

the only part of this demonstration that needs changing is the reason why the boundary term vanishes at the upper limit. When χ_f^- is defined in more detail in Sec. IV, it will be seen that $\chi_f^- - \varphi_f$ vanishes at large positive z for fixed z and y unless the scattering angle is 180°. In this exceptional case, the integral over z' must be defined in the Abelian sense, and the convergence factor then causes the boundary term to vanish at the upper limit.

IV. ITERATION SCHEME

In order to make use of Eq. (2.19), the unknown exact wave function ψ_f^- must be replaced by an approximate wave function or, more systematically, by the leading term or terms of a series expansion. For example, Eq. (2.20) resulted from replacing ψ_f^- by the leading term of its Born series. At high energies, a better choice should be the modified plane wave χ_f^-, which is a good approximation to ψ_f^- in the potential region provided that $kR \gg 1$, $U \ll k^2$, and $(U/k^2)(UR/k) \ll 1$.[4] (The potential is assumed to be smooth and to occupy a region of dimension R.) Postponing until Sec. V a further discussion of this approximation, we consider here the problem of expanding ψ_f^- in a series having χ_f^- as its leading term.

For convenience of notation we shall actually work with ψ_0^+ instead of ψ_f^-; one can be obtained from the other by use of the relation[8]

$$\psi_f^-(\mathbf{r}) = [\psi_{-f}^+(\mathbf{r})]^*, \tag{4.1}$$

where $-f$ refers to the wave vector $-\mathbf{k}_f$. Similarly, χ^- and χ^+ are related by

$$\chi_f^-(\mathbf{r}) = [\chi_{-f}^+(\mathbf{r})]^* = \exp[i\mathbf{k}_f\cdot\mathbf{r} - i\,\delta_{-f}(\mathbf{r})], \tag{4.2}$$

$$\delta_{-f}(\mathbf{r}) = -(2k)^{-1}\int_0^\infty U(\mathbf{r} + \hat{k}_f s)\,ds. \tag{4.3}$$

The phase modification is nonzero if $\mathbf{r}$ lies in the potential or in the backward cylinder with axis in the direction $-\hat{k}_f$ (a semi-infinite cylinder such that a straight line proceeding from $\mathbf{r}$ in the direction $\hat{k}_f$ pierces the potential).

Saxon and Schiff[4] obtained a series for ψ_0^+ with χ_0^+ as leading term by iterating an integral equation for ψ_0^+. We shall instead obtain an integral equation for the exact Green's function and substitute its iteration series in a suitable expression for ψ_0^+, to be derived in the next paragraph. Although our procedure is more complicated, the results are in one respect simpler.

Whereas Saxon and Schiff applied Green's theorem to ψ_0^+ and an approximate Green's function, we shall apply it to χ_0^+ and the exact Green's function, which satisfies

$$[\nabla^2 + k^2 - U(\mathbf{r})]G^+(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'). \tag{4.4}$$

From Green's theorem and Eq. (2.8), it follows that

$$\Omega(\mathbf{r}) \equiv \int d\mathbf{S}'\cdot[G^+(\mathbf{r}',\mathbf{r})\nabla'\chi_0^+(\mathbf{r}') - \chi_0^+(\mathbf{r}')\nabla' G^+(\mathbf{r}',\mathbf{r})] \tag{4.5}$$

$$= \chi_0^+(\mathbf{r}) - \int d\mathbf{r}' G^+(\mathbf{r}',\mathbf{r})U_L(\mathbf{r}')\chi_0^+(\mathbf{r}'). \tag{4.6}$$

Equation (4.6) shows that the surface integral Ω satisfies the same Schrödinger equation as ψ_0^+. However, it is not obvious that Ω has the asymptotic form of a plane wave plus outgoing spherical waves [the asymptotic form of the volume integral cannot be obtained by simply substituting for G^+ its asymptotic form, since the integration in Eq. (4.6) extends over both the potential region and the forward cylinder]. To show that Ω is indeed ψ_0^+, we observe that the same procedure, applied to φ_0 instead of χ_0^+, leads to a familiar equation[9] for ψ_0^+, with no difficulties about the asymptotic form:

$$\psi_0^+(\mathbf{r}) = \int d\mathbf{S}'\cdot[G^+(\mathbf{r}',\mathbf{r})\nabla'\varphi_0(\mathbf{r}') - \varphi_0(\mathbf{r}')\nabla' G^+(\mathbf{r}',\mathbf{r})] \tag{4.7}$$

$$= \varphi_0(\mathbf{r}) - \int d\mathbf{r}' G^+(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\varphi_0(\mathbf{r}'). \tag{4.8}$$

But the surface integrals (4.5) and (4.7) are equal, for $\chi_0^+ - \varphi_0$ and its gradient are zero on the surface of a large sphere except at its intersection with the forward cylinder, while $G^+(\mathbf{r}',\mathbf{r})$ decreases at large r' as $1/r'$. Finally, by the reciprocity property of the Green's function, Eq. (4.6) becomes

$$\psi_0^+(\mathbf{r}) = \chi_0^+(\mathbf{r}) - \int d\mathbf{r}' G^+(\mathbf{r},\mathbf{r}')U_L(\mathbf{r}')\chi_0^+(\mathbf{r}'). \tag{4.9}$$

This equation bears the same relation to Saxon and Schiff's integral equation for ψ_0^+ as does Eq. (4.8) to the integral equation

$$\psi_0^+(\mathbf{r}) = \varphi_0(\mathbf{r}) - \int d\mathbf{r}' G_0^+(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi_0^+(\mathbf{r}').$$

The iteration series to be substituted for G^+ in Eq. (4.9) is chosen to have as its first term the approximate high-energy Green's function proposed

[8] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press, New York, 1958), p. 422.

[9] G. F. Chew and M. L. Goldberger, Phys. Rev. **87**, 778 (1952).

by Saxon and Schiff[4]:

$$F^+(\mathbf{r}, \mathbf{r}') = G_0^+(\rho) \exp i\,\delta(\mathbf{r}, \mathbf{r}'), \tag{4.10}$$

where

$$\begin{aligned} \boldsymbol{\rho} &= \mathbf{r} - \mathbf{r}', \\ G_0^+(\rho) &= (4\pi\rho)^{-1} \exp ik\rho, \\ \delta(\mathbf{r}, \mathbf{r}') &= -(2k)^{-1} \int_0^\rho U(\mathbf{r} - \hat{\rho}s)\, ds. \end{aligned} \tag{4.11}$$

The approximate Green's function satisfies the differential equation

$$[\nabla^2 + k^2 - U(\mathbf{r}) + W(\mathbf{r}, \mathbf{r}')]F^+(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \tag{4.12}$$

with

$$\begin{aligned} W(\mathbf{r}, \mathbf{r}') = &-\exp[-i\,\delta(\mathbf{r}, \mathbf{r}')]\nabla^2 \\ &\times \exp[i\,\delta(\mathbf{r}, \mathbf{r}')] - (i/k\rho)U(\mathbf{r}). \end{aligned} \tag{4.13}$$

When Green's theorem is applied to G^+ and F^+, the surface integral vanishes and we obtain the integral equation

$$\begin{aligned} G^+(\mathbf{r}, \mathbf{r}') = &F^+(\mathbf{r}, \mathbf{r}') \\ &- \int d\mathbf{r}'' F^+(\mathbf{r}, \mathbf{r}'') W(\mathbf{r}'', \mathbf{r}) G^+(\mathbf{r}'', \mathbf{r}'). \end{aligned} \tag{4.14}$$

Iteration of this equation gives a series for G^+ that can be substituted in Eq. (4.9) to yield the desired series expansion of ψ_0^+:

$$\begin{aligned} \psi_0^+(\mathbf{r}) = \chi_0^+(\mathbf{r}) &- \int d\mathbf{r}' F^+(\mathbf{r}, \mathbf{r}') U_L(\mathbf{r}') \chi_0^+(\mathbf{r}') \\ &+ \int d\mathbf{r}'\, d\mathbf{r}'' F^+(\mathbf{r}, \mathbf{r}'') W(\mathbf{r}'', \mathbf{r}) \\ &\times F^+(\mathbf{r}'', \mathbf{r}') U_L(\mathbf{r}') \chi_0^+(\mathbf{r}') + \cdots. \end{aligned} \tag{4.15}$$

The series obtained by iterating Saxon and Schiff's integral equation differs from this in only one respect: the factor $U_L(\mathbf{r}')$ that precedes $\chi_0^+(\mathbf{r}')$ in all terms but the first of Eq. (4.15) is replaced by the more complicated $W(\mathbf{r}', \mathbf{r}^{(n)})$ of Eq. (4.13). This replacement does not change the values of the individual terms of the series; by a proof that begins with the application of Green's theorem to F^+ and χ_0^+, one can show that

$$\int d\mathbf{r}' F^+(\mathbf{r}, \mathbf{r}')[U_L(\mathbf{r}') - W(\mathbf{r}', \mathbf{r})]\chi_0^+(\mathbf{r}') = 0. \tag{4.16}$$

Before turning to other questions, we should like to mention a further use for Eq. (4.9): it provides an alternative derivation of the exact scattering amplitude in the form of Eq. (3.3). We observe that the argument of ψ_0^+ in Eq. (4.9) occurs in the integrand only as an argument of the exact Green's function. As a result, a familiar integral occurs when Eq. (4.9) is substituted in Eq. (2.2a) and the order of integration is reversed in the second term:

$$\begin{aligned} -4\pi f(\mathbf{k}_f, \mathbf{k}_0) = (\varphi_f, U\chi_0^+) &- \int d\mathbf{r} U_L(\mathbf{r}) \chi_0^+(\mathbf{r}) \\ &\times \int d\mathbf{r}' \varphi_f^*(\mathbf{r}') U(\mathbf{r}') G^+(\mathbf{r}', \mathbf{r}). \end{aligned} \tag{4.17}$$

Now the solution of the Schrödinger equation having the asymptotic form of a plane wave φ_f plus incoming spherical waves is

$$\psi_f^-(\mathbf{r}) = \varphi_f(\mathbf{r}) - \int d\mathbf{r}' G^-(\mathbf{r}, \mathbf{r}') U(\mathbf{r}') \varphi_f(\mathbf{r}'). \tag{4.18}$$

By Eq. (3.2) and the identity

$$[G^-(\mathbf{r}, \mathbf{r}')]^* = G^+(\mathbf{r}', \mathbf{r}),$$

it follows that

$$\psi_{sc}^*(\mathbf{r}) = -\int d\mathbf{r}' G^+(\mathbf{r}', \mathbf{r}) U(\mathbf{r}') \varphi_f^*(\mathbf{r}'). \tag{4.19}$$

This identification of the integral shows Eq. (4.17) to be the same as Eq. (3.3).

V. SMALL-ANGLE AND LARGE-ANGLE APPROXIMATIONS

When ψ_f^- is replaced in Eq. (2.19) by the approximate high-energy wave function χ_f^-, we obtain an approximate scattering amplitude

$$\begin{aligned} &-4\pi f_1(\mathbf{k}_f, \mathbf{k}_0) \\ &= \begin{cases} (\varphi_0, U\chi_0^+) + (\chi_0^-, U_L\chi_0^+), & \theta = 0, \\ (\chi_f^-, U_L\chi_0^+), & \theta > 0. \end{cases} \end{aligned} \tag{5.1}$$

In spite of its very different appearance, this expression is equivalent, as shown already in Sec. III, to the high-energy approximation given by Saxon and Schiff.[4] They have discussed its accuracy, as well as the ranges of energy and angle in which it reduces to the simplified small-angle approximation, Eq. (2.20), or to Schiff's large-angle formula, $(\chi_f^-, U\chi_0^+)$.[3]

To discuss these questions again would surely be superfluous if Saxon and Schiff had not found it necessary to make order-of-magnitude estimates [following their Eq. (32), for example] of some rather complicated integrals containing rapidly oscillating factors in their integrands. Such estimates are very difficult to make with certainty; for instance, the relative magnitudes of two functions are no guide to the relative magnitudes of their Fourier transforms, except for the low-frequency components. In view of this, we have thought it worthwhile to see what conditions of validity can be

established by taking the form (5.1) of f_1 as an alternative starting point and abstaining from order-of-magnitude estimates of the kind just mentioned.

The conclusions that we have reached by this route are very limited. The first is that f_1 reduces to the small-angle approximation for scattering angles $\theta \lesssim 1/kR$; that is, for such small angles, it is immaterial whether ψ_f^- is approximated in Eq. (2.19) by a modified or unmodified plane wave. For reasons to be explained presently, we are not able to extend this conclusion to the wider range of angles, $\theta \ll (kR)^{-\frac{1}{2}}$, given by Saxon and Schiff. For angles near 180°, our attempt to recover the Schiff large-angle formula will serve only to underline the hazards of making order-of-magnitude estimates. An effort to avoid them in a particular case, by an approximate saddle-point integration, will be found to suggest that the Schiff large-angle formula should be multiplied by $\frac{1}{2}$ and its range of validity restricted to avoid overlap with that of the Born approximation. (For a Dirac particle, on the other hand, the Schiff large-angle formula will be obtained without difficulty in Sec. VI.)

For small scattering angles, it is convenient first to rearrange Eq. (5.1) in the form

$$-4\pi f_1(\mathbf{k}_f, \mathbf{k}_0) = (\varphi_f, U\chi_0^+) + (\chi_f^- - \varphi_f, U_L\chi_0^+). \quad (5.2)$$

The first term is the familiar small-angle formula of Eq. (2.20); the second term is a correction whose relative order of magnitude we wish to estimate. (The second term is well-defined, with one exception, because the integrand vanishes except in the potential region and in the intersection of the forward and backward cylinders; at $\theta = 180°$, these cylinders coincide, but convergence can be restored by adding a small positive imaginary part to q_z as in Sec. II.) We suppose that the potential is smooth and occupies a region of dimension R, that $kR \gg 1$ and $U \ll k^2$, and that UR/k is not large compared to unity. Then the only factor in either integrand that can oscillate rapidly in a distance R is $\exp(i\mathbf{q}\cdot\mathbf{r})$. If $\theta \lesssim 1/kR$, this factor too is slowly varying, and a straightforward estimate of orders of magnitude gives roughly UR^3 for the first term of Eq. (5.2) and U^2R^3/k^2 for the second term. Thus the second term is of relative order U/k^2 and can be neglected. But if $\theta \gg 1/kR$, the integrand of each term contains the rapidly oscillating factor $\exp(i\mathbf{q}\cdot\mathbf{r})$, and order-of-magnitude estimates, whether of the individual terms or of their ratio, become unreliable.

At large scattering angles, this difficulty of estimating high-frequency Fourier components is aggravated. Reflection from a one-dimensional barrier will illustrate how one can be deceived by apparent orders of magnitude; the same hazards will then be encountered in a discussion of 180° scattering from a Gaussian potential in three dimensions.

The reflection amplitude from a one-dimensional barrier is[10]

$$r = (2ik)^{-1}(\varphi_f, U\psi_0^+). \quad (5.3)$$

This can be rewritten in the two-potential formalism as

$$2ikr = (\varphi_f, U_S\chi_0^+) + (\psi_f^-, U_L\chi_0^+), \quad (5.4)$$

where

$$\varphi_f(z) = \exp(-ikz), \quad (5.5)$$

$$\chi_0^+(z) = \exp[ikz + i\,\delta_0(z)] = [\chi_f^-(z)]^*, \quad (5.6)$$

$$\delta_0(z) = -(2k)^{-1}\int_{-\infty}^{z} U(z')\,dz', \quad (5.7)$$

$$U_L(z) = -\exp(-i\,\delta_0)(d^2/dz^2)\exp(i\,\delta_0). \quad (5.8)$$

As expected, the first term of Eq. (5.4) is easily shown to vanish. Replacement of ψ_f^- in the second term by χ_f^- gives a high-energy approximation analogous to Eq. (5.1):

$$2ikr_1 = (\chi_f^-, U_L\chi_0^+)$$

$$= -\int_{-\infty}^{\infty} dz \exp(2ikz + i\,\delta_0)\frac{d^2}{dz^2}\exp i\,\delta_0. \quad (5.9)$$

The integral can be rewritten in two ways by substituting the identities

$$\exp(i\,\delta_0)\frac{d^2}{dz^2}\exp i\,\delta_0 = \frac{1}{2}\frac{d^2}{dz^2}\exp(2i\,\delta_0) + \left(\frac{d}{dz}\,\delta_0\right)^2\exp(2i\,\delta_0) \quad (5.10a)$$

$$= \frac{1}{4}\frac{d^2}{dz^2}\exp(2i\,\delta_0) + i\,\frac{1}{2}\left(\frac{d^2}{dz^2}\,\delta_0\right)\exp(2i\,\delta_0). \quad (5.10b)$$

In each case, we integrate the first term by parts to obtain

$$2ikr_1 = (\chi_f^-, [U - (U^2/4k^2)]\chi_0^+) \quad (5.11a)$$

$$= \left(\chi_f^-, \left[\frac{1}{2}U + \frac{i}{4k}\frac{dU}{dz}\right]\chi_0^+\right). \quad (5.11b)$$

A glance at Eq. (5.11a) suggests that the second term is of order U_0/k^2 compared to the first and can

[10] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 1071.

be neglected at high energies, leaving $(\chi_f^-, U\chi_0^+)$ as expected by analogy with the Schiff large-angle formula in three dimensions. A fallacy in this argument is that U^2 usually varies more rapidly than U and consequently has larger high-frequency components. Moreover, a contradictory conclusion is reached by estimating the second term of Eq. (5.11b) to be of order $1/kR$ compared to the first.

We shall try to resolve this dilemma by considering a Gaussian potential, $U = U_0 \exp(-z^2/a^2)$. The integrand of Eq. (5.11a) has no singularities for finite complex z, but the quantity

$$\ln [(\chi_f^-)^* \chi_0^+] = 2ikz - i(U_0/k) \int_{-\infty}^{z} \exp\left(-\frac{z'^2}{a^2}\right) dz' \tag{5.12}$$

has a saddle point at

$$z = ia[\ln (2k^2/U_0)]^{\frac{1}{2}} = iy_0, \tag{5.13}$$
$$U(iy_0) = 2k^2.$$

If the integration contour is shifted from the real axis to the line $z = x + iy_0$, then the real part of Eq. (5.12) has a sufficiently sharp maximum as x goes through zero that the variation of the remaining terms of the integrand can be neglected, provided that $y_0 \ll ka^2$. Instead of recording the rather cumbersome result of the saddle-point integration, we observe only that $U^2/4k^2$ has the same value as $U/2$ at the saddle point; thus, in this approximation, we simply recover the first term of Eq. (5.11b).

A better approximation should result from applying the same procedure to Eq. (5.11b), because $dU/dz = -2zU/a^2$ varies less rapidly than U^2. Indeed, only z need be replaced by its value at the saddle point to obtain a small correction term:

$$2ikr_1 \approx \tfrac{1}{2}(\chi_f^-, U\chi_0^+)[1 + (ka^2)^{-1} y_0]. \tag{5.14}$$

If the saddle point is defined more carefully by adding $\ln U$ to Eq. (5.12), the algebra becomes more complicated but the saddle point is shifted by a negligible amount to approximately $iy_0 - i(2k)^{-1}$.

An objection to this saddle-point approximation is that the real part of Eq. (5.12) does not continue to decrease with further increase of $|x|$ but oscillates and reaches a local maximum (never as large as the one at the saddle point) whenever $|x|$ is an integral multiple of $\pi a^2/y_0$. However, if $y_0 \lesssim \pi a$, i.e., if $U_0/k^2 \gtrsim 10^{-4}$, the heights of these subsidiary maxima decrease rapidly from one to the next. Even at the first and largest of them, the exponential of the real part is small compared to its value at the saddle point, and the exponential of the imaginary part is oscillating rapidly. Consequently, we believe that the value of the integral comes almost entirely from the saddle point.

Since the high-energy approximation requires $ka \gg 1$ and $(U_0/k^2)(U_0 a/k) \ll 1$, we find that r_1 is half as large as the analog of the Schiff large-angle formula in the range of parameters $10^{-4} \lesssim U_0/k^2 \ll (ka)^{-\frac{1}{2}}$. No inconsistency with the Born approximation arises from the factor $\frac{1}{2}$, because the second Born approximation for a Gaussian potential is large compared to the first in this range.

The factor $\frac{1}{2}$ does not seem to be a peculiarity of the one-dimensional case. In three dimensions, the approximate amplitude for 180° scattering is

$$-4\pi f_1(-\mathbf{k}_0, \mathbf{k}_0) = (\chi_f^-, U_L \chi_0^+)$$
$$= -\int d\mathbf{r} \exp(2ikz + i\,\delta_0)\nabla^2 \exp i\,\delta_0. \tag{5.15}$$

As in one dimension, we avoid terms explicitly quadratic in U by substituting an identity similar to Eq. (5.10b):

$$\exp(i\,\delta_0)\nabla^2 \exp i\,\delta_0$$
$$= \tfrac{1}{4}\nabla^2 \exp 2i\,\delta_0 + \tfrac{1}{2}i(\nabla^2\,\delta_0) \exp 2i\,\delta_0. \tag{5.16}$$

When the first term is integrated by parts, the surface integral vanishes by the reasoning applied earlier to Eq. (2.16), and the volume integral is just one-half the Schiff large-angle formula. If the second term is evaluated for a Gaussian potential, $U = U_0 \exp(-r^2/a^2)$, Eq. (5.15) becomes

$$-4\pi f_1 = \int d\mathbf{r} \exp(2ikz + 2i\,\delta_0)$$
$$\times [\tfrac{1}{2}U - \tfrac{1}{2}i(ka^2)^{-1} zU$$
$$- 2ia^{-4}(x^2 + y^2 - a^2)\,\delta_0]. \tag{5.17}$$

The integrations over x and y can be carried out exactly, a convenient variable being $t = \exp[-(x^2 + y^2)/a^2]$. The first two terms present no difficulties; the third term, which is defined in the Abelian sense by the convergence factor $\exp(-\epsilon z)$, is first integrated by parts with respect to z and then with respect to t. The result is

$$-4\pi f_1 = \pi a^2 \int_{-\infty}^{\infty} dz \exp(2ikz + 2i\,\delta_0)\tfrac{1}{2}U(z)$$
$$\times \{[1 - i(ka^2)^{-1} z - (ka)^{-2}](2i\,\delta_0)^{-1}$$
$$\times [1 - \exp(-2i\,\delta_0)] + (ka)^{-2}\}. \tag{5.18}$$

In this last equation, but not in Eq. (5.17), U and δ_0 are functions of z alone: $U(z)$ stands for $U_0 \exp(-z^2/a^2)$ and δ_0 is related to it by Eq. (5.7). The terms in $(ka)^{-2}$ come from the third term of Eq. (5.17).

As in the earlier discussion of the reflection amplitude, we estimate the relative importance of the slowly varying factors by evaluating them at the same saddle point, $z = iy_0$. Admittedly, the variation of $[1 - \exp(-2i\,\delta_0)]$ is not slow near the saddle point, but its value remains very close to unity. The term in $(ka^2)^{-1}z$ is then of relative order y_0/ka^2, and the square bracket containing this term is effectively unity. The last term in Eq. (5.18) is of relative order $(ka)^{-2}\,\delta_0 \approx (ky_0)^{-1} \ll 1$. We conclude that only the first term of Eq. (5.17) is important, again provided that $y_0 \lesssim \pi a$:

$$-4\pi f_1(-\mathbf{k}_0, \mathbf{k}_0) \approx \tfrac{1}{2}(\chi_f^-, U\chi_0^+). \tag{5.19}$$

One would like to know whether Eq. (5.19) is correct for potentials other than a Gaussian, in a suitable range of parameters, and whether it can be extended to scattering angles other than 180°. The assumption of a Gaussian potential was not used in obtaining this expression directly from the first term of Eq. (5.16), and we speculate that this term will in general have substantially larger high-frequency components than the second term because it contains the square of the z derivative of the potential. As in the Gaussian case, the effect of its more rapid variation will be compensated by its quadratic dependence on U_0 when U_0 becomes sufficiently small that the Born approximation is valid. The first term leads directly to the right-hand side of Eq. (5.19) also at scattering angles other than 180° provided that χ_f^- is approximated by $\varphi_f \exp(-i\,\delta_0)$. We have not been able to estimate reliably the range of angles about 180° in which no serious error is caused by this approximation.

VI. DIRAC SCATTERING

In order to describe high-energy potential scattering of physical electrons, one must use the Dirac equation to satisfy the requirements of special relativity. We shall find that the two-potential formalism developed earlier for the Schrödinger equation can be applied also to the single-particle Dirac equation with only minor changes. Aside from the complications of spin, the resulting high-energy approximation is in fact simpler in the Dirac case; for 180° scattering, in particular, we shall recover the Schiff large-angle formula[3] with no factor $\frac{1}{2}$ and with no additive terms. These simplifications occur because the Dirac Hamiltonian is linear rather than quadratic in space derivatives.

The Dirac equation for a particle in a scalar potential $V(\mathbf{r})$ is[11]

$$[E - H_0 - V(\mathbf{r})]\psi(\mathbf{r}) = 0, \tag{6.1}$$

where

$$H_0 = i\hbar c\boldsymbol{\alpha}\cdot\nabla - \beta mc^2. \tag{6.2}$$

If no potential is present, the plane-wave solutions with positive energy will be denoted by

$$\begin{aligned} \varphi_i(\mathbf{r}) &= u_i(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{r}), \quad i = \pm\tfrac{1}{2}, \\ k^2 &= (E/\hbar c)^2 - k_c^2, \\ k_c &= mc/\hbar. \end{aligned} \tag{6.3}$$

The four-component spinors u_i satisfy the orthogonality relations

$$u_i^\dagger u_j = (E/mc^2)\,\delta_{ij} = \gamma\,\delta_{ij}, \tag{6.4}$$

$$u_i^\dagger \beta u_j = -\delta_{ij}. \tag{6.5}$$

The exact amplitude for scattering from an initial state with wave vector $\mathbf{k}_0$ and spin s_0 (spinor u_i with $i = s_0$) to a final state with $\mathbf{k}_f$ and s_f is given by

$$-4\pi f(\mathbf{k}_f, s_f; \mathbf{k}_0, s_0) = (\varphi_f, U\psi_0^+) = (\psi_f^-, U\varphi_0), \tag{6.6}$$

$$U(\mathbf{r}) = (2m/\hbar^2)V(\mathbf{r}).$$

The differential cross section $|f|^2$ must of course be averaged over initial spins if the beam is unpolarized and summed over final spins if the spin direction is not observed.

To split the potential into two parts, we again use a plane wave modified by a phase factor that corrects for the change of wavelength in the potential region:

$$\begin{aligned} \chi_0^+(\mathbf{r}) &= \varphi_0(\mathbf{r}) \exp[i\,\delta_0(\mathbf{r})], \\ \delta_0(\mathbf{r}) &= -\gamma(2k)^{-1} \int_0^\infty U(\mathbf{r} - \hat{k}_0 s)\, ds. \end{aligned} \tag{6.7}$$

The only differences from the Schrödinger case are that the plane waves are now spinors and that δ_0 is now proportional to $\gamma = E/mc^2$. The origin of the factor γ becomes obvious when the relativistic expression for the wave number is expanded to first order in V. The Dirac equation satisfied by the modified plane wave is

$$[E - H_0 - V_s(\mathbf{r})]\chi_0^+ = 0, \tag{6.8}$$

$$V_s(\mathbf{r}) = -i\hbar c \exp(-i\,\delta_0)\boldsymbol{\alpha}\cdot\nabla \exp i\,\delta_0 = \hbar c\boldsymbol{\alpha}\cdot\nabla\,\delta_0. \tag{6.9}$$

To express the scattering amplitude in two-potential form, we again integrate the transition current between $(\psi_f^- - \varphi_f)$ and $(\chi_0^+ - \varphi_0)$ over the

[11] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., p. 329.

surface of a large sphere:

$$\int d\mathbf{S}\cdot(\psi_f^- - \varphi_f)^\dagger \boldsymbol{\alpha}(\chi_0^+ - \varphi_0)$$

$$= \int d\mathbf{r}\nabla\cdot[(\psi_f^- - \varphi_f)^\dagger \boldsymbol{\alpha}(\chi_0^+ - \varphi_0)]. \quad (6.10)$$

The surface integral vanishes because the factor $(\chi_0^+ - \varphi_0)$ limits the integration to the intersection of the forward cylinder with the sphere, while $(\psi_f^- - \varphi_f)$ decreases asymptotically as $1/r$. By substituting Eqs. (6.1) and (6.8) in the volume integral and using Eq. (6.6), we obtain

$$-4\pi f = (\varphi_f, U_S\chi_0^+) + (\psi_f^-, U_L\chi_0^+), \quad (6.11)$$

where

$$U_S = (2m/\hbar^2)V_S = 2k_c\boldsymbol{\alpha}\cdot\nabla\ \delta_0, \quad (6.12)$$

$$U_L = U - U_S. \quad (6.13)$$

As in Sec. II, the two terms of Eq. (6.11) can be defined separately in the Abelian sense. The first term again contributes only to exactly forward scattering:

$$(\varphi_f, U_S\chi_0^+) = \begin{cases} (\varphi_f, U\chi_0^+), & \theta = 0, \\ 0 \quad , & \theta > 0. \end{cases} \quad (6.14)$$

(Even at zero angle, it must be remembered that φ_f and φ_0 may describe different spin states.) To prove Eq. (6.14), we first write out the matrix element in detail:

$$(\varphi_f, U_S\chi_0^+) = -2ik_c u_f^\dagger \boldsymbol{\alpha} u_0 \times \int d\mathbf{r}\ (\exp i\mathbf{q}\cdot\mathbf{r})\nabla \exp i\ \delta_0. \quad (6.15)$$

In the case of forward scattering, the spinor product is proportional to the incident current density if the initial and final spin states are the same, and vanishes otherwise:

$$k_c u_f^\dagger(\mathbf{k}_0)\boldsymbol{\alpha}u_0(\mathbf{k}_0) = -\mathbf{k}_0\ \delta(s_f, s_0). \quad (6.16)$$

Use of Eq. (6.4) and the second of Eqs. (6.7) leads at once to

$$(\varphi_f, U_S\chi_0^+) = \gamma\ \delta(s_f, s_0)\int d\mathbf{r}U \exp i\ \delta_0 = (\varphi_f, U\chi_0^+), \quad \theta = 0. \quad (6.17)$$

Since this proof makes no demands on the spatial dependence of φ_f, we observe for future reference that also

$$(\chi_f^-, U_S\chi_0^+) = (\chi_f^-, U\chi_0^+), \quad \theta = 0. \quad (6.18)$$

For nonzero angles, we perform an integration by parts with respect to z in Eq. (6.15):

$$(\varphi_f, U_S\chi_0^+) = -2k_c(q_z + i\epsilon)^{-1}u_f^\dagger\boldsymbol{\alpha}u_0 \times \left\{\iint_{-\infty}^{+\infty} dx\,dy \exp(iq_x x + iq_y y) \times [\exp(iq_z z - \epsilon z)\nabla \exp i\ \delta_0]_{z=-\infty}^{+\infty} + i\gamma(2k)^{-1}\int d\mathbf{r} \exp(i\mathbf{q}\cdot\mathbf{r})\nabla(U \exp i\ \delta_0)\right\}. \quad (6.19)$$

The boundary term vanishes at the upper limit because of the convergence factor and at the lower limit because of the factor $\nabla \exp(i\ \delta_0)$. Integration of the second term by parts transfers the gradient operator to the factor $\exp(i\mathbf{q}\cdot\mathbf{r})$, the surface integral vanishing because the potential vanishes at large distances. The second half of Eq. (6.14) now follows from the identity

$$u_f^\dagger\boldsymbol{\alpha}u_0\cdot\mathbf{q} = 0. \quad (6.20)$$

Alternatively, the two parts of Eq. (6.14) can be proved in a unified way by observing that

$$\lim_{\epsilon\to 0} u_f^\dagger\boldsymbol{\alpha}u_0\cdot(\mathbf{q} + i\epsilon\hat{z})(q_z + i\epsilon)^{-1} = \begin{cases} -\delta(s_f, s_0)(k/k_c), & \theta = 0, \\ 0 \quad , & \theta > 0. \end{cases} \quad (6.21)$$

The exact scattering amplitude can now be written as

$$-4\pi f = \begin{cases} (\varphi_f, U\chi_0^+) + (\psi_f^-, U_L\chi_0^+), & \theta = 0, \\ (\psi_f^-, U_L\chi_0^+) \quad , & \theta > 0. \end{cases} \quad (6.22)$$

As in the Schrödinger case, replacement of ψ_f^- by φ_f gives the familiar approximation

$$-4\pi f \approx (\varphi_f, U\chi_0^+), \quad (6.23)$$

where we have used Eq. (6.14). A better replacement for the exact wave function is the modified plane wave

$$\chi_f^-(\mathbf{r}) = \varphi_f(\mathbf{r}) \exp[-i\ \delta_{-f}(\mathbf{r})], \quad (6.24)$$

$$\delta_{-f}(\mathbf{r}) = -\gamma(2k)^{-1}\int_0^\infty U(\mathbf{r} + \hat{k}_f s)\,ds. \quad (6.25)$$

The parameters are assumed to satisfy the same conditions as in the Schrödinger case, with U replaced by γU; in addition, we assume that $\gamma \gg 1$. Because of Eq. (6.18), the resulting high-energy approximation is simpler at 0° than in the Schrödinger case:

$$-4\pi f_1 = \begin{cases} (\varphi_f, U\chi_0^+) \ , & \theta = 0, \\ (\chi_f^-, U_L\chi_0^+), & \theta > 0. \end{cases} \quad (6.26)$$

For small scattering angles $\theta \lesssim 1/kR$, it is again immaterial whether a modified or unmodified plane wave is used as the approximate wave function, and we are again unable to extend this conclusion to the wider range of angles $\theta \ll (kR)^{-\frac{1}{2}}$.[3] We first rearrange Eq. (6.26) in the form

$$-4\pi f_1 = (\varphi_f, U\chi_0^+) + (\chi_f^- - \varphi_f, U_L\chi_0^+), \qquad U_L = U - 2k_c\boldsymbol{\alpha}\cdot\nabla\,\delta_0. \tag{6.27}$$

If $\gamma UR/k$ is not large compared to unity, the integrals contain no rapidly oscillating factors, and their orders of magnitude can be safely estimated. On evaluating the matrix elements of $\boldsymbol{\alpha}$, the terms in α_x and α_y are found to be at most of order θ relative to $(\varphi_f, U\chi_0^+)$. When the remaining terms of U_L are combined in the form $U(1 + cv^{-1}\alpha_z)$, where v is the speed of the particle, their contribution is at most of order $1/\gamma$ relative to $(\varphi_f, U\chi_0^+)$, and only of order θ^2/γ if the spin state is unchanged.

At a scattering angle of 180°, Eq. (6.26) will be shown to reduce to the Schiff large-angle formula[3] with no approximations:

$$-4\pi f_1 = (\chi_f^-, U\chi_0^+), \quad \theta = 180°. \tag{6.28}$$

We consider first the matrix element

$$(\chi_f^-, U_s\chi_0^+) = -2ik_c u_f^\dagger \boldsymbol{\alpha} u_0 \times \int d\mathbf{r}\, \exp(i\mathbf{q}\cdot\mathbf{r} + i\,\delta_{-f})\nabla \exp i\,\delta_0. \tag{6.29}$$

The phase modification δ_{-f} is equal to δ_0 for $\theta = 180°$; in contrast with Eq. (5.16), we have

$$(\exp i\,\delta_0)\nabla \exp i\,\delta_0 = \tfrac{1}{2}\nabla \exp(2i\,\delta_0). \tag{6.30}$$

Thus, Eq. (6.29) has the same structure for 180° scattering as Eq. (6.15), and the same steps that were used earlier to prove the second half of Eq. (6.14) now lead to

$$(\chi_f^-, U_s\chi_0^+) = 0, \quad \theta = 180°. \tag{6.31}$$

Equation (6.28) follows immediately, and its derivation clearly remains valid in a range of angles about 180° provided that χ_f^- is approximated by $\varphi_f \exp(-i\,\delta_0)$. As in the Schrödinger case, we are unable to estimate reliably the accuracy of this approximation.

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Perturbation Theory and Lie Algebras

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An approach to perturbation theory is considered based on the formula $\exp(-iB)\,A\,\exp(iB) = A\,\exp(iB]$), where $[AB] = AB - BA$ is the commutator. The operators A constitute a linear space $\mathfrak{A}$ and the operators B considered are such that $B]$ take $\mathfrak{A}$ into itself. The present discussion considers the case where $\mathfrak{A}$ is finite dimensional with coordinates $c_1, \cdots, c_n$; i.e., $\mathfrak{A}$ is isomorphic with the set of n-dimensional vectors $\mathbf{c}$. Under these circumstances sufficient conditions for the basic formula are given in terms of the "analytic vectors" of Nelson. The set, $\mathfrak{B}$, of B's available can be considered closed under the processes of taking linear combinations and forming the commutator. Thus $\mathfrak{B}$ is a Lie algebra. Exponentiation leads to a Lie group of operators U, and A and A' are said to be B equivalent if $A' = U^{-1}AU$. For $\mathfrak{A}$ finite dimensional each B is associated with an $n \times n$ matrix, b, which specifies the operation $B]$ relative to the vectors $\mathbf{c}$. Effectively then, $\mathfrak{B}$ is finite dimensional. The matrices b form a Lie algebra with a corresponding Lie group of matrices u such that A and A' are B equivalent if and only if the corresponding two vectors $\mathbf{c}$ and $\mathbf{c}'$ are u images; i.e., $\mathbf{c}' = u\mathbf{c}$. Computationally, therefore, the set of A' equivalent to a given A is obtained by considering the orbit of a given vector $\mathbf{c}$ under the Lie group; i.e., the set of $u\mathbf{c}$. A neighborhood $\mathfrak{A}'$ of a given A consists of those operators A' in the form $A + \delta A$ where δA is arbitrary except for a restriction on the size of its coordinates, c_i. Given A, a neighborhood $\mathfrak{A}'$ can be found for which one can obtain by a well-known construction on the orbits a set of functionally complete and functionally independent invariants for B equivalence. Computationally global and rational invariants are desirable and these can be obtained in the form of similarity invariants, provided that $\mathfrak{A}$ can be mapped onto a set of $n \times n$ matrices a in such a way that if $\mathbf{c}$ corresponds to a, then $b\mathbf{c}$ corresponds to $a' = [ab]$. If the sets $\mathfrak{A}$ and $\mathfrak{B}$ are identical such a mapping is immediately available and if, in addition, the corresponding Lie algebra is semisimple, in general, given A, the A's in some neighborhood are each equivalent to an A'' which is a function of A. This corresponds to a case in which a very simple perturbation of A levels occurs. Two examples are discussed.

INTRODUCTION

PERTURBATION theory is concerned with establishing the spectral characteristics of an operator $A' = A + \delta A$, where A is an operator whose spectral resolution is known and δA is a "perturbation." Procedures for investigating this problem are of great practical importance (cf. Dalgarno; Dalgarno and Stewart; Dirac; Gell-Mann and Goldberger; Gunthard and Primas; Hugenholtz; Karplus *et al.*; March and Young; Nakanishi; Nambu; Schwartz; Speisman; Sysmanik; Young).[1] In the classic approach, one chooses a coordinate system or its continuous equivalent in which A is diagonal and seeks a unitary operator U such that $U^{-1}A'U$ is also diagonal; i.e., commutes with A and may even be a function of A. However, it is a well-known result of Weyl that, even when δA is completely continuous, A' may have a different spectral type from A (cf. Aronszajn; Kuroda; Rosenbloom) and because of this the structure of $A + \delta A$ has been intensely investigated (cf. S. Goldberg; V. N. Goldberg; Kato; Porath; Zaidman). These investigations have often been based very strongly on the spectral structure of A (cf. Castoldi; Faddeev and Ladyzenskaya; Folguel; Friedrichs; Rellich; Rosenblum; Schroder; Van Hove).

There is however another procedure by which off diagonal terms can be eliminated. We denote $AB - BA$ by $[AB]$ and write U in the form $\exp(iB)$. One has the formal relationship

$$\begin{aligned}\exp(-iB)A\,\exp(iB) &= A + [AiB] + (1/2!)[[AiB]iB] \\ &\quad + (1/3!)([]^3A(iB])^3 + \cdots \\ &= (\text{say})\ A\,\exp(iB]) \qquad (1)\end{aligned}$$

to specify a rotation (cf. Foldy and Wouthuysen; Garrido and Pascual; Newton and Wigner; Pryce). The commutator operator has been investigated from a number of points of view (cf. van Kampen; Kermack and McCrea; Putnam; Putnam and Wintner; Sack; Vidav). We consider then a linear set $\mathfrak{A}$ of operators A and suppose that $iB]$ takes $\mathfrak{A}$ into itself. Formally, (1) implies that $\exp(iB])$ also takes $\mathfrak{A}$ into itself. If $B_1, B_2, \cdots$ is a sequence of B's for which $iB_\alpha]$ takes $\mathfrak{A}$ into itself, then formally $\sum \mu_\alpha B_\alpha$ also has this property and the "diagonalization" of $A' = A + \delta A$ then consists in choosing the μ_α so that $A'' = A' \exp(i \sum \mu_\alpha B_\alpha])$ does not have off-diagonal terms. If the operator A, whose spectral resolution has determined the coordinate system, has simple spectrum, this can be accomplished by choosing the μ_α so that A'' is in the set of A's which commute with A.

The present discussion considers the case where $\mathfrak{A}$ is n dimensional. If $A_1, \cdots, A_n$ is a basis for $\mathfrak{A}$, we use the notation $A = \sum_{\alpha=1}^{n} c_\alpha A_\alpha = \mathbf{c}\cdot\mathbf{A}$; i.e.,

[1] See the references given at the end of this paper.

$\mathbf{A}$ is a vector $\{A_1, \cdots, A_n\}$ and $\mathbf{c}$ is the vector $\{c_1, \cdots, c_n\}$. We suppose that each such A has a closure $\bar{A}$. Since $iB]$ takes $\mathfrak{A}$ into itself, there is an $n \times n$ matrix b, which has the corresponding effect on the vector $\mathbf{c}$; i.e., $\mathbf{c}\cdot\mathbf{A}(iB]) = (b\mathbf{c})\cdot\mathbf{A}$. Under these circumstances, sufficient conditions can be formulated in terms of the "analytic vectors" of Nelson for the basic formula (1) to hold for a given element f (cf. Nelson). These conditions can be fulfilled on a nondense subset of Hilbert space and thus we can consider rotating A' on linear subspace rather than on the whole space.

If $\mathfrak{A}$ is isomorphic with a linear vector space $\mathfrak{C}$ to each B for which $iB]$ takes $\mathfrak{A}$ into itself, we have a transformation b of $\mathfrak{C}$ into itself. The set of such B is of course linear and furthermore if certain domain conditions are verified, $[B_1B_2]$ is such a B, if B_1 and B_2 are. The correspondence $B \sim b$ is linear and $[B_1B_2]$ will correspond to $[b_1b_2]$. If $\mathfrak{C}$ is finite dimensional, the set of b's constitutes a finite-dimensional Lie algebra and a finite-dimensional linear set $\mathfrak{B}_f$ of B's can be obtained which are in one-to-one correspondence with the b's. We suppose that there is an appropriate domain such that for every B in $\mathfrak{B}_f$, the basic formula (1) holds.

The set of b's constitutes a finite-dimensional Lie algebra. Exponentiation and multiplication of a finite number of exponents will yield the corresponding Lie group of elements, u [cf. Chevalley (1946)]. In view of (1), we also have for each B of $\mathfrak{B}_f$, a $V = \exp(iB)$ which corresponds to the Lie-group element, $v = \exp b$, in such a way that if A and A' are two operators of $\mathfrak{A}$ with corresponding $\mathbf{c}$ and $\mathbf{c}'$ in $\mathfrak{C}$, then $V^{-1}AV = A'$ on an appropriate domain is equivalent to $v\mathbf{c} = \mathbf{c}'$. Clearly a product U of a finite number of such V's will also correspond to the product u of the corresponding v in such a way that $U^{-1}AU = A'$ on an appropriate domain is equivalent to $u\mathbf{c} = \mathbf{c}'$. We say that A and A' are B equivalent if there is such a U such that $U^{-1}AU = A'$ on an appropriate domain and it is clear that B equivalence for A and A' corresponds to $u\mathbf{c} = \mathbf{c}'$ for a u in the Lie group.

The finite-dimensional set $\mathfrak{B}_f$ is linear but not necessarily closed under the operation of forming the commutator. If there is a finite-dimensional set $\mathfrak{B}_f'$ of B's which contains $\mathfrak{B}_f$ and closed under forming the commutator, then $\mathfrak{B}_f'$ is a finite-dimensional Lie algebra and sufficient conditions are known so that one can consider the set of U's as a unitary representation of the corresponding Lie group (cf. Nelson, Theorem 5, p. 602). In general we are concerned with the unitary character of the individual U's either on the whole space or on an appropriate subspace and this can be investigated directly. For instance, if B is self-adjoint, $\exp(iB)$ is unitary (cf. Stone).

The B equivalence of A and A' corresponds to the existence of a u in the Lie group for the Lie algebra of the b's such that $u\mathbf{c} = \mathbf{c}'$. Thus the problem of determining the set of A' equivalent to a given A is the same as determining the "orbit" of $\mathbf{c}$; i.e., the set of elements in the form $u\mathbf{c}$ for u in the Lie group. The topological character of the set of orbits which occur in a representation of a Lie group has been extensively investigated (cf. Cartan; Conner; Conner and Floyd; Karube; Mills and Seligman; Montgomery; Montgomery and Yang; Montgomery and Zippen; Mostov; Nono) and a study of B equivalence could be based on these, in particular, on the theory of "cross-sections."

However, it is possible to present a somewhat more elementary discussion using a construction given by Weyl and a choice of coordinate systems similar to those described by Pontrjagin. Let A be given and the corresponding vector $\mathbf{c}$. A "neighborhood" of A consists of the $A' = A + \delta A$ where δA has a $\mathbf{c}$ in a neighborhood of the origin. Let $\mathfrak{R}_c$ consist of the vectors $b\mathbf{c}$ in $\mathfrak{C}$, b as defined above. Let $\mathfrak{S}_c$ denote a set complementary to $\mathfrak{R}_c$ in $\mathfrak{C}$ in the linear sense. Let A'' denote an element in the form $A + \partial A$ where ∂A has a $\mathbf{c}$ in $\mathfrak{S}_c$. One can show that there is a neighborhood of A such that every A' in this neighborhood is equivalent to an A'' in the form specified. The set of operators A for which $\mathfrak{S}_c$ has minimum dimensions, has a complement in $\mathfrak{A}$ of lower dimensionality and for an A in this set, if a coordinate system in $\mathfrak{S}_c$ is given with coordinates $z_1, \cdots, z_p$, then the coordinates of the vector corresponding to ∂A constitute, locally, a functionally complete and functionally independent system of invariants for B equivalence within the neighborhood of A.

However, from the computational point of view it is desirable to obtain global and rational invariants for B equivalence. This can be done if the vectors $\mathbf{c}$ can be mapped on $n \times n$ matrices a, $\mathbf{c} \to a(\mathbf{c})$, in such a way that for the b defined above which corresponds to the operation $iB]$ we have $[a(\mathbf{c})b] = a(b\mathbf{c})$. This implies that $\exp b\ a(\mathbf{c}) \exp(-b) = a(\mathbf{c}) \exp(b]) = a\ (\exp b\mathbf{c})$ and thus $a(u\mathbf{c})$ is obtained from $a(\mathbf{c})$ by a similarity transformation and all similarity invariants of $a(\mathbf{c})$ are invariants for A under B equivalence. If the mapping $\mathbf{c} \to a(\mathbf{c})$ is one-to-one, all invariants of B equivalence can be expressed in terms of the elements of the matrix

$a(\mathbf{c})$ (the similarity invariants are examples of this), but if the mapping $\mathbf{c} \to a(\mathbf{c})$ is not one-to-one, the situation is more complex.

A mapping $\mathbf{c} \to a(\mathbf{c})$ is immediately available if the set of A's coincides with the set of B's; i.e., we take $a(\mathbf{c})$ to be the b matrix associated with A. If, under these circumstances, the Lie algebra of the b's is semisimple, then (in general) A' is B equivalent with an A'' which commutes with A.

In view of the detailed investigations of Lie algebras and Lie groups now available, the present discussion could be continued into a categorical specification of the case considered (cf. Borel; Chevalley). But the assumption of $\mathfrak{A}$ finite dimensional is intended merely to develop background material for the more interesting and more pertinent infinite-dimensional case, which will be considered in the future.

Normally the unitary equivalence of the A's relative to B's would be studied by the use of the ring of operators determined by the B and A's. (cf. Kadison and Singer). However, under the circumstances indicated above, a smaller structure can be used; i.e., the B set itself, and this is significant in the infinite-dimensional case. The relation between B equivalence and more general equivalence relations is also extremely important.

Our discussion concludes with consideration of two examples. Operators p and q are defined on the set of summable squared functions of x for $-\infty < x < \infty$, by $qf = xf(x)$, $pf = i(d/dx)f(x)$. One example has A_1, A_2, A_3 defined as p, q and the identity; the other is based on p^2, q^2, and $2qp + 1$. Apparently if p or q occur to a higher degree in similar examples, one does not have a finite dimensional $\mathfrak{A}$.

SECTION 1

We consider a finite-dimensional linear set $\mathfrak{A}$ of operators A on Hilbert space with basis $A_1, \cdots, A_n$ and an operator B such that for every A in $\mathfrak{A}$, $[AB]$ is in $\mathfrak{A}$. (This assumption will be modified by domain restrictions later.)

The commutator $[AB]$ as an operator can be iterated

$$\begin{aligned} [[AB]B] &= (\square)^2 A(B])^2 \\ [[[AB]B]B] &= (\square)^3 A(B])^3 \\ &\cdots . \end{aligned} \tag{1.1}$$

We ignore the multiplicity of the first bracket and hence can express a polynomial or power series in the commutator operator with a single first bracket. For instance

$$[A \exp(B]) = \sum_{\alpha=0}^{\infty} (\alpha!)^{-1} (\square)^{\alpha} A(B])^{\alpha}. \tag{1.2}$$

In this terminology we wish to establish the relation

$$\exp(-iB)A \exp(iB) = [A \exp(iB]), \tag{1.3}$$

which is the formal basis for the study of equivalence. Our procedures are analogous to those of Nelson and we use his terminology for analytic vector. The type of generality we want is determined by various practical considerations and thus it is desirable to make the current discussion self-contained. Thus no properties of the operators not explicitly given here will be used. This permits one to apply these formulas to cases where operators are not known to be self-adjoint and on sets of elements in Hilbert space not known to be dense.

Lemma 1.1. *Let $A_1, \cdots, A_n$ be n operators such that the linear combination, $A = \sum_{\alpha=1}^{n} c_\alpha A_\alpha$ has a closure $\bar{A}$. Let f be an element of the Hilbert space $\mathfrak{H}$ and B an operator such that*

$$[A_i B]f = \sum_{\alpha} b_{\alpha i} A_\alpha f \tag{1.4}$$

and such that f and $A_i f$ are analytic vectors for B. Then there exists an $s > 0$, such that if $|z| < s$, then

$$\exp(-Bz)\bar{A} \exp(Bz)f = [A \exp(zB])f. \tag{1.5}$$

Let $\mathbf{c}$ denote the vector $\{c_1, \cdots, c_n\}$. We define

$$||\mathbf{c}||_m = \max_\alpha |c_\alpha| \tag{1.6}$$

and use the notation $\mathbf{A} = \{A_1, \cdots, A_n\}$ and $\mathbf{c}\cdot\mathbf{A}$ as in the introduction. Equation (1.4) is equivalent to

$$[\mathbf{c}\cdot\mathbf{A}\, B]f = (b\mathbf{c})\cdot\mathbf{A}f \tag{1.7}$$

for all $\mathbf{c}$ and for the matrix $b = \{b_{ij}\}$. There is a $C \geq 0$ determined by the matrix b such that

$$||b\mathbf{c}||_m = ||\mathbf{c}'||_m \leq C\, ||\mathbf{c}||_m \tag{1.8}$$

for all $\mathbf{c}$. The obvious triangle property of $||\ ||_m$ can be used then to show the existence of

$$[\mathbf{c}\cdot\mathbf{A} \exp(tB])f = (\exp tb)\mathbf{c}\cdot\mathbf{A}f \tag{1.9}$$

for every complex t and

$$\begin{aligned} &[[\mathbf{c}\cdot\mathbf{A} \exp(t_1 B]) \exp(t_2 B]) \\ &\qquad = [\mathbf{c}\cdot\mathbf{A} \exp\{(t_1 + t_2)B]\}. \end{aligned} \tag{1.10}$$

Since $A_i f$ is an analytic vector for B, it is in the domain of B^p for $p = 1, 2, \cdots$. We define

$$B^p\mathbf{A} = \{B^p A_1, \cdots, B^p A_n\} \tag{1.11}$$

and there is an $s_i > 0$ such that

$$\sum_{\alpha=0}^{\infty} \frac{s_i^\alpha \, ||B^\alpha A_i f||}{\alpha!} < \infty. \tag{1.12}$$

Thus we can find a $s > 0$ and a K such that for every i,

$$||B^\alpha A_i f|| \leq K\alpha! \, s^{-\alpha}. \tag{1.13}$$

Now Eqs. (1.7), (1.8), and (1.13) imply

$$\begin{aligned} ||B^\alpha[A(B])^\beta f|| &= ||B^\alpha(b^\beta \mathbf{c})\cdot \mathbf{A} f|| \\ &= ||(b^\beta \mathbf{c})\cdot B^\alpha \mathbf{A} f|| \\ &\leq C^\beta \, ||\mathbf{c}||_m \, (\sum_\gamma ||B^\alpha A_\gamma f||) \\ &\leq ||\mathbf{c}||_m \, KnC^\beta \alpha! \, s^{-\alpha} = \text{(say) } K'C^\beta \alpha! \, s^{-\alpha} \\ &\quad \text{for } K' = ||\mathbf{c}||_m \, Kn. \end{aligned} \tag{1.14}$$

[In the current discussion of the basic formula (1.3), the finite dimensionality of the set $\mathfrak{A}$ is used only in the derivation of (1.14).] It is worthwhile to point out here precisely what is needed to obtain (1.14) by the above argument independently of the finite-dimensionality assumption.

We suppose that the set $\mathfrak{A}$ is isomorphic to a linear vector space $\mathfrak{C}$ with norm $||\mathbf{c}||_1$ and let A correspond to $\mathbf{c}$. Let a subset $\mathfrak{A}_1$ of $\mathfrak{A}$ be specified. (In the finite-dimensional case $\mathfrak{A}_1$ is the set $A_1, \cdots, A_n$ but it may be $\mathfrak{A}$ itself in some cases.) Let $\mathfrak{F}$ denote a set of elements, g, in Hilbert space, such that there is a g corresponding to each A in $\mathfrak{A}_1$. For instance if f is in the domain of every A in $\mathfrak{A}_1$, then the set $\mathbf{A}_1 f$ which consists of the Af, A in $\mathfrak{A}_1$ is such an $\mathfrak{F}$. The sum, $\mathfrak{F}_1 + \mathfrak{F}_2$ can be defined as the $\mathfrak{F}$ for which $g = g_1 + g_2$ where g_1, g_2, and g correspond to the same A in $\mathfrak{A}_1$ and similarly $c\mathfrak{F}_1$ for a scalar c is the set $\mathfrak{F}$ of g in the form cg_1, g, and g_1 corresponding to the same A. Thus the set of $\mathfrak{F}$'s constitutes a linear vector space and we suppose a norm $||\mathfrak{F}||_2$ is defined at least for a subset of $\mathfrak{F}$'s which will constitute a normed linear vector space with the above definitions of $+$ and $c\,\cdot$. If Bg is defined for every g in $\mathfrak{F}$, we define $\tilde{B}\mathfrak{F}$ as the set of Bg's for g in $\mathfrak{F}$.

The three critical assumptions we need for the above discussion of (1.14) are:

(1) If $A \sim \mathbf{c}$, $||Af|| \leq ||\mathbf{c}||_1 \, ||\mathbf{A}_1 f||_2$.

(2) $\mathbf{A}_1 f$ is an analytic vector for $\tilde{B}$; i.e., there is an $s > 0$, such that

$$\sum_{\alpha=0}^{\infty} s^\alpha (\alpha!)^{-1} \, ||\tilde{B}^\alpha \mathbf{A}_1 f||_2 < \infty.$$

(3) The transformation b on $\mathfrak{C}$ corresponding to $B]$ should be bounded.

These are adequate to replace the finite dimensionality of $\mathfrak{A}$ and of course the condition of analyticity for the $A_i f$ in the present lemma. However the other conditions such as the analyticity of f relative to the transformation B and the existence of the closure of A must be retained.]

Let

$$\begin{aligned} g_{pq}^{PQ} &= \sum_{\alpha=p}^{P} \sum_{\beta=q}^{Q} (\alpha! \, \beta!)^{-1} t^\alpha B^\alpha [A(tB])^\beta f \\ &= \left\{ \sum_{\alpha=p}^{P} (\alpha!)^{-1} t^\alpha B^\alpha \right\} \left\{ \sum_{\beta=q}^{Q} (\beta!)^{-1} [A(tB])^\beta \right\} f \end{aligned} \tag{1.15}$$

and

$$k_P = \sum_{\alpha=0}^{P} \sum_{\beta=P+1}^{2P-\alpha} (\alpha!)^{-1} t^\alpha (\beta!)^{-1} B^\alpha [A(tB])^\beta f \tag{1.16}$$

and

$$k_P' = \sum_{\alpha=P+1}^{2P} \sum_{\beta=0}^{2P-\alpha} (\alpha!)^{-1} t^\alpha B^\alpha (\beta!)^{-1} [A(tB])^\beta f. \tag{1.17}$$

Now (1.14) permits one to apply the usual limiting arguments to show both the existence of certain limits and the relations

$$\begin{aligned} \lim_{P\to\infty} g_{0\,0}^{P\,P} &= \lim_{P\to\infty} (\lim_{Q\to\infty} g_{0\,0}^{P\,Q}) \\ &= \exp(tB)[A \exp(tB])f \end{aligned} \tag{1.18}$$

and

$$\lim_{P\to\infty} k_P = 0 \quad \text{and} \quad \lim_{P\to\infty} k_P' = 0 \tag{1.19}$$

for $|t| < s$.

The assumption that $A_i f$ and f are analytic vectors implies that f and $A_i f$ are in the domain of B^p, $p = 1, 2, \cdots$. We also have the relation

$$AB^p f = \sum_{\alpha=0}^{p} \binom{p}{\alpha} B^\alpha [A(B])^{p-\alpha} f \tag{1.20}$$

which can be proven inductively. It is valid for $p = 1$. The induction must be concerned only with operations on the left since only one f is involved. The result is assumed for $AB^{p-1}f$ and, since A is arbitrary, for $[AB]B^{p-1}f$. Then the relation $AB^p f = BAB^{p-1}f + [AB]B^{p-1}f$ and the addition formula for binary coefficients yields the result for p. Since A is arbitrary, we also get the corresponding $[AB]$ result.

Now (1.20) yields by summing from 0 to $2P$

$$A\left\{ \sum_{\beta=0}^{2P} (\beta!)^{-1} t^\beta B^\beta \right\} f$$

$$= \sum_{\beta=0}^{2P} \sum_{\alpha=0}^{\beta} \{\alpha!(\beta-\alpha)!\}^{-1}(tB)^{\alpha}[A(tB])^{\beta-\alpha}f$$

$$= \sum_{\alpha=0}^{2P} \sum_{\beta=0}^{2P-\alpha} (\alpha!\,\beta!)^{-1}(tB)^{\alpha}[A(tB])^{\beta}f$$

$$= g_{00}^{PP} + k_P + k_P'. \tag{1.21}$$

Since f is an analytic vector for B, we have the existence of

$$\sum_{\beta=0}^{\infty} (\beta!)^{-1}(tB)^{\beta}f = \exp(tB)f \tag{1.22}$$

for t in a certain neighborhood of the origin. We can adjust the s of (1.13) so that (1.22) converges for $|t| < s$. Now (1.18) and (1.19) imply that the right-hand side of (1.21) has a limit as $P \to \infty$. Furthermore A has a closure $\bar{A}$ and hence (1.22) and the above yields

$$\bar{A}(\exp tB)f = \exp tB[A \exp(tB])f. \tag{1.23}$$

Since the $A_i f$ are analytic vectors for B, one can readily show that $\exp(-tB)$ and $\exp(tB)$ are inverses on the linear combinations of the $A_i f$ for $|t| \leq s$. Since $[A \exp(tB])f$ is such a linear combination, Eq. (1.23) implies the desired Eq. (1.5).

SECTION 2

Lemma 2.1. *Let $A_1, \cdots, A_n$ be n operators with the property that each linear combination $A = \mathbf{c}\cdot\mathbf{A}$ has a closure, $\bar{A}$. Let an operator B, a set $\mathfrak{D}$ in $\mathfrak{H}$ and an $n \times n$ matrix b, $\{b_{ij}\}$, be given with the property that if f is in $\mathfrak{D}$*

(1) *f is in domain of A_i*
(2) $[A_i B]f = \sum_{\alpha=1}^{n} b_{\alpha i} A_\alpha f$
(3) *f is an analytic vector for B*
(4) *$A_i f$ is an analytic vector for B*
(5) *For $0 \leq t \leq T$, $\exp(itB)f$ is in $\mathfrak{D}$.*

Then for $0 \leq t < T$ and all f in $\mathfrak{D}$:

$$\exp(-itB)A \exp(itB)f = [A \exp(iBt])f. \tag{2.1}$$

(Note that no denseness or completeness requirement is imposed on $\mathfrak{D}$.)

Proof. For $f \in \mathfrak{D}$, $A_i f$ exists and hence Af. Thus $\bar{A}f = Af$. Now let a t with $0 < t < T$ be given and a $f \in \mathfrak{D}$. Consider then a t' with $0 \leq t' \leq t$. It is clear that the hypothesis of Lemma 1.1 holds for $\exp(it'B)f$ and thus there exists an $s > 0$, dependent on t' such that if $|z| < s$

$$\exp(-zB)A \exp(zB) \exp(it'B)f = [A \exp(zB]) \exp(it'B)f. \tag{2.2}$$

To each such t', we define the neighborhood consisting of those real t'' for which $|t'' - t'| < s/2$. These neighborhoods are defined for the real t' such that $0 \leq t' \leq t$. Since this set is compact, a finite number of these neighborhoods cover this interval in an overlapping manner. Let $0 = t_0 < t_1 < \cdots < t_p = t$ denote the center points of these neighborhoods and s_α the value of s corresponding to t_α.

Since the neighborhoods overlap, for each α there is a t' such that

$$|t' - t_\alpha| < s_\alpha/2 \text{ and } |t' - t_{\alpha+1}| < s_{\alpha+1}/2. \tag{2.3}$$

Depending on whether s_α is larger than $s_{\alpha+1}/2$ or not, we have

$$|t_{\alpha+1} - t_\alpha| < s_\alpha \quad \text{or} \quad |t_{\alpha+1} - t_\alpha| < s_{\alpha+1}. \tag{2.4}$$

The last inequality implies that for $A' = \mathbf{c}\cdot\mathbf{A}$

$$\exp\{i(t_{\alpha+1} - t_\alpha)B\}A' \times \exp\{i(t_\alpha - t_{\alpha+1})B\} \exp(it_{\alpha+1}B)f = [A' \exp\{i(t_\alpha - t_{\alpha+1})B]\} \exp(it_{\alpha+1}B)f. \tag{2.5}$$

Now let $A = [A' \exp\{i(t_\alpha - t_{\alpha+1})B]\}$. This implies then that for all A

$$[A \exp\{i(t_{\alpha+1} - t_\alpha)B]\} \exp(it_\alpha B)f = \exp\{-i(t_{\alpha+1} - t_\alpha)B\}A \times \exp\{i(t_{\alpha+1} - t_\alpha)B\} \exp(it_\alpha B)f. \tag{2.6}$$

This also holds for the case $|t_{\alpha+1} - t_\alpha| < s_\alpha$.

Suppose now that for t_α we have for all A'

$$\exp(-it_\alpha B)A' \exp(it_\alpha B)f = [A' \exp(it_\alpha B])f. \tag{2.7}$$

Let $A' = [A \exp\{i(t_{\alpha+1} - t_\alpha)B]\}$ in (2.7) and apply $\exp(-it_\alpha B)$ to (2.6). One then obtains by (1.10),

$$\exp(-it_{\alpha+1}B)A \exp(it_{\alpha+1}B)f = [[A \exp\{i(t_{\alpha+1} - t_\alpha)B]\} \exp(it_\alpha B])f = [A \exp(it_{\alpha+1}B])f. \tag{2.8}$$

Since this will hold for $\alpha = 0$, we have it then also for $t = t_p$, Q.E.D.

We consider now a set of B's, with the property that $[AB]$ is in $\mathfrak{A}$ for each A in $\mathfrak{A}$. A linear combination of B's with this property has this property also and thus we can suppose that we are dealing with a linear set of such B's. This set we denote $\mathfrak{B}$. Now suppose B_1 and B_2 are two elements of $\mathfrak{B}$ for which (1.4) holds on a set $\mathfrak{D}$. This implies that for $i = 1, 2$

$$[\mathbf{c}\cdot\mathbf{A}\, B_i] = (b_i\mathbf{c})\cdot\mathbf{A}f \tag{2.9}$$

[see (1.7)] for f in $\mathfrak{D}$ and also

$$([b_1b_2]\mathbf{c})\cdot\mathbf{A}f = [[\mathbf{c}\cdot\mathbf{A}\,B_2]B_1]f - [[\mathbf{c}\cdot\mathbf{A}\,B_1]B_2]f$$
$$= [\mathbf{c}\cdot\mathbf{A}[B_2B_1]]f. \qquad (2.10)$$

Thus we can suppose that the set $\mathfrak{B}$ is both linear and closed under the operation of forming the commutator and this also holds for the set $\mathfrak{b}$ of b's. Both sets are, therefore, Lie algebras and the mapping $B \to b$ is a homomorphism. If $\mathfrak{N}_B$ is the set of B's which are mapped on the zero $n \times n$ matrix, then there exists a finite dimensional linear set of B's, $\mathfrak{B}_f$ which are mapped in a one to one way and linearly onto $\mathfrak{b}$. From the point of view of computational effectiveness, we need only concern ourselves with the properties of the B's in $\mathfrak{B}_f$.

Assumption. Let $\mathfrak{A}$ and $\mathfrak{B}_f$ be two finite-dimensional linear sets of operators on Hilbert space and $\mathfrak{D}$ a linear set in Hilbert space which is in the domain of each A in $\mathfrak{A}$. Let $A_1, \cdots, A_n$ denote a basis for $\mathfrak{A}$.

We assume

(1) *To each B in $\mathfrak{B}$, there is a matrix b, $\{b_{ij}\}$, such that*

$$i[A_iB]f = \sum_{\alpha=1}^{n} b_{\alpha i}A_\alpha f \qquad (2.11)$$

for $f \in \mathfrak{D}$. If $\mathbf{c}\cdot\mathbf{A}$ denotes $\sum_{\alpha=1}^{n} c_\alpha A_\alpha$ this can also be written

$$i[\mathbf{c}\cdot\mathbf{A}\,B]f = (b\mathbf{c})\cdot\mathbf{A}f \qquad (2.12)$$

(2) *For each A in $\mathfrak{A}$, there is a closure $\bar{A}$ and for B in $\mathfrak{B}_f$, f in $\mathfrak{D}$ we have for $A = \mathbf{c}\cdot\mathbf{A}$*

$$\exp(-iB)\bar{A}\exp(iB)f = [A\exp(iB)]f = \exp b\mathbf{c}\cdot\mathbf{A}f \qquad (2.13)$$

(3) *The set $\mathfrak{b}$ of matrices b is closed relative to the operation of forming the commutator and hence, since it is linear, is a Lie algebra.*

Since $\mathfrak{b}$ is a Lie algebra, exponentiation and repeated multiplications determine a Lie group $\mathfrak{g}$ (cf. Chevalley or Pontrjagin).

Definition. If $\mathfrak{A}$, $\mathfrak{B}_f$, and $\mathfrak{b}$ are as in the above assumption and $\mathfrak{g}$ is the Lie group generated by $\mathfrak{b}$, then two operators A and A' of $\mathfrak{A}$ will be said to be B equivalent if for the vectors $\mathbf{c}$ and $\mathbf{c}'$ such that $A = \mathbf{c}\cdot\mathbf{A}$, $A' = \mathbf{c}'\cdot\mathbf{A}$, there exists a u in $\mathfrak{g}$ such that $\mathbf{c}' = u\mathbf{c}$.

Lemma 2.2. The relation B equivalence is transitive and reflexive. If A and A' are B equivalent, and the set $\mathfrak{D}$ in the assumption is invariant under the operators $V = \exp(iB)$ for B in $\mathfrak{B}_f$, then there exists an operator U in the form $V_1 \cdot \cdots \cdot V_r$ where $V_\alpha = \exp(iB_\alpha)$ such that $U^{-1}AUf = A'f$ for all f in $\mathfrak{D}$.

The first sentence is a consequence of the group property of the u's. If $V = \exp(iB)$, then $g = Vf$ is in $\mathfrak{D}$ and hence for A in $\mathfrak{A}$ we have $\bar{A}g = Ag$. Thus (2.13) becomes $V^{-1}AVf = f$. If we have two such V's, V_1, V_2,

$$(V_1V_2)^{-1}AV_1V_2f$$
$$= V_2^{-1}V_1^{-1}AV_1V_2f = V_2^{-1}(V_1^{-1}AV_1)V_2f$$
$$= V_2^{-1}(\exp b_1\mathbf{c}\cdot\mathbf{A})V_2f = \exp b_2 \exp b_1\mathbf{c}\cdot\mathbf{A}f. \qquad (2.14)$$

Repeated application of this argument will yield the desired result.

We now explore the definition of B equivalence. The characteristics of the operators U or V_i do not enter into this discussion.

The set of matrices u are usually described as a "representation" of an abstract Lie group and the set $\mathbf{c}'$ in the form $u\mathbf{c}$ constitute an "orbit" for $\mathbf{c}$ in this "representation."

SECTION 3

We suppose that $\mathfrak{A}$ and $\mathfrak{B}_f$ are as in the assumption of Sec. 2 and let $B_1, \cdots, B_m$ be a basis for $\mathfrak{B}_f$ and let $b_1, \cdots, b_m$ denote the corresponding matrices b. Let $b = \sum_{\alpha=1}^{n} \mu_\alpha b_\alpha$ and $v = \exp b$. The set of $\mathbf{c}'$ in the form $\mathbf{c}' = v\mathbf{c}$ in general has dimensionality less than m, the number of parameters μ. The set of v in the form $v = \exp b$ fill out a neighborhood of the identity in the Lie group and thus for a neighborhood of the origin, B equivalence for A and A' is equivalent to the existence of such a v with $\mathbf{c}' = v\mathbf{c}$.

We seek a complete set of local "invariants" for the orbit relationship; i.e., we want a set of functions of the coordinates of $\mathbf{c}'$, $f_1, \cdots, f_k$ such that $f_i(\mathbf{c}) = f_i(\mathbf{c}')$, if and only if $\mathbf{c}' = v\mathbf{c}$. It is desirable that these f's be functionally independent.

Let $\mathfrak{C}$ denote the set of $\mathbf{c}'$. If we fix $\mathbf{c}$, the relation

$$(\sum \mu_\alpha b_\alpha)\mathbf{c} = \mathbf{c}' \qquad (3.1)$$

describes a linear transformation T_c from $\mathfrak{b}$ to $\mathfrak{C}$. There is a set $\mathfrak{N}_c$ of b's for which

$$b\mathbf{c} = 0, \qquad (3.2)$$

and a set $\mathfrak{R}_c$ of $\mathbf{c}'$ which constitutes the range of T_c; i.e., those $\mathbf{c}'$ in the form $b\mathbf{c}$ for some b and the given $\mathbf{c}$. Let $\mathfrak{S}_c$ denote a set of $\mathbf{c}'$ which is complementary to $\mathfrak{R}_c$ and let us choose a basis for the $\mathbf{c}'$

$$\mathbf{c}_1, \cdots, \mathbf{c}_p, \quad \mathbf{c}_{p+1}, \cdots, \mathbf{c}_n, \qquad (3.3)$$

such that $\mathbf{c}_1, \cdots, \mathbf{c}_p$ is a basis for $\mathfrak{S}_c$ and $\mathbf{c}_{p+1}, \cdots, \mathbf{c}_n$ is a basis for $\mathfrak{R}_c$. Let $\mathfrak{b}^*$ denote a set of b's complementary to $\mathfrak{N}_c$ and let

$$b_1, \cdots, b_{n-p}, \qquad b_{n-p+1}, \cdots, b_{m^*}, \tag{3.4}$$

where $b_1, \cdots, b_{n-p}$ is a basis for $\mathfrak{b}^*$ and $b_{n-p+1}, \cdots, b_{m^*}$ is a basis for $\mathfrak{N}_c$. We can suppose $\mathbf{c}_{p+\alpha} = b_\alpha \mathbf{c}$ for $\alpha = 1, \cdots, n-p$. Now consider the set of vectors

$$\mathbf{c}'' = \mathbf{c} + \sum_{\alpha=1}^{p} z_\alpha \mathbf{c}_\alpha. \tag{3.5}$$

By a "neighborhood of the origin" in the set $\mathfrak{s}_c$, we mean the set of $\sum_{\alpha=1}^{p} z_\alpha \mathbf{c}_\alpha$ for which $|z_\alpha| < \delta$ for some specified positive δ and this expression will be applied to other linear sets. Similarly we consider the set of vectors

$$\mathbf{c}' = \mathbf{c} + \sum_{\alpha=1}^{p} x_\alpha \mathbf{c}_\alpha + \sum_{\alpha=p+1}^{n} y_\alpha \mathbf{c}_\alpha. \tag{3.6}$$

We now consider $\mathbf{c}''$ and $\mathbf{c}'$ as given by (3.5) and (3.6) and the relation

$$\exp\left(\sum_{\alpha=1}^{n-p} \mu_\alpha b_\alpha\right)\mathbf{c}'' = \mathbf{c}'. \tag{3.7}$$

It is clear that this relation is equivalent to n relations

$$\begin{aligned} x_\alpha &= F_\alpha(z_1, \cdots, z_p, \mu_1, \cdots, \mu_{n-p}) \\ y_\alpha &= G_\alpha(z_1, \cdots, z_p, \mu_1, \cdots, \mu_{n-p}), \end{aligned} \tag{3.8}$$

where the F_α and G_α are analytic functions of the indicated variables and for $\mu_i = 0$, these relations become

$$x_\alpha = z_\alpha, \; y_\alpha = 0. \tag{3.9}$$

Lemma 3.1. *There is a neighborhood of the origin in the space* $\mathfrak{C}$, $\sum_{\alpha=1}^{p} |x_\alpha|^2 + \sum_{\alpha=p+1}^{n} |y_\alpha|^2 < \delta$, *such that on this neighborhood there exists analytic functions*

$$\begin{aligned} z_\alpha &= \phi_\alpha(x_1, \cdots, x_p, y_{p+1}, \cdots, y_n) \\ \mu_\alpha &= \psi_\alpha(x_1, \cdots, x_p, y_{p+1}, \cdots, y_n) \end{aligned} \tag{3.10}$$

which are inverse to the relation (3.9).

Proof. It follows from (3.9) that if zero is substituted on both sides of (3.8) it is satisfied. We must show that the Jacobean of the Eqs. (3.8) is not zero at zero.

If we take differentials of (3.7) at the zero point we have by (3.5) and (3.6):

$$\sum_{\alpha=1}^{p} dz_\alpha \mathbf{c}_\alpha + \sum_{\alpha=1}^{n-p} d\mu_\alpha b_\alpha \mathbf{c} = \sum_{\alpha=1}^{p} dx_\alpha \mathbf{c}_\alpha + \sum_{\alpha=p+1}^{n} dy_\alpha \mathbf{c}_\alpha. \tag{3.11}$$

By (3.1) we have that

$$\sum_{\alpha=1}^{n-p} d\mu_\alpha b_\alpha \mathbf{c} = T_c\left(\sum d\mu_\alpha b_\alpha\right) \tag{3.12}$$

and since the range of T_c, $\mathfrak{R}_c$, is determined by $\mathbf{c}_{p+1}, \cdots, \mathbf{c}_n$, it follows that (3.11) is equivalent to

$$\sum_{\alpha=1}^{n-1} d\mu_\alpha b_\alpha \mathbf{c} = T_\alpha\left(\sum d\mu_\alpha b_\alpha\right) = \sum_{\alpha=p+1}^{n} dy_\alpha \mathbf{c}_\alpha \tag{3.13}$$

and

$$\sum_{\alpha=1}^{p} dz_\alpha \mathbf{c}_\alpha = \sum_{\alpha=1}^{p} dx_\alpha \mathbf{c}_\alpha. \tag{3.14}$$

At the zero point, the Eqs. (3.8) specify a linear transformation of the vectors

$$dz_1, \cdots, dz_p, \quad d\mu_1, \cdots, d\mu_{n-p}$$

onto the vectors

$$dx_1, \cdots, dx_p, \quad dy_{p+1}, \cdots, dy_n.$$

The Jacobean is the determinant of this transformation regarded as a linear transformation of n space. Now T_c takes $\mathfrak{b}^*$ in a one to one manner into $\mathfrak{R}_c$ and consequently (3.13) and (3.14) imply that this linear transformation is nonsingular and hence the Jacobean is not zero, Q.E.D.

SECTION 4

Lemma 3.1 describes the relation $v\mathbf{c}'' = \mathbf{c}'$ for a v in the form $\exp\left(\sum_{\alpha=1}^{n-p} \mu_\alpha b_\alpha\right)$. The more general case for v must be considered. To do this we must get a number of results on the product of such v's. These results are either in Pontrjagin or are minor variations from results given there. The proofs are relatively straightforward in our present context and are merely indicated here.

Consider now a finite Lie algebra which consists of $n \times n$ matrices b which are linear combinations of a basis $b_1, \cdots, b_m$. We have

$$[b_i b_j] = \sum_\alpha c_{ij}^\alpha b_\alpha. \tag{4.1}$$

Lemma 4.1. *If* b *and* b' *are matrices, then*

$$b' b^r = \sum_{\alpha=0}^{r} \binom{r}{\alpha} b^\alpha ([]^{r-\alpha} b'(b])^{r-\alpha}, \tag{4.2}$$

where $([]^0 b'(b])^0 = b'$.

This is simply the n-dimensional matrix equivalent of (1.20).

Lemma 4.2. *Le* $b(t)$ *be a matrix function, with derivative* $b'(t)$. *Then*

$$\frac{d}{dt} b(t)^n = \sum_{\gamma=0}^{n} \binom{n}{n-\gamma} b^\gamma ([]^{n-1-\gamma} b'(b])^{n-1-\gamma} \tag{4.3}$$

This follows from (4.2) by a straightforward ma-

nipulation. Similarly, we obtain

Lemma 4.3. *If $b(t)$ is a matrix function with a continuous derivative b' on a closed interval $c_1 \leq t \leq c_2$, then for this interval*

$$(d/dt)\{\exp b(t)\} = \exp b(t)[b'g(b]), \tag{4.4}$$

where

$$g(x) = (\exp x - 1)/x \tag{4.5}$$

Lemma 4.4. *Let a_0 be a given constant matrix and $a(t)$ a matrix function of t with a continuous derivative on some closed interval $0 \leq t \leq c$. Then the differential equation*

$$db/dt = b[a'g(a]) \tag{4.6}$$

[see (4.5) above] *has a unique solution $b = \exp\{a(t)\}a_0$ in the t interval $0 \leq t \leq c$, if $b(0) = \exp\{a(t_0)\}a_0$.*

In view of Lemma 4.3, we must establish the uniqueness. Now (4.6) can be regarded as n^2 equations which express the n^2 derivatives of the components of b as linear combinations with coefficients which are continuous functions of t on the interval. The solution of such a system is uniquely specified by its initial condition. [Since $\exp\{a(t_0)\}$ is nonsingular, an arbitrary choice of a_0 corresponds to an arbitrary choice of b_0.]

Lemma 4.5. *Let $\mathfrak{b}$ denote a Lie algebra of $n \times n$ matrices with basis $b_1, \cdots, b_m$; i.e., we have*

$$[b_i b_j] = \sum_\alpha c_{ij}^\alpha b_\alpha \tag{4.7}$$

Let r be an integer, $1 \leq r < m$. There exists an $\eta_1 > 0$ and $\eta_2 > 0$ such that for $\sum_{\alpha=1}^r \mu_\alpha^2 < \eta_1$ and $\sum_{\alpha=r+1}^m \mu_\alpha^2 < \eta_2$, there exists $\nu_1, \cdots, \nu_m$ which are functions of $\mu_1, \cdots, \mu_m$ such that

$$\exp\left(\sum_{\alpha=1}^m \mu_\alpha b_\alpha\right) = \exp\left(\sum_{\alpha=1}^r \nu_\alpha b_\alpha\right)\exp\left(\sum_{\alpha=r+1}^m \nu_\alpha b_\alpha\right) \tag{4.8}$$

Proof. Let us consider the equation

$$\exp\left(\sum_{\alpha=1}^r \mu_\alpha b_\alpha + t\sum_{\alpha=r+1}^m \mu_\alpha b_\alpha\right) = \exp\left\{\sum_{\alpha=1}^r \nu_\alpha(t) b_\alpha\right\}\exp\left\{\sum_{\alpha=r+1}^m \nu_\alpha(t) b_\alpha\right\} \tag{4.9}$$

as determining ν_α as functions of t. At $t = 0$, this has a solution $\nu_\alpha = \mu_\alpha$, $\alpha = 1, \cdots, r$, $\nu_\alpha = 0$, $\alpha = r+1, \cdots, m$. Now let

$$b(t) = \sum_{\alpha=1}^r \mu_\alpha b_\alpha + t\sum_{\alpha=r+1}^m \mu_\alpha b_\alpha \tag{4.10}$$

$$b^0 = \sum_{\alpha=r+1}^m \mu_\alpha b_\alpha \tag{4.11}$$

$$b^* = \sum_{\alpha=1}^r \nu_\alpha(t) b_\alpha \tag{4.12}$$

$$b^\dagger = \sum_{\alpha=r+1}^m \nu_\alpha(t) b_\alpha \tag{4.13}$$

Differentiating and using (4.9) yield

$$[b^0 g(b]) = [[b^{*\prime} g(b]) \exp(b^\dagger]) + [b^{\dagger\prime} g(b^\dagger]) \tag{4.14}$$

Because of (4.7), both sides of (4.14) can be expressed as a linear combination of $b_1, \cdots, b_m$. Hence (4.14) can be regarded as m equations on $\nu_1, \cdots, \nu_m$ and their first derivatives. These equations are linear in the derivatives of $\nu_1, \cdots, \nu_m$. At $t = 0$, (4.14) reduces to

$$\left[b^0 g\left(\sum_{\alpha=1}^r \mu_\alpha b_\alpha\right)\right] = \sum_{\alpha=1}^m \nu_\alpha'(t) b_\alpha \tag{4.15}$$

It follows then that there is a t interval $0 \leq t \leq c$ and a $\nu_1, \cdots, \nu_m$ neighborhood of $\mu_1, \cdots, \mu_r, 0, \cdots, 0$ within which it is possible to solve the m differential equations equivalent to (4.14) for $\nu_1', \cdots, \nu_m'$. This yields m differential equations depending on the parameters $\mu_{r+1}, \cdots, \mu_m$ and with initial conditions $\mu_1, \cdots, \mu_r, 0, \cdots, 0$ for $\nu_1, \cdots, \nu_m$. The existence theory for differential equations (cf. Miller and Murray) shows that there exists η_1 and η greater than 0 and a t interval $0 \leq t \leq c$ such that there is a solution $\nu_\alpha(t, \mu_1, \cdots, \mu_m)$ of (4.14) on this t interval defined for every set of μ's for which $\sum_{\alpha=1}^r \mu_\alpha^2 < \eta_1$ and $\sum_{\alpha=r+1}^m \mu_\alpha^2 < \eta$.

Let us consider then such a solution of the differential equation (4.14). Then differentiating the right side of (4.9) and using (4.14), we obtain

$$(d/dt)\{\exp(b^*)\exp(b^\dagger)\} = \exp b^* \exp b^\dagger [b^0 g(b]) \tag{4.16}$$

We also have

$$(d/dt)(\exp\{b(t)\}) = \exp\{b(t)\}[b^0 g(b]) \tag{4.17}$$

Let

$$D(t) = \exp(b^*)\exp(b^\dagger) - \exp(b(t)) \tag{4.18}$$

Then (4.16) and (4.17) imply

$$(d/dt)\{D(t)\} = D(t)[b^0 g(b]) \tag{4.19}$$

By Lemma 4.4, $D(t) = a_0 \exp b(t)$. But $D(0) = 0$ and hence $a_0 = 0$ and thus $D(t) = 0$, for the solution of (4.14) which we obtained. This is easily seen to be equivalent to the conclusion of Lemma 4.5 with $\eta_2 = c^2\eta$. [See discussion between (4.15) and (4.16) above.]

The essential part of the above discussion is to obtain a system of m equations by means of (4.14) and then pass to n^2 relations by the argument of (4.16) to (4.18). The following is proved in a similar fashion.

Lemma 4.6. *Let $\epsilon > 0$ be given. There exists an $\eta_1 > 0$ and $\eta_2 > 0$, such that if $\sum_{\alpha=1}^{m} \mu_\alpha^2 < \eta_1$ and $\sum_{\alpha=1}^{m} \mu_\alpha'^2 < \eta_2$, then there exists a set $\nu_1, \cdots, \nu_m$ with $\sum \nu_r^2 < \epsilon$ for which*

$$\exp\left(\sum_{\alpha=1}^{m} \mu_\alpha b_\alpha\right) \exp\left(\sum_{\alpha=1}^{m} \mu_\alpha' b_\alpha\right) = \exp\left(\sum \nu_\alpha b_\alpha\right). \tag{4.20}$$

Lemma 4.7. *Let u_i be an exponential in the form $\exp(\sum \mu_\alpha b_\alpha)$ for $i = 1, \cdots, r$. Then there is a neighborhood of the origin such that if for $i = 1, \cdots, r$, the corresponding $\sum \mu_\alpha b_\alpha$ are in this neighborhood and for $j < r$, $\prod_{\alpha=1}^{j} u_\alpha$ is an exponential in this neighborhood in the specified form, then $\prod_{\alpha=1}^{r} u_\alpha$ is also an exponential in this form.*

Lemma 4.7 follows from Lemma 4.6 by an obvious induction. This lemma is essentially the statement that $\mu_1, \cdots, \mu_m$ can be used as a coordinate system for the local group obtained by exponentiation from the Lie algebra of the b's (cf. Pontrjagin).

Lemma 4.8. *Let $\mathfrak{U}$ denote the set of vectors $\mathbf{c}'$ in the form*

$$\mathbf{c}' = \exp\left(\sum_{\alpha=1}^{n-p} \mu_\alpha b_\alpha\right)\mathbf{c}, \tag{4.21}$$

where $\mathbf{c}$ is given as in Sec. 3 above and $b_1, \cdots, b_{n-p}$ are as in (3.4). *Let u denote an exponential $\exp(\sum_{\alpha=1}^{m} \mu_\alpha b_\alpha)$. The set $\mathfrak{U}$ is of $n - p$ dimensions and there exists a neighborhood of the origin such that if $\sum_{\alpha=1}^{n} \mu_\alpha b_\alpha$ is in this neighborhood then $u\mathbf{c}$ is in $\mathfrak{U}$.*

Proof. Consider the $\mathbf{c}'$ in the form given by Eq. (3.6). The $\mathbf{c}_\alpha$ are linearly independent and hence the $\sum_{\alpha=p+1}^{n} y_\alpha \mathbf{c}_\alpha$ will form an $n - p$ dimensional set if the y_α's are arbitrary. Furthermore, if the x_α are given as analytic functions of $y_{p+1}, \cdots, y_n$, the $\mathbf{c}'$ will still constitute an $n - p$ dimensional set. Now the set $\mathfrak{U}$ of (4.21) can be obtained by setting $z_\alpha = 0$ in (3.7). [See Eq. (3.5).] But the argument of Lemma 3.1 shows that for $z = 0$, we can insert the second set of equations of (3.8) and express the $\mu_1, \cdots, \mu_{n-p}$ as functions of $y_{p+1}, \cdots, y_n$ and if we substitute these in the first set of (3.8) with $z = 0$ we will have x_α as an analytic function of $y_{p+1}, \cdots, y_n$ for $\alpha = 1, \cdots, p$. To each choice then of $y_{p+1}, \cdots, y_n$ in the neighborhood, in which we can insert $y_\alpha = G_\alpha$, we have then a $\mathbf{c}'$ in the form specified for which there is a set $\mu_1, \cdots, \mu_{n-p}$ which yields that $\mathbf{c}'$ is in the set $\mathfrak{U}$. This shows then that $\mathfrak{U}$ contains the set of $\mathbf{c}'$ in the form specified; i.e., with the $y_{p+1}, \cdots, y_n$ arbitrary and x_α as a function of the y's. On the other hand, the second set of equations of (3.8) shows that for $z_\alpha = 0$, the $\mu_1, \cdots, \mu_{n-p}$ determine the y's and hence every $\mathbf{c}'$ in $\mathfrak{U}$ is in the form specified. Thus $\mathfrak{U}$ is $n - p$ dimensional.

Now let $u = \exp(\sum_{\alpha=1}^{m} \mu_\alpha b_\alpha)$. Let us apply Lemma 4.5 and, for an appropriate neighborhood, express u in the form $u = u'u''$ where

$$u' = \exp\left(\sum_{\alpha=1}^{n-p} \nu_\alpha b_\alpha\right), \quad u'' = \exp\left(\sum_{\alpha=n-p+1}^{m} \nu_\alpha' b_\alpha\right) \tag{4.22}$$

Since $b_{n-p+1}, \cdots, b_m$ is a basis for $\mathfrak{N}_c$ [cf. (3.2) and (3.4)]

$$\left(\sum_{\alpha=n-p+1}^{m^*} \nu_\alpha' b_\alpha\right)\mathbf{c} = 0 \tag{4.23}$$

and $u''\mathbf{c} = \mathbf{c}$. Hence we have $u\mathbf{c} = u'u''\mathbf{c} = u'\mathbf{c}$ which is in $\mathfrak{U}$.

SECTION 5

Theorem. We make the assumption of Sec. 2 and specify an $A = \mathbf{c}\cdot\mathbf{A}$ by means of the vector $\mathbf{c}$. Let $n - p$ denote the dimensionality of $\mathfrak{R}_c$, the set of vectors in the form $b\mathbf{c}$. Then p is the same for all $\mathbf{c}'$ equivalent to $\mathbf{c}$ and the dimensionality of the set of A' equivalent to A is $n - p$. If $\mathfrak{S}_c$ is a set complementary to $\mathfrak{R}_c$ and $\mathbf{c}_1, \cdots, \mathbf{c}_p$ is a basis for $\mathfrak{S}_c$ and $\mathbf{c}_1, \cdots, \mathbf{c}_n$ a basis for $\mathfrak{C}$, then there exists a neighborhood of A such that for all A' in this neighborhood,

$$A' = A + \sum_{\alpha=1}^{p} x_\alpha A_\alpha + \sum_{\alpha=p+1}^{n} y_\alpha A_\alpha, \tag{5.1}$$

then A' is B equivalent to an A'' in the form

$$A + \sum_{\alpha=1}^{p} z_\alpha A_p. \tag{5.2}$$

Proof. Since $\mathbf{c}' \sim \mathbf{c}$ is equivalent to $\exp b\mathbf{c} = \mathbf{c}'$ and $\exp(-b)\mathbf{c}' = c$, one can readily show that p is the same for $\mathbf{c}$ and $\mathbf{c}'$ if they are equivalent. Lemma 4.8 shows that for each A, there exists a neighborhood for which the set of equivalent A's is $n - p$ dimensional.

The last sentence of the Theorem is essentially Lemma 3.1. For Eqs. (3.10) show how, for an arbitrary set of $x_1, \cdots, x_p, y_{p+1}, \cdots, y_n$, we can find a set of z's and μ's for which (3.7) holds, and hence for which the required B equivalence holds (definition, Sec. 2).

Notice then that the ϕ_α of (3.10) do constitute a complete set of invariants for the restricted type of B equivalence associated with $\sum_{\alpha=1}^{n-p} \mu_\alpha B_\alpha$ [see (3.7)] and for the appropriate neighborhood. Two A' in the form (5.1) will be equivalent under this restricted B equivalence to the same A'' in the form (5.2) if and only if all the ϕ_α functions agree. Now an A' in the form (5.1) will be equivalent to a set $\mathfrak{U}'$ of dimension $n - p'$. This $\mathfrak{U}$ must include the set of those equivalent to a transformation in the form (5.2) under the restricted B set and argument of the proof of Lemma 4.8 with the specified values of z_α will show that the latter set has dimension $n - p$. Hence $n - p' \geq n - p$ and the ϕ_α will constitute a set of invariants for the full B equivalence if the equality holds.

Corollary 1. *Given an A, there exists a neighborhood such that for all A' in this neighborhood $p' \geq p$.*

Since p is positive and integral, there is a least value that it assumes. Suppose A has been chosen so that p has this value. Then in a neighborhood $p' = p$ and we have a local set of invariants. If we recall the definition of p [cf. (3.3)], we see that there must be a determinant of order $n - p$ in the matrix for T_c which is not zero. For A' in the form (5.1) this determinant becomes a polynomial in $x_1, \cdots, x_p, y_{p+1}, \cdots, y_n$ and hence not zero except on a set of dimensionality lower than n.

Corollary 2. *If p_0 is the minimum value assumed by p, then p assumes the value p_0 except possibly on a set of dimensionality less than n and we can in each neighborhood find an A for which there is a neighborhood for which p_0 invariants can be defined so that two A's in this neighborhood are B equivalent if and only if they have the same values for these invariants.*

SECTION 6

We have seen that B equivalence relations can be specified by the equation

$$\exp\left(\sum_{\alpha=1}^{m} \mu_\alpha b_\alpha\right)\mathbf{c} = \mathbf{c}', \tag{6.1}$$

(see Sec. 2).

As indicated in the previous section, in general, the dimensionality of the set of $\mathbf{c}'$ is less than n. Thus given a $\mathbf{c}$ in the form (3.6) with $\mathbf{c}$ chosen so as to make p a minimum, there will be p functions ϕ_α of (3.10) such that two such $\mathbf{c}'$ will be equivalent if they have the same values of ϕ_α. [Each is equivalent to a $\mathbf{c}''$ in the form (3.5) under an appropriate exponential transformation and Lemma 4.6 permits us to compound exponentials into a single exponential.] These p functions are then a set of invariants. However they are basically nonunique because of the possible arbitrariness in the choice of $\mathbf{c}_1, \cdots, \mathbf{c}_p$. (Since these are merely required to determine a manifold complementary to $\mathfrak{R}_c$, we may substitute for $\mathbf{c}_1, \cdots, \mathbf{c}_p$ any set

$$\mathbf{c}'_\alpha = \sum_{\beta=1}^{p} a_{\alpha\beta}\mathbf{c}_\beta + \sum_{p+1}^{n} b_{\alpha\beta}\mathbf{c}_\beta \tag{6.2}$$

provided that the determinant of the $a_{\alpha\beta}$ matrix is not zero. The transformation rule for the new ϕ_α is readily determined in terms of the original set.) It is also true that these invariants are defined in a local manner and, while analytic extension is possible, this process presents grave computational problems.

It seems desirable therefore to replace these invariants if possible by similarity invariants. Suppose for instance that we have a linear mapping of the vectors $\mathbf{c}$ onto $n \times n$ matrices a, $\mathbf{c} \to a(\mathbf{c})$ in such a way that

$$[ba(\mathbf{c})] = a(b\mathbf{c}). \tag{6.3}$$

This relation and the linearity of the mapping of $\mathbf{c}$ onto a shows that for an arbitrary polynomial

$$P([b)a(\mathbf{c})] = a\{P(b)\mathbf{c}\} \tag{6.4}$$

and by a well known limiting procedure

$$\exp ba(\mathbf{c}) \exp(-b) = \exp([b)a(\mathbf{c})] = a(\exp b\mathbf{c}). \tag{6.5}$$

Thus (6.3) implies that a (exp $b\mathbf{c}$) is obtained from $a(\mathbf{c})$ by a similarity transformation using the matrix exp $(-b)$. Furthermore this result implies that even when a number of exponentials are applied in sequence, the resulting matrix is still obtainable by a similarity from the original. Thus similarity invariants of the matrix $a(\mathbf{c})$ are preserved when $\mathbf{c}$ is replaced by an equivalent $\mathbf{c}$ under the whole non local group and yield therefore invariants.

Lemma 6.1. *If we have a linear mapping of the vectors $\mathbf{c}$ onto matrices $a(\mathbf{c})$ such that* (6.3) *holds, then* (6.5) *holds and all similarity invariants of $a(\mathbf{c})$ are invariants of B equivalence in the global sense.*

Naturally one must not expect the similarity invariants to be complete. This is true even if we consider invariants for only those similarities associated with transformations in the form exp (b). For suppose

$$a(\mathbf{c}') = \exp ba(\mathbf{c}) \exp(-b) = a(\exp b\mathbf{c}) \tag{6.6}$$

[the second equality follows from (6.5)] or

$$a(\mathbf{c}' - \exp b\mathbf{c}) = 0. \tag{6.7}$$

Thus the first equality of (6.6) implies simply that

$$\mathbf{c}' = (\exp b)\mathbf{c} + \mathbf{c}'', \tag{6.8}$$

where $\mathbf{c}''$ is such that $a(\mathbf{c}'') = 0$. Hence:

Lemma 6.2. *If the mapping* $\mathbf{c} \to a(\mathbf{c})$ *is faithful; i.e., one to one, then equivalence under the similarities is the form* exp (b) a exp $(-b)$ *for the* $a(\mathbf{c})$ *determines the equivalence of the* $\mathbf{c}$.

Let $\mathfrak{Q}$ denote the set of $\mathbf{c}$'s for which $a(\mathbf{c}) = 0$.

SECTION 7

The condition of Lemma 6.2 is too restrictive in general although there are certain interesting examples where it is fulfilled. However, to obtain precise information concerning the b equivalence situation, we apply an argument similar to the argument of Lemma 3.1.

We consider a fixed c and the corresponding $a(\mathbf{c})$ and define a transformation from the set of b's to the a's by means of the equation

$$T_a b = [a(\mathbf{c}), b] = a' = a(b\mathbf{c}). \tag{7.1}$$

Let ρ_a denote the range of T_a. We recall that $\mathfrak{R}_c$ consists of the vectors in the form $b\mathbf{c}$. It is clear from (7.1) that ρ_a consists of matrices in the form $a(b\mathbf{c})$. We can consider the set $\mathfrak{N}'$ of those vectors in the form $b\mathbf{c}$ for which $a(b\mathbf{c}) = 0$. Thus $\mathfrak{N}' = \mathfrak{Q}\cdot\mathfrak{R}_c$ for $\mathfrak{Q}$ as defined after Lemma 6.2 in the previous section. The vectors $\mathbf{c}_{p+1}, \cdots, \mathbf{c}_n$ of (3.3) which form a basis for $\mathfrak{R}_c$ can be chosen in such a way that $\mathbf{c}_{p+1}, \cdots, \mathbf{c}_{p+k}$ form a basis for $\mathfrak{N}'$. Then

$$a(\mathbf{c}_{p+k+1}), \cdots, a(\mathbf{c}_n) \tag{7.2}$$

are linearly independent. The vectors $\mathbf{c}_1, \cdots, \mathbf{c}_p$ determine a manifold $\mathfrak{S}_c$ complementary to $\mathfrak{R}_c$. These can be chosen so that if $\mathfrak{Q}$ is the set of vectors $\mathbf{c}$ for which, $a(\mathbf{c}) = 0$, then $\mathbf{c}_{r+1}, \cdots, \mathbf{c}_p$ determine a complementary manifold for $\mathfrak{N}'$ relative to $\mathfrak{Q}$ and $\mathbf{c}_1, \cdots, \mathbf{c}_r$ determine a manifold complementary to that containing $\mathfrak{R}_c$ and $\mathfrak{Q}$. Thus an arbitrary vector $\mathbf{c}'$ can be written

$$\mathbf{c}' = \mathbf{c} + \sum_{\alpha=1}^{r} x'_\alpha \mathbf{c}_\alpha + \sum_{\alpha=r+1}^{p} x''_\alpha \mathbf{c}_\alpha + \sum_{\alpha=p+1}^{p+k} y'_\alpha \mathbf{c}_\alpha + \sum_{\alpha=p+k+1}^{n} y''_\alpha \mathbf{c}_\alpha. \tag{7.3}$$

The first two sums are in $\mathfrak{S}_c$, the last two in $\mathfrak{R}_c$; the second and third are in $\mathfrak{Q}$.

Correspondingly,

$$a' = a(\mathbf{c}') = a(\mathbf{c}) + \sum_{\alpha=1}^{r} x'_\alpha a_\alpha + \sum_{\alpha=p+k+1}^{n} y''_\alpha a_\alpha, \tag{7.4}$$

where $a_\alpha = a(\mathbf{c}_\alpha)$. By the above construction

$$a(\mathbf{c}_\alpha) = 0 \quad \text{for} \quad r < \alpha \leq p + k. \tag{7.5}$$

We recall that $\mathfrak{N}_c$ has been defined as the set of b's for which $b\mathbf{c} = 0$. We now consider a larger set of b's for which $a(b\mathbf{c}) = 0$. If this set is termed $\mathfrak{N}_c^\ddagger$, then $\mathfrak{N}_c \subset \mathfrak{N}_c^\ddagger$. We also have that

$$\mathbf{c}_{\alpha+p} = b_\alpha \mathbf{c} \tag{7.6}$$

by (3.4) and $b_1, \cdots, b_k$ are in $\mathfrak{N}_c^\ddagger$ by the choice of $\mathbf{c}_p, \cdots, \mathbf{c}_{p+k}$ above. Thus [cf. (3.4)]

$$b_1, \cdots, b_k, b_{n-p+1}, \cdots, b_m \tag{7.7}$$

is a basis for $\mathfrak{N}_c^\ddagger$ and the

$$b_{k+1}, \cdots, b_{n-p} \tag{7.8}$$

determine a manifold $\mathfrak{b}^\ddagger$ complementary to $\mathfrak{N}_c^\ddagger$. Each $b \in \mathfrak{b}$ can be written $b = b' + b''$ where

$$b' = \sum_{\alpha=1}^{k} \mu_\alpha b_\alpha + \sum_{\alpha=m-p+1}^{m} \mu_\alpha b_\alpha$$
$$b'' = \sum_{\alpha=k+1}^{n-p} \mu_\alpha b_\alpha. \tag{7.9}$$

We can now repeat the argument of Lemma 3.1 relative to the a's rather than the $\mathbf{c}$'s but retaining the connections between $\mathbf{c}$ and a. Consider then the $\mathbf{c}'$ in the form (7.3) and the corresponding $a(\mathbf{c}')$ in the form (7.4). Consider also the corresponding

$${}^u\mathbf{c}'' = \mathbf{c} + \sum_{\alpha=1}^{r} z'_\alpha \mathbf{c}_\alpha + \sum_{\alpha=r+1}^{p} z''_\alpha \mathbf{c}_\alpha + \sum_{\alpha=p+1}^{p+k} z''_\alpha \mathbf{c}_\alpha \tag{7.10}$$

and

$$a({}^u\mathbf{c}'') = a(\mathbf{c}) + \sum_{\alpha=1}^{r} z'_\alpha a(\mathbf{c}_\alpha). \tag{7.11}$$

Consider then the relationship

$$\exp(b'')^u\mathbf{c}'' = \mathbf{c}' \tag{7.12}$$

and the corresponding matrix equation

$$\exp b'' a({}^u\mathbf{c}'') \exp(-b'') = \exp([b'')a(\mathbf{c}'')] = a(\mathbf{c}'). \tag{7.13}$$

This last equation shows by (7.4), (7.9), and (7.11) that

$$x'_\alpha = f'_\alpha(z'_1, \cdots, z'_r, \mu_{k+1}, \cdots, \mu_{n-p}) \qquad \alpha = 1, \cdots, r \tag{7.14}$$

$$y''_\alpha = g'_\alpha(z'_1, \cdots, z'_r, \mu_{k+1}, \cdots, \mu_{n-p})$$
$$\alpha = p + k + 1, \cdots, n.$$

The Jacobian argument of Lemma 3.1 is now applicable and shows that Eqs. (7.14) can be inverted and thus

$$z'_\alpha = \phi'_\alpha(x'_1, \cdots, x'_r, y''_{p+k+1}, \cdots, y''_n)$$
$$\alpha = 1, \cdots, r \qquad (7.15)$$
$$\mu_\alpha = \psi'_\alpha(x'_1, \cdots, x'_r, y''_{p+k+1}, \cdots, y''_n)$$
$$\alpha = k + 1, \cdots, n - p.$$

But we can also consider $\mathbf{c}''$ as given by (3.5) and for this we will have

$$a(\mathbf{c}'') = a(\mathbf{c}) + \sum_{\alpha=1}^{r} z_\alpha a(\mathbf{c}_\alpha). \qquad (7.16)$$

Then (3.7) implies

$$\exp\left(\sum_{\alpha=1}^{n-p} \mu_\alpha b_\alpha\right) a(\mathbf{c}'') \exp\left(-\sum_{\alpha=1}^{n-p} \mu_\alpha b_\alpha\right) = a(\mathbf{c}'), \qquad (7.17)$$

and this again yields

$$x'_\alpha = f_\alpha(z_1, \cdots, z_r, \mu_1, \cdots, \mu_k, \mu_{k+1}, \cdots, \mu_{n-p})$$
$$y''_\alpha = g_\alpha(z_1, \cdots, z_r, \mu_1, \cdots, \mu_k, \mu_{k+1}, \cdots, \mu_{n-p}). \qquad (7.18)$$

Now clearly (7.14) corresponds to the case $\mu_1 = \cdots = \mu_k = 0$. Since the Eqs. (7.14) can be inverted, it follows that for a neighborhood of these values of $\mu_1, \cdots, \mu_k$ it must be possible to solve (7.18) for $z_1, \cdots, z_r, \mu_{k+1}, \cdots, \mu_{n-p}$.

$$z_\alpha = \phi_\alpha(x'_1, \cdots, x'_r, y''_{p+k+1}, \cdots, y''_n, \mu_1, \cdots, \mu_k)$$
$$\alpha = 1, \cdots, r,$$
$$\mu_\alpha = \psi_\alpha(x'_1, \cdots, x'_r, y''_{p+k+1}, \cdots, y''_n, \mu_1, \cdots, \mu_k)$$
$$\alpha = k + 1, \cdots, n - p. \qquad (7.19)$$

Now the z_α, $\alpha = 1, \cdots, r$ cannot be regarded as invariants for the matrix $a(\mathbf{c}')$ since they depend on the quantities $\mu_1, \cdots, \mu_k$ which are not associated with this matrix. However, if we eliminate these quantities between these expressions, we will get $r - k'$ expressions

$$Z_\alpha(z_1, \cdots, z_r, x'_1, \cdots, x'_r, y''_{p+k+1}, \cdots, y''_n) = 0 \qquad (7.20)$$

which are expressible purely in terms of matrix coefficients. We have $k' \leq k$. The similarity invariants must yield equations of this type when they do not yield expressions which are identically zero. One equates the invariant expression in terms of x' and y'' to the corresponding expression in z.

Notice that, in general, given $a(\mathbf{c})$, $a(\mathbf{c}'')$ will not be determined unless $k' = 0$. This would happen if either $k = 0$ or the ϕ_α in (7.19) do not contain $\mu_1, \cdots, \mu_k$ since (7.19) shows that the z_α, which determine $a(\mathbf{c}'')$ by (7.16), depend on $\mu_1, \cdots, \mu_k$ which are not specified by $a(\mathbf{c})$. These possibilities can be explored but we will not do so at present.

Lemma 7.1. *Let a linear mapping* $\mathbf{c} \to a(\mathbf{c})$ *where* a *is an* $n \times n$ *matrix, such that* (6.3) *holds. Let* $\mathfrak{Q}$ *denote the set of vectors* $\mathbf{c}$ *for which* $a(\mathbf{c}) = 0$. *Suppose* $\mathbf{c}$ *is given and* $\mathfrak{R}_c$ *denotes the vectors in the form* $b\mathbf{c}$. *Let* $\mathfrak{N}'$ *denote the intersection of* $\mathfrak{R}_c$ *and* $\mathfrak{Q}$. $\mathfrak{N}'$ *is the set of vectors in the form* $\mathbf{c}' = b\mathbf{c}$ *for which* $a(\mathbf{c}') = 0$. *Let* k *denote the dimensionality of* $\mathfrak{N}'$ *and* $p - r + k$ *denote the dimensionality of* $\mathfrak{Q}$. *If* $\mathbf{c}'$ *is an arbitrary vector in a certain neighborhood of* $\mathbf{c}$ [*cf.* (3.6)], *then* $a(\mathbf{c}')$ *is equivalent under similarities determined by exponentials* exp (b) *to matrices* $a(\mathbf{c}'')$ *determined by* r *constants* $z_1, \cdots, z_r$. *There is a non-negative integer* $k' \leq k$ *such that there are* $r - k'$ *relations between the coefficients of the* $a(\mathbf{c}')$ *matrix and* $z_1, \cdots, z_r$. [*See* (7.19) *and* (7.20) *above.*] *The similarity invariants are either identically zero or yield relations of this character.* (*See the discussion after* (7.20).) *The matrix* $a(\mathbf{c}'')$ *is determined by* $a(\mathbf{c}')$ *if and only if* $k' = 0$.

Lemma 7.1 shows the limitations which appear when one endeavors to consider the matrices $a(\mathbf{c})$ instead of $\mathbf{c}$ themselves. If we let $q = p - r + k$ denote the dimensionality of $\mathfrak{Q}$, and $q' = p - r + k'$, then instead of p invariants for the c's, we have $p - q'$ relations on the elements of the a's. Since $q' \leq q$, if the dimensionality of $\mathfrak{Q}$ is zero, we have equivalence. However the relations for the a elements obtained when they exist are useful in the global study of B equivalence.

SECTION 8

We consider the special case in which the A_i and B_i's coincide. We have a basis for the set $\mathfrak{A}$, $A_1, \cdots, A_n$, with

$$i[A_i A_j] = \sum_{\alpha=1}^{n} a_{ij}^\alpha A_\alpha. \qquad (8.1)$$

For the vectors $\mathbf{c} = \{c_1, \cdots, c_n\}$, constituting an n-dimensional space $\mathfrak{C}$, we have a correspondence with the linear combinations of the $A_1, \cdots, A_n$

$$\mathbf{c} \sim A = \sum c_\alpha A_\alpha = \mathbf{c} \cdot \mathbf{A}. \qquad (8.2)$$

We also have a correspondence with the $n \times n$

matrices

$$a = a(\mathbf{c}) = \{\sum_{\beta} a^i_{j\beta} c_\beta\} \quad i, j = 1, \cdots, n, \tag{8.2'}$$

such that by (8.1) we have

$$i[\mathbf{c}\cdot\mathbf{A}\ \mathbf{c}'\cdot\mathbf{A}] = \{a(\mathbf{c}')\mathbf{c}\}\cdot\mathbf{A}. \tag{8.3}$$

Thus if $A = \mathbf{c}\cdot\mathbf{A}$, $B = \mathbf{c}'\cdot\mathbf{A}$, $b = a(\mathbf{c}')$ we have

$$i[\mathbf{c}\cdot\mathbf{A}\ B] = (b\mathbf{c})\cdot\mathbf{A}.$$

Hence by (8.3)

$$\begin{aligned}\{a(b\mathbf{c})\mathbf{c}''\}\cdot\mathbf{A} &= i[\mathbf{c}''\cdot\mathbf{A}\ b\mathbf{c}\cdot\mathbf{A}] = i[\mathbf{c}''\cdot\mathbf{A}\ i[\mathbf{c}\cdot\mathbf{A}\ B]] \\ &= i[i[\mathbf{c}''\cdot\mathbf{A}\ \mathbf{c}\cdot\mathbf{A}]\ B] - i[i[\mathbf{c}''\cdot\mathbf{A}\ B]\ \mathbf{c}\cdot\mathbf{A}] \\ &= (b\{a(\mathbf{c})\}\mathbf{c}'')\cdot\mathbf{A} - (\{a(\mathbf{c})b\}\mathbf{c}'')\cdot\mathbf{A} \\ &= \{[ba(\mathbf{c})]\mathbf{c}''\}\cdot\mathbf{A} \end{aligned} \tag{8.4}$$

This implies

$$a(b\mathbf{c})\mathbf{c}'' = [ba]\mathbf{c}'' \tag{8.5}$$

for all $\mathbf{c}''$ and hence

$$a(b\mathbf{c}) = [ba]. \tag{6.3}$$

Thus, if $A_i = B_i$, we have a correspondence $\mathbf{c} \sim a(\mathbf{c})$, of the type of Sec. 6. The set $\mathfrak{Q}$ consists of those $\mathbf{c}$ for which

$$a(\mathbf{c}) = 0. \tag{8.6}$$

Now Eq. (8.3) implies

$$a(\mathbf{c}')\mathbf{c} = -a(\mathbf{c})\mathbf{c}'. \tag{8.7}$$

For a given $\mathbf{c}$, the transformation T_c has been defined for the set $b = a(\mathbf{c}')$ with range $\mathfrak{R}_c$ included in $\mathfrak{C}$ with

$$T_c b = \mathbf{c}'' \text{ equivalent to } b\mathbf{c} = \mathbf{c}''. \tag{8.8}$$

But by (8.7) this could be stated

$$T_c a(\mathbf{c}') = \mathbf{c}'' \text{ equivalent to } -a(\mathbf{c})\mathbf{c}' = \mathbf{c}''. \tag{8.9}$$

Thus $\mathfrak{R}_c$ is also the range of $a(\mathbf{c})$.

In Sec. 3, a number of sets were mentioned. One of these is $\mathfrak{R}_c$ which is also seen to be the range of the transformation $a(\mathbf{c})$. Another is the set $\mathfrak{S}_c$ which is defined as complementary to $\mathfrak{R}_c$ in $\mathfrak{C}$. We also have $\mathfrak{N}_c$, the set of those b's for which $b\mathbf{c} = 0$ and a set $\mathfrak{b}^*$ complementary to $\mathfrak{N}_c$ in the set of b's. The set $\mathfrak{S}_c$ and $\mathfrak{b}^*$ are not uniquely determined, but, in this case, a specific choice can be made, in terms of the structure of the transformation associated with $a(\mathbf{c})$. It will be convenient to denote both the matrix $a(\mathbf{c})$ and its associated transformation by $a(\mathbf{c})$.

The associated structure is part of the Jordan structure of $a(\mathbf{c})$. The Jordan structure of $a(\mathbf{c})$ is not available, in general, since normally some characteristic roots of $a(\mathbf{c})$ are complex. But certain constructions can be completed in the real field. Let $\phi(\lambda)$ denote the minimal polynomial for $a(\mathbf{c})$. This $\phi(\lambda)$ is a factor of the characteristic polynomial for $a(\mathbf{c})$, with leading coefficient one, characterized by the statement that $\phi\{a(\mathbf{c})\} = 0$, but no proper factor of ϕ has this property. This $\phi(\lambda)$ has real coefficients. [Note that since the elements of a are real, $\phi(a) = 0$ implies $\bar{\phi}(a) = 0$ and hence $\phi' = \frac{1}{2}(\phi + \bar{\phi})$ is of the same degree as ϕ with leading coefficient one and such that $\phi'(a) = 0$. Thus $\phi = \phi'$ which has real coefficients.] We can write $\phi(\lambda)$ as

$$\phi(\lambda) = \lambda^s \psi(\lambda) \tag{8.10}$$

where ψ does not have λ as a factor. Let $\mathfrak{M}_1$ denote the vectors $\mathbf{c}'$ such that

$$\psi\{a(\mathbf{c})\}\mathbf{c}' = 0 \tag{8.11}$$

and $\mathfrak{N}_1$ denote the set for which

$$a(\mathbf{c})^s\mathbf{c}' = 0. \tag{8.12}$$

Now $\mathfrak{M}_1$ and $\mathfrak{N}_1$ are supplementary. Furthermore $a(\mathbf{c})$ has an inverse on $\mathfrak{M}_1$ and $\mathfrak{M}_1 \subset \mathfrak{R}_c$. We also have that $a(\mathbf{c})$ takes $\mathfrak{N}_1$ into a subset $\mathfrak{N}_1'$ of itself. Thus $\mathfrak{N}_1' = \mathfrak{R}_c\cdot\mathfrak{N}_1$. We choose a $\mathfrak{S}_c$ so that $\mathfrak{S}_c \oplus \mathfrak{N}_1' = \mathfrak{N}_1$. Then

$$\mathfrak{R}_c = \mathfrak{N}_1' \oplus \mathfrak{M}_1 \tag{8.13}$$

and

$$\mathfrak{C} = \mathfrak{N}_1 \oplus \mathfrak{M}_1 = \mathfrak{S}_c \oplus \mathfrak{N}_1' \oplus \mathfrak{M}_1 = \mathfrak{S}_c \oplus \mathfrak{R}_c. \tag{8.14}$$

The set $\mathfrak{N}_c$ consists of those $b = a(\mathbf{c}')$ for which $b\mathbf{c} = 0$. In view of (8.9), this is equivalent to $a(\mathbf{c})\mathbf{c}' = 0$ and we let $\mathcal{P}_0$ consist of those $\mathbf{c}'$ for which

$$a(\mathbf{c})\mathbf{c}' = 0. \tag{8.15}$$

Clearly, $\mathcal{P}_0 \subset \mathfrak{N}_1$, by (8.12). Let $\mathcal{P}_1$ be complementary to $\mathcal{P}_0$ in $\mathfrak{N}_1$. Let $\mathcal{W} = \mathcal{P}_1 \oplus \mathfrak{M}_1$. Now $\mathcal{W}$ and $\mathcal{P}_0$ are complementary and thus if $\mathbf{c}'$ is in $\mathcal{W}$, then $a(\mathbf{c}')\mathbf{c} = -a(\mathbf{c})\mathbf{c}'' \neq 0$. Thus $\mathfrak{b}^*$ can be taken as those $b = a(\mathbf{c}')$ for $\mathbf{c}'$ is in $\mathcal{W}$.

Lemma 8.1. *For the case in which* $\mathfrak{A} = \mathfrak{B}$, *a natural mapping* $\mathbf{c} \to a(\mathbf{c})$ *of Sec.* 6 *is available. Furthermore, given* $\mathbf{c}$, *the sets* $\mathfrak{R}_c$ *and* $\mathfrak{S}_c$ *of Sec.* 3, *following* (3.2), *can be obtained by means of the sets* $\mathfrak{M}_1$ *and* $\mathfrak{N}_1$

[*cf.* (8.11) *and* (8.12)] *as follows. Let* $\mathfrak{N}_1^r = \mathfrak{R}_e \cdot \mathfrak{N}_1$. *Then* $\mathfrak{R}_e = \mathfrak{M}_1 \oplus \mathfrak{N}_1^r$ *and* $\mathfrak{S}_e$ *can be chosen as a complement to* $\mathfrak{N}_1^r$ *relative to* $\mathfrak{N}_1$.

The set $\mathfrak{N}_e$, *which has been defined in* (3.2) *as the set of b's for which* $b\mathbf{c} = 0$, *consists of those* $b = a(\mathbf{c}')$ *for which* $a(\mathbf{c})\mathbf{c}' = 0$. *Let* $\mathcal{P}_0$ *consist of the* $\mathbf{c}'$ *for which* $a(\mathbf{c})\mathbf{c}' = 0$. *Then* $\mathcal{P}_0 \subset \mathfrak{N}_1$ *and let* $\mathcal{P}_1$ *be complementary to* $\mathcal{P}_0$ *in* $\mathfrak{N}_1$. *Let* $\mathfrak{W} = \mathcal{P}_1 \oplus \mathfrak{M}_1 \subset \mathfrak{C}$. *The set* $\mathfrak{b}^*$, *which has been defined in* (3.4) *as a complementary set for* $\mathfrak{N}_e$ *can be taken as the set of b in form* $a(\mathbf{c}')$ *with* $\mathbf{c}'$ *in* $\mathfrak{W}$.

Now consider $a(\mathbf{c})$ on $\mathfrak{N}_1$. Since $a(\mathbf{c})$ is nil-potent, we can reduce $a(\mathbf{c})$ on $\mathfrak{N}_1$ to a Jordan normal form. This means we have a set of linearly independent vectors

$$\mathbf{e}_{ij}, \quad i = 1, \cdots, p, \quad j = 0, 1, \cdots, j_i, \tag{8.16}$$

which constitute a basis for $\mathfrak{N}_1$ and such that

$$a(\mathbf{c})\mathbf{e}_{ij} = \mathbf{e}_{ij-1}, \quad i = 1, \cdots, p, \quad j = 1, \cdots, j_i \tag{8.17}$$

and

$$a(\mathbf{c})\mathbf{e}_{i0} = 0, \qquad i = i, \cdots, r. \tag{8.18}$$

The $\mathbf{e}_{i0}$ can be chosen so that a subset determines $\mathfrak{Q}$ [see (8.6) and (8.7)].

We also introduce vectors

$$\text{I.} \qquad \mathbf{c}_{r+1}, \cdots, \mathbf{c}_n \tag{8.19}$$

which form a basis for $\mathfrak{M}_1$.

Although the choice of the $\mathbf{e}_{ij}$ is not unique, in general, the $\mathbf{e}_{ij}$ are easily constructed and hence permit a relatively simple statement of our results. We denote the linearly independent set of vectors (8.19) by I, and define other linearly independent vectors by

$$\begin{aligned} &\text{II.} && \mathbf{e}_{ij}, \quad j_i \geq 0, \quad j < j_i \\ &\text{III.} && \mathbf{e}_i j_i, \quad i = 1, \cdots, p \\ &\text{IV.} && \mathbf{e}_{ij}, \quad j_i > 0, \quad j \geq 1 \\ &\text{V.} && \mathbf{e}_{i_0}, \quad i = 1, \cdots, p \end{aligned} \tag{8.20}$$

Notice that II and III are disjoint and together determine $\mathfrak{N}_1$ and that a similar statement holds for IV and V. Furthermore, the set II determines $\mathfrak{N}_1^r$ by (8.17) and consequently III can be used to determine $\mathfrak{S}_e$. (It may be mentioned that for every permissible $\mathfrak{S}_e$ a normal form of the above sort can be set up with the corresponding set III determining $\mathfrak{S}_e$.) The set $\mathcal{P}_0$ is determined by the set V and a set $\mathcal{P}_1$ can be determined by IV.

Lemma 8.2. *The sets I and II determine* $\mathfrak{R}_e$. *We can take the set* $\mathfrak{S}_e$ *as that determined by III. The set V determines a linear set of vectors* $\mathbf{c}'$ *such that* $a(\mathbf{c}')$ *is in* $\mathfrak{N}_e$. *The sets I and IV determine a linear set of vectors* $\mathbf{c}'$ *such that the set of* $a(\mathbf{c}')$ *can be taken to be* $\mathfrak{b}^*$.

This lemma translates the results of Lemma 8.1 to the present situation.

Theorem. Let sets of operators $\mathfrak{A}$ *and a set* $\mathfrak{D}$ *in Hilbert space be given for which* (8.1) *and assumption I of Sec.* 2 *holds, with the* B_i *replaced by* A_i *and* $\mathfrak{B}$ *replaced by* $\mathfrak{A}$. *A correspondence* $\mathbf{c} \sim A \to a(\mathbf{c})$ *is specified by* (8.2) *and* (8.2′). *Consider then a given A and the corresponding* $\mathbf{c}$ *and* $a(\mathbf{c})$. *Let* $\phi(\lambda) = \lambda^s\psi(\lambda)$ *denote the minimal polynomial for* $a(\mathbf{c})$ [*cf.* (8.10)]. *Let* $\mathfrak{M}_1$ *denote the null manifold of* $\psi(a)$ *and* $\mathfrak{N}_1$, *the null manifold for* a^s [*cf.* (8.11) *and* (8.12)]. *Let r denote the dimension of* $\mathfrak{N}_1$. *Let* $\mathbf{c}_{r+1}, \cdots, \mathbf{c}_n$ *denote a basis for* $\mathfrak{M}_1$ [*cf.* (8.19)] *and* $\mathbf{e}_{ij}$, $i = 1, \cdots, p$, $j = 0, 1, \cdots, j_i$ *denote a basis for* $\mathfrak{N}_1$ *which corresponds to the Jordan structure of a in* $\mathfrak{N}_1$ [*cf.* (8.20)]. *We define*

$$C_i = \mathbf{c}_i \cdot \mathbf{A}, \quad i = p + 1, \cdots, n \tag{8.21}$$

$$E_{ij} = \mathbf{e}_{ij} \cdot \mathbf{A}, \; i = 1, \cdots, p, \; j = 0, \cdots, j_i \tag{8.22}$$

The C_i *and* E_{ij} *are linearly independent and together constitute a basis for the set* $A_1, \cdots, A_n$. *For each* $\eta > 0$ *a neighborhood of A can be defined as the transformations in the form*

$$A' = A + \sum x_{\alpha\beta}E_{\alpha\beta} + \sum y_\alpha C_\alpha \tag{8.23}$$

with $x_{\alpha\beta}$ *and* y_α *real and such that*

$$x_{\alpha\beta}^2 + y_\beta^2 < \eta^2. \tag{8.24}$$

Let A″ denote a transformation in the form

$$A'' = A + \sum_\alpha z_\alpha E_{\alpha j_\alpha}. \tag{8.25}$$

Let B′ denote a transformation in the form

$$B' = \sum_{\beta>0} \mu'_{\alpha\beta}E_{\alpha\beta} + \sum \mu_\alpha C_\alpha \tag{8.26}$$

and B a similar transformation without the restriction $\beta > 0$. *Then there exists an* $\eta > 0$ *such that for every A′ of* (8.23) *there exists a B′ and A″ such that on* $\mathfrak{D}$

$$\exp B'A'' \exp(-B') = A' \tag{8.27}$$

Also there is an $\eta_2 > 0$, *with the property that if* B *is such that*

$$\sum \mu_{\alpha\beta}'^2 + \sum \mu_\alpha^2 < \eta_2^2 \tag{8.28}$$

then there exists a B' *such that on* $\mathfrak{D}$

$$\exp BA \exp(-B) = \exp B'A \exp(-B') \tag{8.29}$$

Let A *be chosen so that* p *is a minimum* [*cf.* (8.20)]. *Then the* η *which determines an* A *neighborhood* [*cf.* (8.23) *and* (8.24)] *and the* η_2 *which determines a* B *neighborhood* [*cf.* (8.26) *and* (8.28)] *can be chosen so that if there is* A', A'' *in the* A *neighborhood* [*cf.* (8.23) *and* (8.25)] *and a* B *in the* B *neighborhood for which*

$$\exp BA'' \exp(-B) = A', \tag{8.30}$$

then there is also a B' [*cf.* (8.26)] *for which*

$$\exp(B')A'' \exp(-B') = A'. \tag{8.31}$$

If

$$\exp(B)A \exp(-B) = A' \tag{8.32}$$

then $a(\mathbf{c})$ *and* $a(\mathbf{c}')$ *are equivalent under a similarity. If* k *is the dimensionality of* $\mathfrak{Q}$, *the set of* $\mathbf{c}$ *for which* $a(\mathbf{c}) = 0$, *then there exists a* k' *such that* $0 \leq k' \leq k$ *such that there are* $p - k'$ *invariants of* B *equivalence which depend only on the components of the matrix* $a(\mathbf{c})$ *and these must contain all similarity invariants of the matrix* $a(\mathbf{c})$.

We next show: *The set of matrices* $a(\mathbf{c}')$ *with* $\mathbf{c}'$ *in* $\mathfrak{N}_1$ *is closed under the operation of forming the commutator.*

Proof. We can characterize the set of $\mathbf{c}'$ in $\mathfrak{N}_1$ by the property that there exists a positive integer s' such that

$$([])^{s'}a(\mathbf{c}')(a(\mathbf{c})])^{s'} = 0. \tag{8.33}$$

For by (6.3) and (8.5)

$$a\{a(\mathbf{c}')\mathbf{c}\} = [a(\mathbf{c}'), a(\mathbf{c})] = -a\{a(\mathbf{c})\mathbf{c}'\} \tag{8.34}$$

and consequently (6.3) yields

$$([])^{s'}a(\mathbf{c}')(a(\mathbf{c})])^{s'} = (-1)^{s'}a\{a(\mathbf{c})^{s'}\mathbf{c}'\}. \tag{8.35}$$

Thus if $\mathbf{c}' \in \mathfrak{N}_1$, (8.10) implies (8.33) for $s' \geq s$. Now the set of $\mathbf{c}'$ which satisfy (8.33) is a linear set. It includes $\mathfrak{N}_1$. Now if it were a proper linear extension of $\mathfrak{N}_1$, it would have an intersection with $\mathfrak{M}_1$ which contains a non-zero $\mathbf{c}'$. Since $a(\mathbf{c})$ takes $\mathfrak{M}_1$ into itself and has an inverse on $\mathfrak{M}_1$, $a(\mathbf{c})^{s'}\mathbf{c}'$ is not zero for $\mathbf{c}$ in $\mathfrak{M}_1$ and for every s'. By (8.6) and (8.7) $\mathfrak{Q}\cdot\mathfrak{M}_1$ consists simply of the zero vector and thus $a(a(\mathbf{c})^{s'}\mathbf{c}') \neq 0$. Hence (8.35) and (8.33) yield a contradiction which shows that $\mathfrak{N}_1$ is characterized by (8.33).

It is a simple consequence of the Jacobian identity that

$$([])^n[b', b'']a])^n = \sum_\alpha \binom{n}{\alpha} ([])^\alpha b'(a])^\alpha ([])^{n-\alpha} b''(a])^{n-\alpha} \tag{8.36}$$

(cf. Weyl, p. 70). This implies that if (8.33) holds for $b' = a(\mathbf{c}')$ and s' and for $b'' = a(\mathbf{c}'')$ and s'', then it holds for $[b', b'']$ and $s = s' + s''$. Since the set of $a(\mathbf{c})$ is closed under commutation, $[a(\mathbf{c}'), a(\mathbf{c}'')]$ must be in the form $a(\mathbf{c}^*)$ for which (8.33) holds and hence $\mathbf{c}^*$ must be in $\mathfrak{N}_1$. Consequently the $a(\mathbf{c}')$ with $\mathbf{c}'$ in $\mathfrak{N}_1$ are seen to form a Lie subgroup. This Lie subgroup will be called the zero group for $a(\mathbf{c})$ (cf. Weyl).

In the particular case in which the $a(\mathbf{c})$ are semi-simple, and $\mathfrak{C}$ is chosen so that p is a minimum, the zero subgroup will be Abelian, $\mathfrak{Q}$ will be $\{0\}$ and $k = 0$ (cf. Weyl, p. 86.)

Corollary. If the set of $a(\mathbf{c})$ *is a semi-simple Lie algebra and* A *is chosen so that* p *is a minimum, then the* $\sum_\alpha z_\alpha E_\alpha j_\alpha$ *coincides with* $\sum_\alpha z_\alpha E_{\alpha 0}$ *and this set constitutes an Abelian ring which contains* A. *In this case,* $k = 0$ *and every invariant is expressible in terms of the components of* $a(\mathbf{c})$.

This means that every operator of the neighborhood in the given set can be formally rotated into an operator which commutes with the original A. If A and the rotated A' have a common set of characteristic vectors, the variation in the characteristic values between these two operators is determined by the invariants. This difference is in a special case in quantum mechanics the variation of the energy due to the perturbation.

SECTION 9

There are two relatively straightforward examples available to illustrate the theory. These are based on the Hilbert space $\mathfrak{L}_2$ of summable squared functions $f(x)$ defined for $-\infty < x < \infty$. We introduce the operators q and p by the equations

$$qf = xf(x), \quad pf = i\, df/dx. \tag{9.1}$$

For the present we will ignore domain questions which have been thoroughly explored in other contexts; i.e., we will just proceed formally.

Example 1 is obtained by taking $A_0 = 1$ (the identity) $A_1 = q$, $A_2 = p$. Then $i[A_1A_2] = A_0$ and of course $i[A_0A_1] = i[A_0A_2] = 0$. We obtain a set of B_i's by letting $A_i = B_i$. If $\mathbf{c} = \{c_0, c_1, c_2\}$ denotes a vector with three components, $A = \mathbf{c}\cdot\mathbf{A}$, and $B = \mu_0A_0 + \mu_1A_1 + \mu_2A_2$, then

$$i[AB] = (c_1\mu_2 - \mu_1c_2)A_0 = (b\mathbf{c})\cdot\mathbf{A} \tag{9.2}$$

for

$$b = \begin{vmatrix} \mu_2 & 0 & 0 \\ -\mu_1 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix}. \tag{9.3}$$

Consider now a $\mathbf{c}$ for which $c_1^2 + c_2^2 > 0$. Then in terms of Sec. 3, $\mathfrak{R}_c = k\mathbf{c}_0$ and we have a complementary set to $\mathfrak{R}_c$ determined by $\mathbf{c}_1$ and $\mathbf{c}_2$. We can choose $\mathfrak{b}^*$ as the multiples of b_1 which corresponds to the B for which $\mu_2 = c_1$ and $\mu_1 = -c_2$ [see (9.3)]. Notice that $0 = b_1^2 = b_1^3 = \cdots$. It is immediately apparent that the set of $\mathbf{c}'$ equivalent to $\mathbf{c}$ is given by

$$\mathbf{c}' = \mathbf{c}\exp \mu b_1 = \{c_0 + \mu(c_1^2 + c_2^2), c_1, c_2\}. \tag{9.4}$$

Thus two, A and A' are B equivalent if and only if they differ by a multiple of A_0. The coefficients c_1 and c_2 are B invariants.

Example 2. Let

$$A_1 = 8^{-\frac{1}{2}}(-p^2),\ A_2 = 8^{-\frac{1}{2}}q^2,\ A_3 = \tfrac{1}{2}qp + \tfrac{1}{4}i. \tag{9.5}$$

We then have

$$i[A_1A_2] = A_3,\ i[A_3A_1] = A_1,\ i[A_2A_3] = A_2. \tag{9.6}$$

Thus we can use for B_1, B_2, B_3 the corresponding A_i's. If we correspond to B, the matrix b by the equation

$$[\mathbf{c}\cdot\mathbf{A}\,B] = (b\cdot\mathbf{c})\mathbf{A} \tag{9.7}$$

then

$$A_1 \simeq a_1 = \begin{vmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & 0 \end{vmatrix},$$

$$A_2 \simeq a_2 = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{vmatrix}, \tag{9.8}$$

$$A_3 \simeq a_3 = \begin{vmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{vmatrix}.$$

This is a case where we may take $a(\mathbf{c})$ equal to the corresponding b. (see Sec. 8).

$$a(\mathbf{c}) = \begin{vmatrix} -c_3 & 0 & c_1 \\ 0 & c_3 & -c_2 \\ c_2 & -c_1 & 0 \end{vmatrix}. \tag{9.9}$$

Clearly $a(\mathbf{c}) = 0$ implies $\mathbf{c} = 0$. Thus every invariant function is a function of the matrix elements and every similarity invariant of $a(\mathbf{c})$ is an equivalence invariant. The characteristic polynomial of $a(\mathbf{c})$ is

$$|a(\mathbf{c}) - \lambda| = \begin{vmatrix} -\lambda - c_3 & 0 & c_1 \\ 0 & c_3 - \lambda & -c_2 \\ c_2 & -c_1 & -\lambda \end{vmatrix} \tag{9.10}$$

$$= -\lambda^3 + (c_3^2 + 2c_1c_2)\lambda.$$

We have therefore the invariant

$$\Delta(\mathbf{c}) = c_3^2 + 2c_1c_2. \tag{9.11}$$

Notice that if $\Delta \neq 0$, 0 is a simple root. Thus the range of $a(\mathbf{c})$ which is also $\mathfrak{R}_c$ is two dimensional.

Furthermore if $\Delta(\mathbf{c}) \neq 0$, $\mathbf{c}$ is not in the range of $a(\mathbf{c})$. For suppose we can find an x, y, z such that $\mathbf{c} = a(\mathbf{c})\{x, y, z\}$ or

$$\begin{aligned} c_1 &= -c_3x + c_1z \\ c_2 &= c_3y - c_2z \\ c_3 &= c_2x - c_1y. \end{aligned} \tag{9.12}$$

If we multiply these equations by c_2, c_1, and c_3, respectively, and add, we obtain $c_3^2 + 2c_1c_2 = 0$. Thus $\mathbf{c}$ is not in the range of $a(\mathbf{c})$ and the set $\{k\mathbf{c}\}$ of multiples of $\mathbf{c}$ is a complementary manifold to $\mathfrak{R}_c$. Our result in Sec. 3 shows that there is a neighborhood of $\mathbf{c}$ such that for every $\mathbf{c}'$ in this neighborhood we have $\mathbf{c}'$ equivalent to $(1 + z)\mathbf{c}$ and if the neighborhood is taken small, z will be small. Because of the invariant character of Δ, we must have

$$\Delta(\mathbf{c}') = (1 + z)^2\,\Delta(\mathbf{c})\,. \tag{9.13}$$

Thus the $\mathbf{c}'$ with $\Delta(\mathbf{c}') = \Delta(\mathbf{c})$ in this neighborhood have $z = 0$ or $z = -2$. But the latter possibility is excluded if the neighborhood is small enough. Hence, if $\Delta(\mathbf{c}) \neq 0$ then there is a neighborhood of $\mathbf{c}$, such that all $\mathbf{c}'$ with $\Delta(\mathbf{c}') = \Delta(\mathbf{c})$ in this neighborhood are equivalent to $\mathbf{c}$. Thus if we consider the connected sheet of the surface $\Delta(\mathbf{c}') = \Delta$ which contains $\mathbf{c}$, all these $\mathbf{c}'$ are equivalent $\mathbf{c}$. It is also true that every $\mathbf{c}'$ equivalent to $\mathbf{c}$ must be connected to it by a path consisting of equivalent $\mathbf{c}''$. Thus by these rather simple arguments, we have established

Lemma 9.1. *If* $\Delta(\mathbf{c}) \neq 0$, *the set of* $\mathbf{c}'$ *equivalent*

to $\mathbf{c}$ *form the connected sheet of the surface* $\Delta(\mathbf{c}') = \Delta(\mathbf{c})$ *which contains* $\mathbf{c}$.

We must still examine the case $\Delta(\mathbf{c}) = 0$. The argument of (9.12) in this case shows that we can consider, in general, one equation to be a consequence of the other two if $\mathbf{c} \neq 0$. Now let $\mathbf{c} \neq 0$ and suppose for definiteness that c_1 is not zero. Then, by using Eqs. (9.12), we can find three vectors $\mathbf{c}_0$, $\mathbf{c}_1$, $\mathbf{c}_2$ with properties

$$\mathbf{c}_0 = \mathbf{c},\ a(\mathbf{c})\mathbf{c}_0 = 0,\ a(\mathbf{c})\mathbf{c}_1 = \mathbf{c}_0,\ a(\mathbf{c})\mathbf{c}_2 = \mathbf{c}_1. \quad (9.14)$$

In particular if we choose $\mathbf{c}_1$ and $\mathbf{c}_2$ with first component zero, we obtain

$$\begin{aligned} \mathbf{c}_1 &= \{0, -c_3/c_1, 1\} \\ \mathbf{c}_2 &= \{0, -1/c_1, 0\}. \end{aligned} \quad (9.15)$$

Equations (9.14) imply that $a(\mathbf{c})$ has a nil-potency of three and hence its range $\mathcal{R}_c$ is two dimensional and the multiples $\{z\mathbf{c}_2\}$ of $\mathbf{c}_2$ form a complementary set.

Again our basic equivalence result shows that there is a neighborhood of $\mathbf{c}$ such that every $\mathbf{c}'$ in this neighborhood is equivalent to a $\mathbf{c}''$ in the form

$$\mathbf{c}'' = \mathbf{c} + z\mathbf{c}_2 = \{c_1, c_2 - z/c_1, c_3\}.$$

Since $\Delta(\mathbf{c}) = 0$, $\Delta(\mathbf{c}'') = -2z$. Hence if $\mathbf{c}'$ in this neighborhood has $\Delta(\mathbf{c}') = 0$, then $z = 0$ and $\mathbf{c}'$ is equivalent to $\mathbf{c}$. Thus if $\Delta(\mathbf{c}) = 0$ and $c_1 \neq 0$ there is a neighborhood of $\mathbf{c}$ such that all $\mathbf{c}'$ with $\Delta(\mathbf{c}') = 0$ in this neighborhood are equivalent to $\mathbf{c}$.

If $\Delta(\mathbf{c}) = 0$ and $c_1 = 0$, then $c_3 = 0$ and $\mathbf{c} = \{0, c_2, 0\}$ with c_2 not zero. We can apply an argument similar to the above with $\mathbf{c}_0 = \mathbf{c}$, $\mathbf{c}_1 = \{0, 0, 1\}$ and $\mathbf{c}_2 = \{-1/c_2, 0, 0\}$. We obtain a neighborhood whose elements $\mathbf{c}'$ are equivalent to vectors

$$\mathbf{c}'' = \mathbf{c} + z\mathbf{c}_2 = \{-z/c_2, c_2, 0\} \quad (9.16)$$

and the previous argument clearly applies. Thus we have

Theorem. For example 2, *the set of* $\mathbf{c}'$ *equivalent to* $\mathbf{c}$ *form the connected sheet of the surface* $\Delta(\mathbf{c}') = \Delta(\mathbf{c})$ *which contains* $\mathbf{c}$. *If* $\Delta = c_3^2 + 2c_1c_2$ *is positive, the surface is simply connected. If* $\Delta < 0$, *the surface consists of two disjoint sheets. If* $\Delta = 0$, *removing* $\mathbf{c} = 0$ *divides the surface into two disjoint sets which are the nappes of a cone.*

One can readily see that $c_3^2 + 2c_1c_2 = a^2 > 0$ is a hyperboloid of revolution of one sheet while $c_3^2 + 2c_1c_2 = -a^2$ is a hyperboloid of revolution of two sheets. One also has $c_3^2 + 2c_1c_2 = 0$ is a cone with apex at the origin.

The above discussion of the second example has been directed toward illustrating the previous theoretical results. One could also calculate the results directly and this calculation would specify the unitary transformations $\exp(iB)$ which yield the equivalence. These calculations however are quite lengthy and yet do not reveal the structure of the equivalence as well as the above discussion.

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A Procedure for Estimating Eigenvalues*

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A new procedure is given for calculation of lower bounds to the eigenvalues of self-adjoint operators. Computation of the lower bounds is reduced to the solution of linear algebraic problems.

I. INTRODUCTION

In this paper we give a new procedure for the calculation of lower bounds to eigenvalues. We modify the method of intermediate problems[1] based on a comparison of operators[2] by introducing a second projection. Our procedure makes possible the determination of the lower bounds from finite, linear, algebraic computations. The inner products which appear are just those which are needed in the method of truncation.[3,4] Parts of the work presented here were previously summarized.[5]

II. INTERMEDIATE OPERATORS

We suppose A to be a self-adjoint operator in a separable Hilbert space $\mathfrak{H}$ with the inner product (u, v). We assume A is bounded below and that the initial part of its spectrum consists of eigenvalues of finite multiplicity before the first limit point of the spectrum. We denote the ordered eigenvalues by $\lambda_1, \lambda_2, \cdots$, and the corresponding ortho-normal eigenvectors by $u_1, u_2, \cdots$. If the spectrum of A contains limit points we denote the first by λ_*. We assume further that A may be decomposed as the sum of two operators

$$A = A^0 + A', \tag{1}$$

in which A^0 is a self-adjoint operator and A' is a non-negative symmetric operator. We also require that the initial spectrum of A^0 consists of at least a finite number of known eigenvalues $\lambda_1^0, \lambda_2^0, \cdots$ with corresponding known ortho-normal eigenvectors $u_1^0, u_2^0, \cdots$. We denote the first limit point of the spectrum of A^0 by λ_*^0. Denoting the domains of A, A^0, and A' by D_A, D_{A^0}, and $D_{A'}$, respectively, we have $D_A = D_{A'} \cap D_{A^0}$. Since A' is non-negative and $D_A \subset D_{A^0}$ we have

$$A^0 \leq A. \tag{2}$$

Consequently, the ordered eigenvalues of A^0 and A satisfy the inequalities,[6]

$$\lambda_i^0 \leq \lambda_i, \qquad i = 1, 2, \cdots, \tag{3}$$

and

$$\lambda_*^0 \leq \lambda_* . \tag{4}$$

In order to improve the rough lower bounds given by (3) to the eigenvalues of A, we construct a sequence[7] $\{A^k\}$ of self-adjoint operators that satisfy the inequalities $A^0 \leq A^k \leq A^{k+1} \leq A$ so that their eigenvalues give improved lower bounds.

To construct the operators A^k we introduce temporarily the inner product[8] $[u, v]$ defined by $[u, v] = (A'u, v)$ on the elements of $D_{A'}$. Let P^k be the projection with respect to this inner product on the span of the first k vectors of a given sequence $\{p_1, p_2, \cdots\}$ of linearly independent elements of $D_{A'}$. The projection P^k has the explicit representation

$$P^k v = \sum_{i,j=1}^{k} [v, p_i] b_{ij} p_j, \tag{4}$$

where b_{ij} are the elements of the matrix inverse to that with elements $[p_i, p_j]$. For any vector v in $D_{A'}$ the operator $A'P^k v$ is given by

$$A'P^k v = \sum_{i,j=1}^{k} (v, A'p_i) b_{ij} A'p_j. \tag{5}$$

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[2] N. Aronszajn, *Proceedings of the Symposium on Spectral Theory and Differential Problems* (Oklahoma A & M, Stillwater, Oklahoma, 1951) (reprinted in 1955), p. 179.

[3] N. W. Bazley and D. W. Fox, J. Research Natl. Bur. Standards **65B**, 105 (1961).

[4] N. W. Bazley and D. W. Fox, Phys. Rev. **124** 483 (1961).

[5] N. W. Bazley and D. W. Fox, Am. Math. Soc. Notices **8**, 151 (1961).

[6] If A^0 has but n eignevalues before λ_*^0, then we also have that $\lambda_*^0 \leq \lambda_i$ for every $i > n$.

[7] Here we follow the construction of Aronszajn.[2]

[8] We assume here that A' is positive definite; the extension to the semidefinite case is easily made.

Since P^k is a projection we have

$$0 \leq [P^k v, v] \leq [P^{k+1} v, v] \leq [v, v]. \tag{6}$$

It is clear from (5) that $A'P^k$ may be extended by continuity to all of $\mathfrak{H}$. There it is a symmetric operator of finite rank and from (6) satisfies

$$0 \leq A'P^k \leq A'P^{k+1} \leq A'. \tag{7}$$

The operators A^k are now defined by

$$A^k = A^0 + A'P^k; \tag{8}$$

they are clearly self-adjoint, have domains D_{A^k} equal to D_{A^0}, and satisfy the desired inequalities,

$$A^0 \leq A^k \leq A^{k+1} \leq A. \tag{9}$$

Their eigenvalues λ_i^k satisfy the parallel inequalities,

$$\lambda_i^0 \leq \lambda_i^k \leq \lambda_i^{k+1} \leq \lambda_i. \tag{10}$$

The difficulties in the determination of the spectrum of A^k have been discussed elsewhere.[2,3] In order to overcome these difficulties we introduce here smaller operators $A^{l,k}$ of which the spectra can be determined by finite algebraic computations.

III. INTRODUCTION OF A SECOND PROJECTION

For each positive number γ, the operator A^k may be rewritten

$$A^k = [A^0 - \gamma] + [A'P^k + \gamma].$$

Since $A'P^k + \gamma$ is greater than γ, we may introduce for each γ and k a new inner product $\langle u, v \rangle$ defined by

$$\langle u, v \rangle = ([A'P^k + \gamma]u, v) \tag{11}$$

on the elements of $\mathfrak{H}$. Let Q^l be the projection with respect to this inner product on the span of the first l vectors of a given sequence $\{q_1, q_2, \cdots\}$ of linearly independent elements of $\mathfrak{H}$. It follows by arguments similar to those used in establishing (7) that for fixed k and γ

$$0 \leq [A'P^k + \gamma]Q^l \leq [A'P^k + \gamma]Q^{l+1} \leq A'P^k + \gamma. \tag{12}$$

The operators $[A'P^k + \gamma]Q^l$ are bounded, symmetric, and of finite rank. They have the explicit representation

$$[A'P^k + \gamma]Q^l u = \sum_{m,n=1}^{l} (u, [A'P^k + \gamma]q_m) c_{mn} [A'P^k + \gamma]q_n, \tag{13}$$

where c_{mn} are elements of the matrix inverse to that with elements $([A'P^k + \gamma]q_m, q_n)$. We now define the operators $A^{l,k}$ by

$$A^{l,k} = [A^0 - \gamma] + [A'P^k + \gamma]Q^l. \tag{14}$$

It follows that these operators have domains $D_{A^{l,k}}$ equal to D_{A^0} and satisfy the inequalities

$$A^0 - \gamma \leq A^{l,k} \leq A^{l+1,k} \leq A^k \leq A. \tag{15}$$

Their eigenvalues $\lambda_i^{l,k}$ satisfy the parallel inequalities

$$\lambda_i^0 - \gamma \leq \lambda_i^{l,k} \leq \lambda_i^{l+1,k} \leq \lambda_i^k \leq \lambda_i. \tag{16}$$

Conditions sufficient to insure the convergence of the eigenvalues of A^k to those of A have been given by Aronszajn.[2] These conditions also suffice to ensure the convergence of the eigenvalues of $A^{l,k}$ to those of A^k when the q's are complete in $\mathfrak{H}$. Thus under these assumptions the eigenvalues of $A^{l,k}$ converge to those of A as l and k become large.

IV. DETERMINATION OF THE SPECTRUM OF $A^{l,k}$

In general, the determination of the spectrum of $A^{l,k}$ for arbitrarily given elements $q_1, q_2, \cdots, q_l$ is as difficult as that for A^k itself. However, the operator $A^{l,k}$ has been constructed so that a "special choice"[3,9] of the q's is always possible.

In fact, since $[A'P^k + \gamma]^{-1}$ may be regarded as an explicitly known operator[10] on $\mathfrak{H}$, we may make the choice of elements

$$q_i = [A'P^k + \gamma]^{-1} u_i^0, \qquad i = 1, 2, \cdots, l. \tag{17}$$

With this it follows from (13) and (14) that the operator $A^{l,k}$ has the form

$$A^{l,k}u = [A^0 - \gamma]u + \sum_{m,n=1}^{l} (u, u_m^0) c_{mn} u_n^0, \tag{18}$$

where the c_{mn} are now elements of the matrix inverse to that with elements $(u_m^0, [A'P^k + \gamma]^{-1}u_n^0)$.

We observe that the subspace $\mathfrak{M}$ of $\mathfrak{H}$ spanned by $u_1^0, u_2^0, \cdots, u_l^0$ now reduces the operator $A^{l,k}$, and that $A^{l,k}u$ equals $A^0u - \gamma u$ for u orthogonal to $\mathfrak{M}$. Since this is true, $A^{l,k}$ has the same spectrum as $A^0 - \gamma$ on this orthogonal complement. The spectrum of $A^{l,k}$ is completely determined by finding its eigenvectors of the form

$$u = \sum_{i=1}^{l} \beta_i u_i^0. \tag{19}$$

This leads to the algebraic eigenvalue problem

$$\sum_{i=1}^{l} \beta_i [(\lambda_i^0 - \gamma)\, \delta_{ij} + c_{ij} - \lambda\, \delta_{ij}] = 0, \qquad j = 1, 2, \cdots, l. \tag{20}$$

[9] N. W. Bazley, J. Math. Mech. 10, 289 (1961).
[10] See Sec. V.

The eigenvalues $\lambda_i^{l,k}$ are found by ordering those found from (20) with $\lambda_{l+1}^0 - \gamma$, $\lambda_{l+2}^0 - \gamma$, $\cdots$. These give improved lower bounds according to (16).

V. THE OPERATOR $[A'P^k + \gamma]^{-1}$

An expression for $[A'P^k + \gamma]^{-1}$ can be obtained from its spectral resolution. In fact, from the expression,

$$[A'P^k + \gamma]v = \sum_{i,j=1}^{k} (v, A'p_i)b_{ij}A'p_j + \gamma v, \tag{21}$$

it is clear that the subspace of $\mathfrak{H}$ spanned by $A'p_1$, $A'p_2$, $\cdots$, $A'p_k$ reduces $A'P^k + \gamma$. Consequently $A'P^k + \gamma$ has γ as an eigenvalue of infinite multiplicity with characteristic subspace all vectors orthogonal to $A'p_1$, $\cdots$, $A'p_k$. The remaining eigenvalues, $\mu_1 + \gamma$, $\mu_2 + \gamma$, $\cdots$, $\mu_k + \gamma$, all greater than γ, and the corresponding normalized eigenvectors, v_1, v_2, $\cdots$, v_k, are obtained by putting

$$v = \sum_{i=1}^{k} d_i A'p_i, \tag{22}$$

and lead to the algebraic system

$$0 = \sum_{i=1}^{k} d_i[(A'p_i, A'p_j) - \mu(A'p_i, p_j)], \qquad j = 1, 2, \cdots, k. \tag{23}$$

Hence

$$[A'P^k + \gamma]^{-1}u = \sum_{i=1}^{k} \frac{(u, v_i)v_i}{\mu_i + \gamma} + \frac{1}{\gamma}\left[u - \sum_{i=1}^{k} (u, v_i)v_i\right]. \tag{24}$$

The matrix c_{mn} of (18) is just that inverse to the matrix with elements

$$\frac{1}{\gamma}\left\{\delta_{mn} - \sum_{i=1}^{k} \frac{\mu_i}{\mu_i + \gamma}(u_m^0, v_i)(v_i, u_n^0)\right\}, \tag{25}$$

where the v_i's and μ_i's are determined from (22) and (23).

An alternative expression for the matrix given in (25) was suggested to the authors by W. Börsch-Supan. It is

$$\frac{1}{\gamma}\left\{\delta_{mn} - \sum_{i,j=1}^{k} (u_m^0, A'p_i)\, d_{ij}(\gamma)(A'p_j, u_n^0)\right\}, \tag{26}$$

where $d_{ij}(\gamma)$ is the matrix inverse to that with elements $(A'p_i, A'p_j) + \gamma(A'p_i, p_j)$. This expression follows directly from (25) or from initial considerations. The expression (25) requires the explicit solution of the algebraic eigenvalue problem (23); the expression (26) requires the inversion of a $k \times k$ matrix for each value of γ.

VI. DEPENDENCE ON γ

In this section we consider the dependence of the operator $A^{l,k}$ on the parameter γ when the elements q_i are chosen according to (17). First we show that $A^{l,k}$ is monotonically increasing in γ on the space $\mathfrak{M}$ spanned by u_1^0, u_2^0, $\cdots$, u_l^0. In fact, on $\mathfrak{M}$ this operator may be represented by the matrix $\Lambda^0 - \gamma I + C$, where Λ^0 is the diagonal matrix of eigenvalues of A^0, I the identity, and C the matrix introduced in Eq. (18). To demonstrate the monotonicity we show that the matrix,

$$(d/d\gamma)[\Lambda^0 - \gamma I + C] = -I - C(dC^{-1}/d\gamma)C, \tag{27}$$

is positive, or equivalently that

$$-dC^{-1}/d\gamma \geq C^{-2}. \tag{28}$$

Since C is inverse to the matrix having elements $(u_i^0, [A'P^k + \gamma]^{-1}u_j^0)$, it follows that

$$(dC^{-1}/d\gamma)_{ij} = -(u_i^0, [A'P^k + \gamma]^{-2}u_j^0) = -(q_i, q_j). \tag{29}$$

The inequality between quadratic forms corresponding to the matrix inequality (28) may be written

$$\sum_{i,j=1}^{l} \alpha_i\bar{\alpha}_i(q_i, q_j) \geq \sum_{i,j,m=1}^{l} \alpha_i\bar{\alpha}_i(q_i, u_m^0)(u_m^0, q_j). \tag{30}$$

Setting v equal to $\sum_{i=1}^{l} \alpha_i q_i$, (30) becomes

$$(v, v) \geq \sum_{m=1}^{l} (v, u_m^0)(u_m^0, v), \tag{31}$$

which is Bessel's inequality.

The monotonicity of $A^{l,k}$ on $\mathfrak{M}$ implies that the ordered eigenvalues of the matrix problem (20) are also monotonically increasing in γ. Examination of the matrices involved also shows that as γ approaches zero these eigenvalues approach λ_1^0, λ_2^0, $\cdots$, λ_l^0, and as γ approaches infinity they approach the Rayleigh-Ritz upper bounds to the operator $A^0 + A'P^k$ obtained with the trial vectors u_1^0, u_2^0, $\cdots$, u_l^0.

Since $A^{l,k}$ equals $A^0 - \gamma$ on the orthogonal complement of $\mathfrak{M}$, it is there monotonically decreasing in γ and has eigenvalues $\lambda_{l+1}^0 - \gamma$, $\lambda_{l+2}^0 - \gamma$, $\cdots$. Thus for each l and k, the best value of γ for the estimation of λ_ν ($\nu \leq l$) is that value for which $\lambda_{l+1}^0 - \gamma$ is equal to the νth eigenvalue of the matrix problem (20). Suitable choices of γ may be obtained from other (possibly experimental or nonrigorous) estimates of λ_ν.

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A Note on Perturbation Theory in Nearly Periodic Systems

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It is shown that for a particle in periodic or nearly periodic motion, an integrated form of the equations of motion may be the better starting point for an approximate calculation of the orbit. The motion of a charged particle in a static, inhomogeneous magnetic field is used to illustrate how this approach avoids the difficulty of the spurious secular terms to all orders of the approximation.

INTRODUCTION

SINCE there exists no general method capable of yielding exact solutions to nonlinear differential equations, one is usually forced to employ approximate methods. One nonlinear equation frequently encountered in physics is the simple harmonic oscillator equation with a small nonlinear term added. The solutions to such equations cannot differ much from those of the corresponding linear equation, i.e., they must be periodic or nearly periodic. With the nonlinear term small, it would seem natural to try a solution in the form of a power series in the parameter of smallness and to solve the resulting equation order by order, as was done by Poisson and by Poincaré.[1] The zeroth order term would be the solution of the linear equation, which is harmonic in time, t, i.e., of the form $\sin \omega t$. The difficulty with this approach is the appearance in the nth order of the series of so-called secular terms of the form $t^n \sin \omega t$, terms which seem to grow indefinitely, but which in fact arise from an expansion of terms periodic in time. The astronomers Gylden and Lindstedt[2] found a way to eliminate such secular terms in each order of the expansion, and applied their method to problems in celestial mechanics. More recently Krylov and Bogoliubov[3] have adapted this procedure to the theory of nonlinear oscillations.

The purpose of this note is to point out that in dealing with motion which is periodic or nearly periodic, an integrated form of the equations of motion may be the better starting point for an approximate calculation of the orbit. An example is given below to illustrate how this approach avoids the difficulty of spurious secular terms.

[1] H. Poincaré, *Les méthodes nouvelles de la mécanique céleste* (Gauthier-Villars, Paris, 1892), Vol. I.
[2] A. Lindstedt, Mem. Acad. Impériale Sci. St. Petersbourg **31** (1883).
[3] N. Krylov and N. Bogoliubov, *Introduction to Non-Linear Mechanics* (Kiev, U. S. S. R., 1937), in Russian; English version by S. Lefschetz (Princeton University Press, Princeton, New Jersey, 1943).

MOTION IN THE MAGNETIC FIELD: $B(x, y)\mathbf{e}_z$

1. General Results

Let us consider the motion of a nonrelativistic particle of mass m and charge q in the static, inhomogeneous magnetic field, $\mathbf{B} = B(x, y)\mathbf{e}_z$, where $\mathbf{e}_z$ is the unit vector in the z direction. We shall not be concerned with the motion along the z direction, which is unaffected by the magnetic field. Introducing the Larmor frequency, $\Omega(x, y) = qB(x, y)/mc$, the equations of motion take the form:

$$\ddot{x} = \Omega(x, y)\dot{y}, \tag{1}$$

$$\ddot{y} = -\Omega(x, y)\dot{x}, \tag{2}$$

where the dot represents the time derivative. Alternatively the orbit, $x(t')$, $y(t')$, of the particle which at time $t' = t$ has the position x, y and the velocity $\dot{x}$, $\dot{y}$, may be obtained from the integral equations:

$$\int_t^{t'} dt'' \Omega\{x(t''), y(t'')\}\dot{x}(t'') = \dot{x} \sin \tau(t') + \dot{y}\{1 - \cos \tau(t')\}, \tag{3}$$

$$\int_t^{t'} dt'' \Omega\{x(t''), y(t'')\}\dot{y}(t'') = \dot{y} \sin \tau(t') - \dot{x}\{1 - \cos \tau(t')\}, \tag{4}$$

where

$$\tau(t') = \int_t^{t'} dt'' \Omega\{x(t''), y(t'')\}. \tag{5}$$

The integrals in Eqs. (3)–(5) are along the (unknown) particle orbit $x(t'')$, $y(t'')$.

Let us now restrict ourselves to the case

$$\Omega(x, y) = \Omega_0 + \Omega_1(x, y), \tag{6}$$

where Ω_0 is a constant and $|\Omega_1(x, y)| \ll \Omega_0$ for all x, y. While Ω_1 is small in magnitude, no restriction is placed on its derivative, i.e., Ω_1 may vary rapidly over distances of the order of the Larmor radius. Approximate solutions to the equations of motion of charged particles in slowly varying electric and magnetic fields have been developed by Alfvén[4] and more recently by Bogoliubov and Zubarev[5] and by Kruskal.[6] In these treatments the assumption is made that the magnetic field may be represented by: $\mathbf{B}(\mathbf{r}) = \mathbf{B}(\mathbf{r}_0) + (\mathbf{r} - \mathbf{r}_0)\cdot\nabla\mathbf{B}(\mathbf{r}_0)$, over distances from $\mathbf{r}_0$ greater than the Larmor radius. We do not restrict ourselves in this way here.

If we base our perturbation theory on Eqs. (1) and (2), secular terms of the form $t^n \sin \Omega_0 t$ and $t^n \cos \Omega_0 t$ show up in the n'th order. These may of course be eliminated by the method of Krylov and Bogoliubov.[3] However, if we proceed from the integral equations (3) and (4), it is possible to develop a systematic approximation in which spurious terms never appear. With Eq. (6) we may rewrite Eqs. (3) and (4) as follows:

$$\Omega_0\{x(t') - x\} = \dot{x}\sin\tau(t') + \dot{y}\{1 - \cos\tau(t')\} - \int_t^{t'} dt''\Omega_1\{x(t''), y(t'')\} \times [\dot{x}\cos\tau(t'') + \dot{y}\sin\tau(t'')], \quad (7)$$

$$\Omega_0\{y(t') - y\} = \dot{y}\sin\tau(t') - \dot{x}\{1 - \cos\tau(t')\} - \int_t^{t'} dt''\Omega_1\{x(t''), y(t'')\} \times [\dot{y}\cos\tau(t'') - \dot{x}\sin\tau(t'')]. \quad (8)$$

In the last terms of Eqs. (7) and (8) we have inserted the expressions for $\dot{x}(t')$ and $\dot{y}(t')$, which result upon differentiating Eqs. (3) and (4) with respect to t'. To the zeroth order in Ω_1 Eqs. (7) and (8) yield the circular orbit $x_0(t')$, $y_0(t')$:

$$\Omega_0\{x_0(t') - x\} = \dot{x}\sin\tau_0(t') + \dot{y}\{1 - \cos\tau_0(t')\}, \quad (9)$$

$$\Omega_0\{y_0(t') - y\} = \dot{y}\sin\tau_0(t') - \dot{x}\{1 - \cos\tau_0(t')\}, \quad (10)$$

$$\tau_0(t') = \Omega_0(t' - t). \quad (11)$$

The form of Eqs. (7) and (8) immediately suggests the following n'th order approximation, $x_n(t')$, $y_n(t')$, to the orbit:

$$\Omega_0\{x_n(t') - x\} = \dot{x}\sin\tau_n(t') + \dot{y}\{1 - \cos\tau_n(t')\} - \int_t^{t'} dt''\Omega_1\{x_{n-1}(t''), y_{n-1}(t'')\} \times [\dot{x}\cos\tau_{n-1}(t'') + \dot{y}\sin\tau_{n-1}(t'')], \quad (12)$$

$$\Omega_0\{y_n(t') - y\} = \dot{y}\sin\tau_n(t') - \dot{x}\{1 - \cos\tau_n(t')\} - \int_t^{t'} dt''\Omega_1\{x_{n-1}(t''), y_{n-1}(t'')\} \times [\dot{y}\cos\tau_{n-1}(t'') - \dot{x}\sin\tau_{n-1}(t'')], \quad (13)$$

$$\tau_n(t') = \Omega_0(t' - t) + \int_t^{t'} dt''\Omega_1\{x_{n-1}(t''), y_{n-1}(t'')\}. \quad (14)$$

We see that $x_n(t')$ and $y_n(t')$ are expressed as periodic functions of $\tau_n(t')$ plus integrals involving Ω_1. These integrals will be periodic in time only if Ω_1 is itself a periodic function. In general the orbit is not truly periodic, but since the integrands in Eqs. (12)–(14) are bounded functions of t'', the corresponding integrals cannot increase faster than linearly in time. The possibility of a term linear in $(t' - t)$ corresponds to the well-known drift of charged particles in inhomogeneous magnetic fields. Such "secular" terms are real; however, the nonphysical secular terms of the form $t^n \sin \Omega_0 t$, $n > 1$ never appear. This is what we intended to show. From Eqs. (12) and (13) it is clear why terms of the form $t^n \sin \Omega_0 t$ must show up in a solution which is a power series in Ω_1, since such a solution would involve an expansion of $\sin \tau_n$ and $\cos \tau_n$.

2. First-Order Results

It is perhaps of interest to study the first-order orbit, $x_1(t')$, $y_1(t')$, in some detail. For simplicity we shall henceforth assume that Ω_1 depends on only one space variable, say x. Let us also introduce the cylindrical velocity coordinates, v and ϕ,

$$\dot{x} = v\cos\phi, \qquad \dot{y} = v\sin\phi, \quad (15)$$

and the center of gyration, x_c, y_c,

$$x_c = x + \dot{y}/\Omega_0, \qquad y_c = y - \dot{x}/\Omega_0, \quad (16)$$

in terms of which the zeroth-order orbit may be rewritten as follows:

$$\Omega_0\{x_0(t') - x_c\} = v\sin[\Omega_0(t' - t) - \phi], \quad (17)$$

$$\Omega_0\{y_0(t') - y_c\} = v\cos[\Omega_0(t' - t) - \phi]. \quad (18)$$

Turning to the first-order orbit, let us first examine τ_1, which we write:

$$\tau_1(t') = \Omega_0(t' - t) + \Delta\tau_1(t'), \quad (19)$$

[4] H. Alfvén, *Cosmical Electrodynamics* (Clarendon Press, Oxford, England, 1950).

[5] N. Bogoliubov and D. Zubarev, Ukrain. Mat. Zhur **7**, 5 (1955). Translation by B. D. Fried available as a Space Technology Laboratories Report (1960).

[6] M. Kruskal, *Proceedings of the Third International Conference on Ionization Phenomena in Gases* (Venice, 1957), or AEC Report NYO-7903 (1958).

where by Eq. (14)

$$\Delta\tau_1(t') = \int_t^{t'} dt''\Omega_1\{x_0(t'')\}. \tag{20}$$

We now Fourier analyze $\Omega_1(x)$, substitute for $x_0(t'')$ from Eq. (17), and carry out the integration over t''. The result is:

$$\Delta\tau_1(t') = \int_{-\infty}^{\infty} dk\Omega_1(k)e^{ikx_c}\Big\{(t' - t)J_0\Big(\frac{kv}{\Omega_0}\Big) + \sum_{n\neq 0} J_n\Big(\frac{kv}{\Omega_0}\Big)e^{-in\phi}(in\Omega_0)^{-1}(e^{in\Omega_0(t'-t)} - 1)\Big\}, \tag{21}$$

where $\Omega_1(k)$ is the Fourier transform of $\Omega_1(x)$ and where we have used the standard symbols, J_n, for Bessel's functions. The sum in Eq. (21) is periodic in t', whereas the first term is linear in time. Thus we have found a first-order frequency shift from Ω_0, given by:

$$\Delta\Omega = \int_{-\infty}^{\infty} dk\Omega_1(k)e^{ikx_c}J_0\Big(\frac{kv}{\Omega_0}\Big). \tag{22}$$

Employing a well-known integral representation for J_0, the integration over k may be carried out, yielding:

$$\Delta\Omega = \pi^{-1}\int_0^{\pi} d\theta\Omega_1(x_c + v\Omega_0^{-1}\cos\theta), \tag{23}$$

which illustrates that $\Delta\Omega$ is just the average of $\Omega_1(x)$ over the zero-order orbit.

The expression for $y_1(t')$ is obtained from Eq. (13):

$$\Omega_0(y_1(t') - y_c) = v\cos\{\tau_1(t') - \phi\} - \int_t^{t'} dt''\Omega_1\{x_0(t'')\}\dot{y}_0(t''), \tag{24}$$

where we have used the variables introduced in Eqs. (15) and (16). The first term on the right-hand side of Eq. (24) is periodic in time. In order to evaluate the other term, we again Fourier decompose $\Omega_1(x)$, substitute for $x_0(t'')$ and $\dot{y}_0(t'')$ from Eqs. (17) and (18), and integrate over t'':

$$-\int_t^{t'} dt''\Omega_1\{x_0(t'')\}\dot{y}_0(t'') = v\int_{-\infty}^{\infty} dk\Omega_1(k)e^{ikx_c}\Big\{i(t' - t)J_1\Big(\frac{kv}{\Omega_0}\Big) + \sum_{n\neq 0} J_n'\Big(\frac{kv}{\Omega_0}\Big)(n\Omega_0)^{-1}e^{-in\phi}(1 - e^{in\Omega_0(t'-t)})\Big\}, \tag{25}$$

where $J_n'(z) \equiv (d/dz)J_n(z)$. All terms in Eq. (25) are periodic in time, except the first, which represents a drift in the y direction with a velocity, v_d, given by:

$$v_d = iv\Omega_0^{-1}\int_{-\infty}^{\infty} dk\Omega_1(k)e^{ikx_c}J_1\Big(\frac{kv}{\Omega_0}\Big) = v\Omega_0^{-1}\pi^{-1}\int_0^{\pi} d\theta\cos\theta\Omega_1(x_c + v\Omega_0^{-1}\cos\theta). \tag{26}$$

A similar calculation of $x_1(t')$ shows it to be periodic in t', or, as expected, that there is no drift in the x direction when Ω_1 is independent of y.

Finally we note that if $\Omega_1(x)$ varies slowly over distances of the order of the Larmor radius, v/Ω_0, Eq. (26) may be approximated by:

$$v_d = \frac{v}{\Omega_0}\int_0^{\pi}\frac{d\theta}{\pi}\cos\theta\Big[\Omega_1(x_c) + \frac{d\Omega_1}{dx_c}\frac{v}{\Omega_0}\cos\theta\Big] = \frac{1}{2}\Big(\frac{v}{\Omega_0}\Big)^2\frac{d\Omega}{dx_c}, \tag{27}$$

which is the usual first-order orbit theory result.[4]

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Stochastic Models for Many-Body Systems. I. Infinite Systems in Thermal Equilibrium*

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Some model Hamiltonians are proposed for quantum-mechanical many-body systems with pair forces. In the case of an infinite system in thermal equilibrium, they lead to temperature-domain propagator expansions which are expressible by closed, formally exact equations. The expansions are identical with infinite subclasses of terms from the propagator expansion for the true many-body problem. The two principal models introduced correspond, respectively, to ring and ladder summations from the true propagator expansion, but augmented by infinite classes of self-energy corrections. The latter are expected to yield damping of single-particle excitations. The eigenvalues of the ring and ladder model Hamiltonians are real, and they are bounded from below if the pair potential obeys certain conditions. The models are formulated for fermions, bosons, and distinguishable particles. In addition to the ring and ladder models, two simpler types are discussed, one of which yields the Hartree-Fock approximation to the true problem. A novel feature of all the model Hamiltonians (except the Hartree-Fock) is that they contain an infinite number of parameters whose phases are fixed by random choices. Explicit closed expressions are obtained for the Helmholtz free energy of all the models in the classical limit.

1. INTRODUCTION

A DIFFICULTY in calculating the statistical behavior of many-body systems is that some quantities of interest may not have convergent perturbation expansions. If the system is infinite in size, this can occur even when the density of particles is very low and the interparticle forces are very weak. The situation is already present in the classical theory. Consider a gas of classical particles which interact by a repulsive, short-range pair-potential $\lambda V(\mathbf{x})$. If the pressure, expressed as a function of density and temperature, is expanded in powers of the strength parameter λ, the expansion has zero radius of convergence.[1] This suggests that a similar situation may exist in the quantum-mechanical case.

Nonconvergence of interaction-strength expansions is not necessarily a disaster. In the classical example just cited, the expansion almost certainly is asymptotic about $\lambda = 0$, and we may hope that this is true also in some quantum-mechanical cases. However, many physical problems of interest do not exhibit weak interactions. Moreover, certain properties of a quantum-mechanical many-body system may not have even asymptotic expansions as power-series in λ. An example is the one-particle momentum distribution $\sigma(\mathbf{k})$, normalized to unity. For an infinite system, a finite change in $\sigma(\mathbf{k})$ from its form for uncoupled particles means that an *infinite* number of particles are displaced from the momentum levels they would occupy if they were not coupled. In order to form such a state from the uncoupled state, the interaction Hamiltonian must act an infinite number of times; that is, infinite orders of perturbation theory are involved. We expect on physical grounds that the change in $\sigma(\mathbf{k})$ goes to zero as λ does. However, we cannot presume that it must go to zero as some integral power of λ.

In recent years, several formalisms for handling perturbation expansions in the quantum-mechanical many-body problem have been proposed which are related to methods previously used in quantum electrodynamics.[2-10] They produce great simplifications in manipulations and permit one to carry out various formal summations of infinite classes

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[1] One way to obtain this result is the following. Take $\lambda < 0$ (pure *attractive* potential). Then every diagram in the irreducible cluster expansion for pressure gives a negative contribution. The total number of diagrams of order n increases with n faster than any exponential, and a consequence is that the pressure comes out negatively infinite no matter how small $|\lambda|$ is. (Physically, this means the system will collapse.) On the other hand, for $\lambda > 0$, the pressure must approach the perfect gas value as $|\lambda| \to 0$. Therefore the pressure is a nonanalytic function of λ at $\lambda = 0$. [Cf. T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1119 (1957).]

[2] T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955).

[3] E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).

[4] C. Bloch and C. De Dominicis, Nuclear Phys. **7**, 459 (1958).

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[7] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).

[8] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

[9] D. N. Zubarev, Uspekhi Fiz. Nauk. **71**, 71 (1960) [translation: Soviet Phys.—Uspekhi **3**, 320 (1960)].

[10] Extensive further bibliography is given in references 7 and 9.

of terms from the perturbation expansions. These formalisms are a natural choice for investigating quantities, such as $\sigma(\mathbf{k})$, which may not have convergent or asymptotic expansions. However, it can be difficult to know in advance what summations should be carried out in given cases. With sufficient ingenuity, it is possible to sum certain divergent series so as to obtain almost any answer whatever. It is difficult to guess in advance whether adding further infinite classes of terms to a known expansion will improve the answer or make it worse.

In the present paper we shall describe a procedure intended to pick out perturbation-term summations for which certain characteristics are predictable in advance. We shall formulate model Hamiltonians such that the *complete* perturbation expansions to which they lead are formally identical with certain infinite subclasses of terms from the corresponding perturbation expansion for the true Hamiltonian. The model Hamiltonians are Hermitian, conserve momentum, and have eigenvalues which are bounded from below if the pair potential obeys certain restrictions. The predictable characteristics of the model solutions are, first, some general consistency properties which follow automatically from the fact that the solutions describe actual Hamiltonians exactly. These include positive-definiteness of the one-particle energy-momentum distribution function, for example. The further predictable characteristics are those which follow from the boundedness and conservation properties.

In common with the true many-body Hamiltonian, our models (with one exception) are not diagonalizable by known means. They are soluble only in the sense that they yield formally closed integral equations for the propagators that determine the mean energies, mean occupation numbers, etc., which are of statistical-mechanical interest. A feature of the models is that they contain infinite numbers of parameters whose values are chosen at random. We shall therefore call them stochastic models. The random parameters will be described in Secs. 2 and 3.

We shall present two principal types of stochastic models, ladder and ring. They correspond, respectively, to summations of familiar infinite classes of ladder or ring diagrams from the perturbation series for the true Hamiltonian. At the same time, they include certain infinite classes of self-energy corrections to these diagrams. The corrections are of a type expected to contribute to the damping of elementary excitations. In addition to the ladder and ring models, we shall introduce two simpler types. One yields the Hartree-Fock approximation to the true problem (and contains no random parameters). The other also includes the Hartree-Fock diagrams, but with iterated self-energy corrections. The eigenvalues of this last model are not bounded from below for any pair potential, and its validity therefore is quite doubtful.

The models which are described in the present paper yield closed equations only for infinite systems. We shall develop each type of model in two forms: for indistinguishable particles (fermions and bosons) and for distinguishable particles. The analytical treatment will begin with the distinguishable particle models. They admit more immediate physical interpretations. We shall apply to them the Ursell-Mayer irreducible cluster expansion method and thereby obtain an explicit closed expression for the Helmholtz free energy of each model in the classical limit. For the fermion and boson models, we shall use a temperature-domain propagator formalism of the type originated by Matsubara[2] and developed further by Fradkin,[5] Abrikosov *et al.*,[6] Luttinger and Ward,[8] and others. The distinguishable and indistinguishable particle models turn out to give formally identical thermodynamics in the classical limit. Thus, our classical results for the Helmholtz free energy provide some insights into the behavior of the fermion and boson models.

In the paper which follows,[11] we develop more general models which yield closed equations whatever the size of the system. We shall apply them to nonequilibrium as well as equilibrium statistical mechanics. For an infinite system in equilibrium, the generalized models yield the same final equations as the models of the present paper. However, they provide a neater and more satisfactory derivation of these equations. We do not start with the general treatment in the present paper because it requires a more elaborate formalism and therefore does not provide as direct an introduction to the use of the stochastic models.

The derivation of our closed model equations involves a deep-lying convergence question which is described in Sec. 5.1. We make no attempt to answer this question in the present paper. In the following paper, we offer what we hope is a satisfying, although nonrigorous, resolution.

2. MODELS FOR DISTINGUISHABLE PARTICLES

2.1. Nature of the Models

Let us consider a system of N similar but distinguishable particles (of unit mass) which interact

[11] R. H. Kraichnan, J. Math. Phys. **3**, 496 (1962).

through a pair potential $V(\mathbf{x})$. The total Hamiltonian may be written

$$H = \tfrac{1}{2}\sum_n \mathbf{p}_n^2 + \tfrac{1}{2}\sum_{n,m}{}' V(\mathbf{x}_n - \mathbf{x}_m) \qquad (n, m = 1, 2, \cdots, N), \qquad (2.1)$$

where $\sum'$ means that $n = m$ is omitted in the sum. Here $\mathbf{p}_n$ and $\mathbf{x}_n$ are the momentum and position of the nth particle. We shall adopt the artifice of confining the system in a cubical cyclic box of volume Ω. That is, we restrict $V(\mathbf{x})$ to the form

$$V(\mathbf{x}) = \sum_{\mathbf{k}} V_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}), \qquad (2.2)$$

where $\mathbf{k}$ takes all the values allowed by cyclic boundary conditions on the walls of the box, and we require that the Schrödinger wave function be a cyclic function of the coordinates of each particle. In the classical case, we assume that a particle which exits through any wall of the box simultaneously re-enters, with the same momentum, through the opposite wall. We shall eventually be interested in the limit $N \to \infty$, $\Omega \to \infty$, with N/Ω finite.

We require that $V(\mathbf{x})$ be real and have reflectional symmetry. These conditions imply

$$V(\mathbf{x}) = V(-\mathbf{x}), \quad V_{\mathbf{k}} = V_{-\mathbf{k}}, \quad V_{\mathbf{k}} = V_{\mathbf{k}}^*. \qquad (2.3)$$

Except where we specify otherwise, we shall assume that $V(\mathbf{x})$ is a smooth, bounded function such that

$$|V_{\mathbf{k}}| = O(\Omega^{-1}), \qquad \Omega \to \infty \quad (\text{all } \mathbf{k}),$$
$$|V_{\mathbf{k}}| \leq O(k^{-2}), \qquad k \to \infty.$$

In particular, this implies that $\int V(\mathbf{x})\, d^3x$ and $\int [V(\mathbf{x})]^2\, d^3x$ exist for $\Omega \to \infty$, where the integration is over the whole box.

We shall call (2.1) the true Hamiltonian, and refer to the statistical mechanical problem associated with it as the true problem.

Now let us consider model Hamiltonians of the form

$$H = \tfrac{1}{2}\sum_n \mathbf{p}_n^2 + \tfrac{1}{2}\sum_{n,m}{}' V^{n,m}(\mathbf{x}_n - \mathbf{x}_m), \qquad (2.4)$$

where $V^{n,m}(\mathbf{x})$ is a pair potential which may be different for each pair of particles n and m. We require that $V^{n,m}(\mathbf{x})$ be real, and we replace (2.3) by

$$V^{n,m}(\mathbf{x}) = V^{m,n}(-\mathbf{x}). \qquad (2.5)$$

Let us write

$$V^{n,m}(\mathbf{x}) = \sum_{\mathbf{k}} V_{\mathbf{k}}^{n,m} \exp(i\mathbf{k}\cdot\mathbf{x}) \qquad (2.6)$$

and define the parameters $\phi_{n,m;\mathbf{k}}$ by

$$V_{\mathbf{k}}^{n,m} = V_{\mathbf{k}}\phi_{n,m;\mathbf{k}}. \qquad (2.7)$$

Then the reality condition and (2.5) imply

$$\phi_{n,m;\mathbf{k}} = \phi_{n,m;-\mathbf{k}}^*, \qquad \phi_{n,m;\mathbf{k}} = \phi_{m,n;-\mathbf{k}}. \qquad (2.8)$$

The true problem, of course, corresponds to $\phi_{n,m;\mathbf{k}} = 1$ for all n, m, and $\mathbf{k}$. In the models with which we shall be concerned here, all the $\phi_{n,m;\mathbf{k}}$ will be assigned unit modulus (except in the Hartree-Fock model where most of them will vanish). However, for each triad n, m, $\mathbf{k}$ the phase of $\phi_{n,m;\mathbf{k}}$ will be assigned by a random choice, subject to (2.8), and to additional constraints which differ for each model. As we shall see, the models so produced have certain properties in common with the true Hamiltonian but lead to a statistical mechanics that can be expressed in closed form in the limit $\Omega \to \infty$.

2.2. Ladder Model

Let us specialize $\phi_{n,m;\mathbf{k}}$ to the form

$$\phi_{n,m;\mathbf{k}} = \exp(-i\mathbf{k}\cdot\mathbf{d}_{n,m}), \qquad \mathbf{d}_{n,m} = -\mathbf{d}_{m,n}, \qquad (2.9)$$

where the $\mathbf{d}_{n,m}$ are constant, real vectors. This clearly satisfies (2.8). Now, for each pair n, m let us give the three vector-components of $\mathbf{d}_{n,m}$ values chosen at random within the interval $(0, L)$, where $L = \Omega^{\frac{1}{3}}$. The choices are to be completely independent for pairs which are not identical. In the x representation, we have

$$V^{n,m}(\mathbf{x}) = V(\mathbf{x} - \mathbf{d}_{n,m}), \qquad (2.10)$$

which permits a very simple interpretation of this model: The pair potential has the same shape as in the true problem, but the particles now collide with ghosts of each other, displaced by the randomly chosen vectors $\mathbf{d}_{n,m}$. For reasons which will appear later, we shall call this the ladder model.

An important feature of the ladder model is immediately apparent from (2.10). If $V(\mathbf{x})$ is non-negative for all $\mathbf{x}$, then $V^{n,m}(\mathbf{x})$ also has this property. It follows that in this case the expectation of H in any quantum-mechanical state is non-negative, or, in other words, that all the eigenvalues of H are non-negative.

At this point, we want to make as clear as possible the precise sense in which our model is stochastic. The values of the $\mathbf{d}_{n,m}$ are chosen at random [subject to (2.9)]. Once chosen, however, they are fixed, and we work thereafter with the definite Hamiltonian embodying these values. In particular, the same choice of the $\mathbf{d}_{n,m}$ will be employed for every member of the canonical or grand canonical ensemble which we use in describing the statistical mechanics of the system. The principal deductions

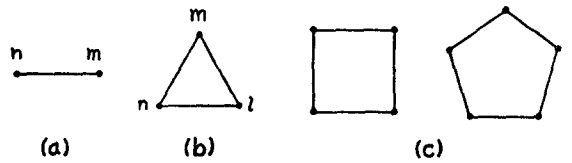

FIG. 1. Some irreducible cluster diagrams.

we shall make about the statistical mechanics of the model will be valid only for *typical assignments* of values for the $\mathbf{d}_{n,m}$, a situation which is familiar in stochastic problems. [Thus $\mathbf{d}_{n,m} = 0$ (all n, m) is a possible result of a random assignment of values, but it is not typical. The probability of this assignment vanishes with extreme rapidity as $N \to \infty$.] Instead of restricting ourselves to typical assignments, we could equivalently employ a statistical distribution of assignments and make our deductions about averages over the distribution. Such a procedure would have some formal advantages, but we feel that the analysis will be clearer if we do not introduce this additional kind of average.

We wish now to investigate the equilibrium thermodynamics of our model in the classical limit. The virial expansion of the Helmholtz free energy per particle for the true problem may be written

$$A = A_0 - \beta^{-1} \sum_{\alpha=1}^{\infty} (\alpha + 1)^{-1} \rho^{\alpha} B_{\alpha}. \tag{2.11}$$

Here $A_0 = \beta^{-1} \{\ln [\rho(2\pi\hbar^2\beta)^{\frac{3}{2}}] - 1\}$ is the Helmholtz function for free particles, ρ is N/Ω, B_{α} is the Mayer irreducible cluster integral for a cluster of $\alpha + 1$ particles, and $\beta = 1/kT$, where k is Boltzmann's constant and T is absolute temperature. Equation (2.11) is formally exact in the limit Ω, $N \to \infty$. In the true problem it makes no difference, of course, which of the N particles are assumed to be in the cluster for which B_{α} is calculated; the interaction of all pairs is identical. If the derivation is retraced with a model potential $V^{n,m}(\mathbf{x})$, it is found that (2.11) is still valid provided that B_{α} is reinterpreted in the following way: It is the average value of the cluster integral when the latter is calculated for all possible choices of the $\alpha + 1$ particles from among the N particles in the system.[12]

Let us write

$$f(\mathbf{x}) = \exp [-\beta V(\mathbf{x})] - 1,$$
$$f^{n,m}(\mathbf{x}) = \exp [-\beta V^{n,m}(\mathbf{x})] - 1. \tag{2.12}$$

Then the model cluster integral B_1 [Fig. 1(a)] is

$$B_1 = N^{-2}\Omega^{-1} \sum_{n,m}{}' \iint f^{n,m}(\mathbf{x}_n - \mathbf{x}_m)\, d^3x_n\, d^3x_m, \tag{2.13}$$

where the integrations are over Ω, and we have replaced $N(N-1)$ by N^2 in anticipation of the limit $N \to \infty$. In the ladder model we have

$$f^{n,m}(\mathbf{x}) = f(\mathbf{x} - \mathbf{d}_{n,m}).$$

Therefore, since $V(\mathbf{x})$ is cyclic, we find

$$B_1 = \int f(\mathbf{x})\, d^3x, \tag{2.14}$$

which is identical with the result for the true problem.

Let us now assume that $V(\mathbf{x})$ has a finite range r_0 and is negligible for $|\mathbf{x}| > r_0$. (Here $\mathbf{x}$ is measured modulo displacement by a cyclic period.) The next irreducible cluster integral [Fig. 1(b)] is

$$B_2 = N^{-3}\Omega^{-2} \sum_{n,m,l}{}' \iiint f^{n,m}(\mathbf{x}_n - \mathbf{x}_m) f^{m,l}(\mathbf{x}_m - \mathbf{x}_l) \times f^{l,n}(\mathbf{x}_l - \mathbf{x}_n)\, d^3x_n\, d^3x_m\, d^3x_l. \tag{2.15}$$

Contributions to this integral can arise only from points which simultaneously satisfy

$$|\mathbf{x}_n - \mathbf{x}_m - \mathbf{d}_{n,m}| \leq r_0, \qquad |\mathbf{x}_m - \mathbf{x}_l - \mathbf{d}_{m,l}| \leq r_0,$$
$$|\mathbf{x}_l - \mathbf{x}_n - \mathbf{d}_{l,n}| \leq r_0. \tag{2.16}$$

However, since the $\mathbf{d}_{n,m}$ have been fixed by random choices, and have values which range over the entire cyclic volume, it will be impossible to satisfy (2.16) for most triads n, m, l. In fact, given a typical assignment of the $\mathbf{d}$'s, it is clear that (2.16) can be satisfied only for a fraction of all triads which is of order r_0^3/Ω. It follows that B_2 vanishes as r_0^3/Ω in the limit $\Omega \to \infty$, $N \to \infty$. Similar considerations show that any given B_{α} ($\alpha > 1$) also vanishes in the limit. The contribution to B_{α} of each irreducible cluster diagram with $\alpha + 1$ particles and γ links vanishes as $(r_0^3/\Omega)^{\gamma-\alpha}$. Actually, the condition we placed on $V(\mathbf{x})$ is stronger than needed to obtain this result. It is sufficient that $f(\mathbf{x})$ be bounded and that $\int |f(\mathbf{x})|\, d^3x$ be finite in the limit.

On the basis of the preceding paragraph, let us assume that the total contribution to (2.11) from *all* B_{α} ($\alpha > 1$) vanishes in the limit. This is a nontrivial assumption. It involves a deep-lying convergence question which we shall discuss, in its quantum-mechanical form, in Sec. 5.1, and at length in the following paper. The essential point is that the number of irreducible diagrams of order α is enormous for $\alpha \sim O(N)$. For the present, we shall simply adopt the assumption. An equivalent assump-

[12] See the Appendix.

tion will be implicit in the discussion of the further classical models of Sec. 2. Retaining, then, only B_1 in the limit, we have

$$A - A_0 = \beta^{-1}a(\beta)\rho, \tag{2.17}$$

where $-2a(\beta)$ is the right side of (2.14). The corresponding equation of state is

$$p = \beta^{-1}\rho[1 + a(\beta)\rho], \tag{2.18}$$

where we define the pressure by the relation $p = \rho^2 (\partial A/\partial\rho)_\beta$.

Equations (2.17) and (2.18) exhibit several properties of interest. First, we note that if $V(\mathbf{x})$ is non-negative everywhere, then $A - A_0$ is non-negative for all β and goes to zero as $\beta \to \infty$. This is consistent with our previous finding that the model potential energy is always non-negative for such $V(\mathbf{x})$.[13] The present result provides some reassurance as to the validity of our formal procedures. A second property shows up most clearly if we take $V(\mathbf{x})$ to be a hard-sphere potential of range r_0. Then we have $a(\beta) = \frac{2}{3}\pi r_0^3$. Now if we increase ρ without limit, we see that, in contrast to the true problem, the ladder model exhibits no saturation; the free energy and pressure continue to rise smoothly.[14]

A third fact of interest is that if $V(\mathbf{x})$ is negative anywhere, we have $\beta^{-1}a(\beta) \to -\infty$ as $\beta \to \infty$. Thus we have $A \to -\infty$ for any ρ, which indicates that there is no lower bound to the potential energy per particle. Furthermore, we have $(\partial p/\partial\rho)_\beta < 0$, for any given ρ, if the temperature is low enough. This suggests that the system then would be unstable to collapse, and, since there is no saturation, that the collapse would be catastrophic once it occurred.[15] In the case of potentials with an attractive part, the ladder model offers the possibility of a valid approximation to the true problem only above a critical temperature for each ρ. It should be viewed with suspicion even above this temperature.

It is clear from (2.17) and (2.18) that the ladder model represents an extremely rudimentary approximation to the classical true problem. The interest of these results lies in the fact that they represent classical limits for the fermion and boson ladder models which we shall introduce in Sec. 3. These models are nontrivial. A similar interest attaches to the further classical results to be presented in the remainder of Sec. 2.

2.3. Ring Model

Instead of adopting (2.9), let us now specialize $\phi_{n,m;\mathbf{k}}$ to the form

$$\phi_{n,m;\mathbf{k}} = \exp[i(\theta_{n;\mathbf{k}} + \theta_{m;-\mathbf{k}})], \tag{2.19}$$

$$\theta_{n;\mathbf{k}} = -\theta_{n;-\mathbf{k}}, \tag{2.20}$$

where the $\theta_{n;\mathbf{k}}$ are real phases. Again we see that (2.8) is satisfied. Let us give the $\theta_{n;\mathbf{k}}$ values chosen at random in the interval $(0, 2\pi)$. The choice is to be made independently for each pair of indices n, $\mathbf{k}$, subject only to (2.20). We shall call the result the ring model, for reasons which will become clear shortly. It represents a rather more drastic mutilation of the true Hamiltonian than does the ladder model. Because the phases $\theta_{n;\mathbf{k}}$ fluctuate randomly as $\mathbf{k}$ changes, the present $V^{n,m}(\mathbf{x})$ are strange potentials which spread out irregularly over the entire cyclic cube.

The ring-model Hamiltonian also has a boundedness property in common with the true Hamiltonian, but a different one than we noted for the ladder model. Let us formally define a self-interaction potential by extending (2.6), (2.7), and (2.19), without change, to the case $n = m$. Then we may rewrite the model interaction Hamiltonian in the form

$$H_i = \tfrac{1}{2}\sum_{n,m} V^{n,m}(\mathbf{x}_n - \mathbf{x}_m) - \tfrac{1}{2}NV(0), \tag{2.21}$$

where the summation now *admits* $n = m$. Using (2.6), (2.19), and (2.20), we find

$$H_i = \tfrac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{k}}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^* - \tfrac{1}{2}NV(0), \tag{2.22}$$

where

$$\rho_{\mathbf{k}} = \sum_n \exp[i(\mathbf{k}\cdot\mathbf{x}_n + \theta_{n;\mathbf{k}})]. \tag{2.23}$$

Now suppose that $V_{\mathbf{k}}$ is non-negative for all $\mathbf{k}$. Then $\sum_{\mathbf{k}} V_{\mathbf{k}}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*$ is a non-negative operator, and it follows that the expectation of the potential energy per particle in any quantum-mechanical state is bounded from below by $-\frac{1}{2}V(0)$.

In the true problem all the $\theta_{n;\mathbf{k}}$ are zero, and $\rho_{\mathbf{k}}$ is a density-operator Fourier component, as introduced by Pines and Bohm[16] and others. In the ring model, we may call $\rho_{\mathbf{k}}$ an effective density component.

The conditions $V(\mathbf{x}) \geq 0$ (all $\mathbf{x}$) and $V_{\mathbf{k}} \geq 0$ (all $\mathbf{k}$) are not mutually exclusive, but they do not

[13] As $\beta \to \infty$, we have $A_0 \to 0$, and at zero temperature A becomes just the potential energy per particle.

[14] The following may make clear how this can happen. Take Ω finite (but $\gg r_0^3$) and place an arbitrarily large number of particles into the cube in any desired positions $\mathbf{x}_n$. Whatever the number of particles, and whatever their positions, it is clear that for every pair n, m there will be many possible choices of $\mathbf{d}_{n,m}$ such that $|\mathbf{x}_n - \mathbf{x}_m - \mathbf{d}_{n,m}| > r_0$.

[15] This statement must be carefully qualified. See the Appendix for a discussion of the condition $(\partial p/\partial\rho)_\beta < 0$.

[16] D. Pines and D. Bohm, Phys. Rev. **85**, 338 (1952).

imply each other. The bounds we have derived therefore suggest that the ladder and ring models have inequivalent domains of validity. Consider, for example, the modified Coulomb potential

$$V_{\mathbf{k}} = \Omega^{-1}4\pi e^2 \exp(-a\,|\mathbf{k}|)k^{-2} \quad (|\mathbf{k}| \geq 1/l), \qquad V_{\mathbf{k}} = 0 \quad (|\mathbf{k}| < 1/l), \tag{2.24}$$

where a and l provide, respectively, a short-range and long-range cutoff. $V_{\mathbf{k}}$ is non-negative and $V(0)$ is finite. Thus the ring model Hamiltonian has a finite lower bound per particle and may be expected to yield healthy results. On the other hand, $V(\mathbf{x}) \geq 0$ is not satisfied for large x, and we cannot make a similar prediction for the ladder model.

If we let $l \to \infty$, then $V(0)$ approaches a finite limit, and we conclude that the long-range character of the Coulomb potential should not pose difficulties for the ring model. In the limit $a \to 0$, however, we have $-\frac{1}{2}V(0) \to -\infty$. In the true problem, the $V_{\mathbf{k}}$ for very high k give a purely repulsive contribution to $V(\mathbf{x})$ and cannot actually cause H_i to be unbounded from below. In the ring model, however, the very high k give rise to attractive as well as repulsive regions in the $V^{n,m}(\mathbf{x})$, because of the fluctuating phases of the $V_{\mathbf{k}}^{n,m}$. Thus we may anticipate trouble in the limit $a \to 0$. We shall see shortly that it actually occurs, at least in the classical case.

The B_α may be evaluated for the ring model by expanding the $f^{n,m}(\mathbf{x})$ as power series in $-\beta$, expanding the $V^{n,m}(\mathbf{x})$ in Fourier series, and then performing the space integrations. We thereby find

$$B_1 = \Omega N^{-2} \sum_{n,m}{}' [-V_0^{n,m} + \tfrac{1}{2}(-\beta)^2 \sum_{\mathbf{k}} V_{\mathbf{k}}^{n,m} V_{-\mathbf{k}}^{n,m} + (1/3!)(-\beta)^3 \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}}^{n,m} V_{\mathbf{k}'}^{n,m} V_{-\mathbf{k}-\mathbf{k}'}^{n,m} + \cdots]. \tag{2.25}$$

By (2.19) and (2.20), we find

$$V_0^{n,m} = V_0, \qquad V_{\mathbf{k}}^{n,m} V_{-\mathbf{k}}^{n,m} = V_{\mathbf{k}} V_{-\mathbf{k}}.$$

Thus the first two terms on the right side of (2.25) are unaffected by the averaging over n and m. All the higher terms, however, involve phases which fluctuate randomly as n and m are varied, except when all the summed indices $\mathbf{k}$, $\mathbf{k}'$, $\cdots$ are either equal and opposite in pairs or zero. The consequence is that none of the higher terms makes a contribution to B_1 in the limit $N \to \infty$, $\Omega \to \infty$.

We shall illustrate by considering the term containing $(-\beta)^3$. The random phase of the summand is

$$(\theta_{n;\mathbf{k}} + \theta_{m;\mathbf{k}}) + (\theta_{n;\mathbf{k}'} + \theta_{m;-\mathbf{k}'}) + (\theta_{n;-\mathbf{k}-\mathbf{k}'} + \theta_{m;\mathbf{k}+\mathbf{k}'}).$$

By (2.20), this expression vanishes for $\mathbf{k} = 0$, $\mathbf{k}' = 0$, or $\mathbf{k} + \mathbf{k}' = 0$. However, it follows readily from the restrictions on $V(\mathbf{x})$, stated after (2.3), that the total contribution to B_1 from these restricted wave-vector combinations vanishes in the limit. For the remaining wave-vector combinations, the phase of the summand changes at random with change of n and m. For a given $\mathbf{k}$ and $\mathbf{k}'$, the averaging over n and m therefore reduces the contribution to B_1 by a factor $\sim N^{-1} = 1/\sqrt{(N^2)}$ from its value in the true problem. The consequence is that the total contribution of the $(-\beta)^3$ term vanishes in the limit. Similar arguments show that all the higher terms vanish also. Thus we have

$$B_1 = \Omega[-\beta V_0 + \tfrac{1}{2}\beta^2 \sum_{\mathbf{k}} (V_{\mathbf{k}})^2], \tag{2.26}$$

where we note $V_{\mathbf{k}} = V_{-\mathbf{k}}$. In obtaining (2.26), we use the fact that the expansion of $f^{n,m}(\mathbf{x})$ in powers of $-\beta$ is absolutely convergent for all β, if $V(\mathbf{x})$ obeys the restrictions imposed after (2.3).

The higher B_α may be evaluated by similar analysis. The result is that the only irreducible Mayer diagrams which give nonvanishing contributions in the limit are the ring diagrams, the first three of which are shown in Figs. 1(b) and 1(c). The surviving contributions from the ring diagrams give

$$B_\alpha = \tfrac{1}{2} \sum_{\mathbf{k}} (-\beta)^{\alpha+1} \Omega^\alpha (V_{\mathbf{k}})^{\alpha+1} \quad (\alpha \geq 2). \tag{2.27}$$

The surviving contributions arise as the products of the terms $\propto -\beta$ in the expansions of all the f factors occurring in the ring diagram integrands. To see how they survive, consider Fig. 1(b). The surviving contribution from this diagram is

$$\tfrac{1}{2}N^{-3} \sum_{n,m,l}{}' \sum_{\mathbf{k}} (-\beta)^3 \Omega^2 V_{\mathbf{k}}^{n,m} V_{\mathbf{k}}^{m,l} V_{\mathbf{k}}^{l,n},$$

and the phase of the summand is

$$(\theta_{n;\mathbf{k}} + \theta_{m;-\mathbf{k}}) + (\theta_{m;\mathbf{k}} + \theta_{l;-\mathbf{k}}) + (\theta_{l;\mathbf{k}} + \theta_{n;-\mathbf{k}}),$$

which vanishes by (2.20).

Inserting (2.26) and (2.27) in (2.11), and performing the sum over α,[17] we find

$$A - A_0 = \tfrac{1}{2}\rho\Omega V_0 - \tfrac{1}{2}(\beta\rho)^{-1}\Omega^{-1} \sum_{\mathbf{k}} [\beta\rho\Omega V_{\mathbf{k}} - \ln(1 + \beta\rho\Omega V_{\mathbf{k}})]. \tag{2.28}$$

It is of interest to compare (2.28) with the well-

[17] E. W. Montroll and J. E. Mayer, J. Chem. Phys. 9, 626 (1941).

known result

$$A - A_0 = -\tfrac{1}{2}\rho\beta^{-1}\Omega f_0 - \tfrac{1}{2}(\beta\rho)^{-1}\Omega^{-1} \cdot \sum_{\mathbf{k}} [-\rho\Omega f_{\mathbf{k}} - \ln(1 - \rho\Omega f_{\mathbf{k}}) - \tfrac{1}{2}\rho^2\Omega^2 f_{\mathbf{k}}^2], \quad (2.29)$$

where $f_{\mathbf{k}}$ is defined by

$$f(\mathbf{x}) = \sum_{\mathbf{k}} f_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}),$$

which Montroll and Mayer[17] obtained by summing all the ring diagrams for the true problem. We shall find that (2.28), and not (2.29), represents the classical limit of the quantum-mechanical ring summation to be carried out in Sec. 4.[18]

From (2.28), we see that $A - A_0$ is bounded from below ($V_{\mathbf{k}} \geq 0$) by

$$-\tfrac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{k}} = -\tfrac{1}{2}V(0),$$

which agrees with the rigorous bound we have previously found for the ring-model potential energy. As in the case of the ladder model, this provides some reassurance as to the validity of our formal procedure. It is clear that if $V_0 = 0$, then $A - A_0$ will actually approach the absolute lower bound as $\beta \to \infty$. [The ln term in (2.28) gives a vanishing contribution in this limit.]

If $V_{\mathbf{k}}$ is given by (2.24), we find that $A - A_0$ converges in the limit $l \to \infty$ and/or $\beta \to \infty$. This supports our anticipation that the long-range part of the potential should not pose difficulties for the ring model. It should be noted that the derivation of (2.28) with potential (2.24) requires that l be kept finite until after the limit $\Omega \to \infty$ is taken. Otherwise, the assumption $V_{\mathbf{k}} = O(\Omega^{-1})$ is violated for very low k.

If now we take $a = 0$, we find $A - A_0 \to -\infty$ as $\beta \to \infty$. Thus, as we anticipated might be so, the ring model is not an admissible approximation in this case. The situation may be substantially improved in the quantum theory, however.

2.4. Random-Coupling and Hartree-Fock Models

We wish now to examine two simpler distinguishable-particle models. In common with the ladder and ring models, they are of interest because their classical thermodynamics represents limits for corresponding fermion and boson models.

Let us now specialize $\phi_{n,m;\mathbf{k}}$ to the form

$$\phi_{n,m;\mathbf{k}} = \exp(i\theta_{n,m;\mathbf{k}}), \quad (2.30)$$

with

$$\theta_{n,m;\mathbf{k}} = -\theta_{m,n;\mathbf{k}}, \qquad \theta_{n,m;\mathbf{k}} = -\theta_{n,m;-\mathbf{k}}, \quad (2.31)$$

where the $\theta_{n,m;\mathbf{k}}$ are real phases. Again (2.8) is satisfied. Let us give the $\theta_{n,m;\mathbf{k}}$ values in the interval $(0, 2\pi)$ determined by independent, random choices for all the combinations of indices, subject only to (2.31). We shall call this the random-coupling model.

There appears to be no lower bound to the potential energy per particle in the random coupling model if we take the limit $N \to \infty$. Consequently, we cannot be sure that the model has any thermodynamic validity. We shall return to this question in a moment.

The B_α for the random-coupling model may be determined by the same formal procedure as we used for the ring model. The result is that B_1 has the value (2.26) and that all the higher B_α vanish in the limit $N \to \infty$, $\Omega \to \infty$. The results for A and p are

$$A - A_0 = \tfrac{1}{2}\rho\Omega V_0 - \tfrac{1}{4}\rho\beta\Omega \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \quad (2.32)$$

and

$$p = \beta^{-1}\rho + \tfrac{1}{2}\rho^2\Omega V_0 - \tfrac{1}{4}\beta\rho^2\Omega \sum_{\mathbf{k}} V_{\mathbf{k}}^2. \quad (2.33)$$

If (2.17) is expanded in powers of $-\beta$, and then expressed in terms of Fourier coefficients, it is easy to verify that (2.32) represents that part of (2.17) which is also contained in (2.28). That is to say, the only contributions to A which survive in the random-coupling model are those which survive in both the ladder and ring models.

From (2.33) we see that if ρ and β are high enough we have $(\partial p/\partial\rho)_\beta < 0$, regardless of the form of $V(\mathbf{x})$. The instability to collapse, thereby indicated,[15] is associated with the lack of a lower bound to the model potential energy. However, if ρ and β are low enough, (2.33) suggests that the random-coupling model may have a stable thermodynamics. We choose to regard that indication with caution.

Our final model is the Hartree-Fock model, which we construct by taking

$$V_0^{n,m} = V_0, \qquad V_{\mathbf{k}}^{n,m} = 0 \qquad (\mathbf{k} \neq 0). \quad (2.34)$$

This is a zeroth model in the sense that there are no randomly chosen parameters at all. It corresponds simply to having each particle move in the uniform potential obtained by averaging the true fields of the other particles over all possible configurations. Only B_1 is nonvanishing in the limit

[18] Our result also resembles (except for the term $\frac{1}{2}\rho\Omega V_0$) the classical limit of a quantum-mechanical ring summation given in reference 3 [Eq. (5.14) of that reference]. However, that summation is based on an activity rather than a density expansion. It corresponds to a sum of pure ring diagrams from the primitive (reducible) classical cluster expansion.

$\Omega \to \infty$, and we have

$$A - A_0 = \tfrac{1}{2}\rho\Omega V_0. \tag{2.35}$$

3. MODELS FOR FERMIONS AND BOSONS

3.1. Nature of the Models

The models described in Sec. 2 involve interaction potentials which are different for different pairs of particles. They are therefore meaningless for indistinguishable particles. In order to construct stochastic models for fermion and boson systems, let us replace (2.1) by the second-quantized true Hamiltonian

$$H = H_0 + H_i, \qquad H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} q_{\mathbf{k}}^\dagger q_{\mathbf{k}}, \tag{3.1}$$

$$H_i = \tfrac{1}{2} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}}\, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q_{\mathbf{k}}^\dagger q_{\mathbf{p}}^\dagger q_{\mathbf{r}} q_{\mathbf{s}}. \tag{3.2}$$

Here $q_{\mathbf{k}}^\dagger$ and $q_{\mathbf{k}}$ are fermion or boson creation and destruction operators for momentum $\mathbf{k}$, $\epsilon_{\mathbf{k}}$ is the free-particle energy $\frac{1}{2}k^2$, and we take $\hbar = 1$. The commutation relations are

$$[q_{\mathbf{k}}, q_{\mathbf{p}}]_{\mp} = 0, \qquad [q_{\mathbf{k}}, q_{\mathbf{p}}^\dagger]_{\mp} = \delta_{\mathbf{kp}}, \tag{3.3}$$

where the plus sign is for fermions and the minus for bosons.

As the general model interaction Hamiltonian, we take

$$H_i = \tfrac{1}{2} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}} \phi_{\mathbf{kprs}}\, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q_{\mathbf{k}}^\dagger q_{\mathbf{p}}^\dagger q_{\mathbf{r}} q_{\mathbf{s}}, \tag{3.4}$$

where the $\phi_{\mathbf{kprs}}$ are c-number parameters which play a role analogous to that of the $\phi_{n,m;\mathbf{k}}$. We leave H_0 unaltered. In correspondence to (2.8), we impose the conditions

$$\phi_{\mathbf{kprs}} = \phi_{\mathbf{srpk}}^*, \qquad \phi_{\mathbf{kprs}} = \phi_{\mathbf{pksr}}. \tag{3.5}$$

The first of these relations ensures the Hermiticity of H_i. The second is suggested by the invariance of (3.2) to the 'particle exchange' $(\mathbf{k}, \mathbf{s}) \rightleftarrows (\mathbf{p}, \mathbf{r})$.

We shall obtain the fermion and boson versions of the ladder, ring, random-coupling, and Hartree-Fock models by making specialized stochastic assignments of values to the $\phi_{\mathbf{kprs}}$. The $\phi_{\mathbf{kprs}}$ will all have unit modulus in the models we shall examine here, except in the Hartree-Fock model, where most of the $\phi_{\mathbf{kprs}}$ will vanish. In Secs. 4 and 5 we shall develop an appropriate propagator formalism for the fermion and boson models and find closed equations which determine the propagators for each model. We shall put off until Sec. 6 a demonstration of the relations among the fermion, boson, and distinguishable-particle models.

3.2. Ladder Model

To construct the fermion or boson ladder model, we take

$$\phi_{\mathbf{kprs}} = \exp\,[i(-\theta_{\mathbf{pk}} + \theta_{\mathbf{rs}})], \tag{3.6}$$

with

$$\theta_{\mathbf{kp}} = \theta_{\mathbf{pk}}. \tag{3.7}$$

We then determine the real phase $\theta_{\mathbf{kp}}$ for each pair $\mathbf{k}$, $\mathbf{p}$ by a random choice in the interval $(0, 2\pi)$. The choices are all independent, subject only to (3.7).

Let us define the quantities

$$\begin{aligned} \chi(\mathbf{x}', \mathbf{x}) &= \Omega^{-1} \sum_{\mathbf{rs}} q_{\mathbf{r}} q_{\mathbf{s}} \\ &\quad \times \exp\,[i(\mathbf{r}\cdot\mathbf{x}' + \mathbf{s}\cdot\mathbf{x} + \theta_{\mathbf{rs}})], \\ \chi^\dagger(\mathbf{x}', \mathbf{x}) &= \Omega^{-1} \sum_{\mathbf{rs}} q_{\mathbf{s}}^\dagger q_{\mathbf{r}}^\dagger \\ &\quad \times \exp\,[-i(\mathbf{r}\cdot\mathbf{x}' + \mathbf{s}\cdot\mathbf{x} + \theta_{\mathbf{rs}})]. \end{aligned} \tag{3.8}$$

In the true problem (all $\theta_{\mathbf{rs}} = 0$), $\chi(\mathbf{x}', \mathbf{x})$ is simply the two-particle amplitude $\psi(\mathbf{x}')\psi(\mathbf{x})$, where $\psi(\mathbf{x})$ is the destruction field in x space. We may call $\chi(\mathbf{x}', \mathbf{x})$ the effective two-particle amplitude in the ladder model. By straightforward Fourier analysis, we find

$$H_i = \tfrac{1}{2} \iint V(\mathbf{x} - \mathbf{x}')\chi^\dagger(\mathbf{x}', \mathbf{x})\chi(\mathbf{x}', \mathbf{x})\, d^3x\, d^3x'. \tag{3.9}$$

If $V(\mathbf{x}) \geq 0$ for all $\mathbf{x}$, H_i is a positive-definite operator, and it follows that the eigenvalues of H are all non-negative. This is the same bound which we obtained in Sec. 2 for the distinguishable-particle ladder model.

It is not obvious that the present model will be an admissible approximation to the true problem if $V(\mathbf{x})$ is a hard-sphere potential, although this was clearly the case for the distinguishable-particle ladder model. A sufficient condition for admissibility would appear to be that the relation

$$\chi(\mathbf{x}', \mathbf{x}) \mid \Phi\rangle = 0, \qquad (|\mathbf{x} - \mathbf{x}'| \leq r_0), \tag{3.10}$$

where r_0 is the hard-sphere diameter, be satisfied for as rich a manifold of states Φ in the model as in the true problem. We have not investigated this question.

3.3. Ring Model

To construct the fermion or boson ring model, we take

$$\phi_{\mathbf{kprs}} = \exp\,[i(\bar{\theta}_{\mathbf{ks}} + \bar{\theta}_{\mathbf{pr}})], \tag{3.11}$$

where

$$\bar{\theta}_{\mathbf{ks}} = -\bar{\theta}_{\mathbf{sk}}. \tag{3.12}$$

We fix the real phases $\bar{\theta}_{\mathbf{ks}}$ by random choices in the interval $(0, 2\pi)$, subject only to (3.12).

In analogy to (2.23), let us introduce the effective density-component operators

$$\rho_{\mathbf{m}} = \sum_{\mathbf{k}} q_{\mathbf{k}}^{\dagger} q_{\mathbf{k+m}} \exp(i\bar{\theta}_{\mathbf{k},\mathbf{k+m}}). \tag{3.13}$$

By (3.12), they satisfy $\rho_{\mathbf{m}} = \rho_{-\mathbf{m}}^{\dagger}$. It follows from (3.3) and (3.12) that for either fermions or bosons the ring model H_i may be rewritten

$$H_i = \tfrac{1}{2} \sum_{\mathbf{k}} V_{\mathbf{k}} \rho_{\mathbf{k}}^{\dagger} \rho_{\mathbf{k}} - \tfrac{1}{2} V(0) N, \tag{3.14}$$

where

$$N = \sum_{\mathbf{k}} N_{\mathbf{k}}, \qquad N_{\mathbf{k}} = q_{\mathbf{k}}^{\dagger} q_{\mathbf{k}}.$$

As in (2.22), we note that the first term on the right side of (3.14) is a positive-definite operator if $V_{\mathbf{k}} \geq 0$ for all $\mathbf{k}$. It follows that the fermion and boson ring models exhibit the same lower bound on H as did the distinguishable-particle ring model.

A third model, which has no analog in the distinguishable case, may be constructed by taking

$$\phi_{\mathbf{kprs}} = \exp[i(\bar{\theta}_{\mathbf{kr}} + \bar{\theta}_{\mathbf{ps}})] \tag{3.15}$$

and requiring the $\bar{\theta}_{\mathbf{kr}}$ to obey (3.12). We may call this the exchange model. Hybrid models may also be constructed, by taking $\phi_{\mathbf{kprs}}$ as a linear combination of the forms for the ladder, ring, and exchange models. We shall not discuss these cases in this paper.

3.4. Random-Coupling and Hartree-Fock Models

To construct the fermion and boson versions of the random-coupling model, we take

$$\phi_{\mathbf{kprs}} = \exp(i\theta_{\mathbf{kprs}}), \tag{3.16}$$

with

$$\theta_{\mathbf{kprs}} = -\theta_{\mathbf{srpk}}, \quad \theta_{\mathbf{kprs}} = \theta_{\mathbf{pksr}}, \quad \theta_{\mathbf{kprs}} = \theta_{\mathbf{pkrs}}, \tag{3.17}$$

and fix the phases $\theta_{\mathbf{kprs}}$ by independent random choices for each combination of indices $(\mathbf{k}, \mathbf{p}, \mathbf{r}, \mathbf{s})$, subject only to (3.17). As in the distinguishable-particle random coupling model, there appears to be no lower bound on the potential energy per particle when the system is infinite. This suggests that results obtained from the random-coupling model be viewed with skepticism. It perhaps should be pointed out that our random-coupling models are unrelated to the random-phase approximation employed by Pines and Bohm[16] and others. We make no assumption about the phase correlations among the dynamic variables.

The fermion or boson Hartree-Fock model is given by the assignment

$$\phi_{\mathbf{kppk}} = \phi_{\mathbf{kpkp}} = 1, \qquad \phi_{\mathbf{kprs}} = 0 \quad (\mathbf{k} \neq \mathbf{r} \text{ or } \mathbf{s}). \tag{3.18}$$

This model contains no randomly chosen parameters. We shall see in Sec. 5 that it yields simply the Hartree-Fock approximation to the true problem, in the limit $\Omega \to \infty$.

4. TEMPERATURE-DOMAIN PROPAGATOR FORMALISM

The equilibrium statistical mechanics of the fermion and boson models can be investigated most neatly by means of the temperature-domain propagator formalism and its associated diagram technique.[2,5,6,8] Since our models differ from the true Hamiltonian only by the replacement

$$V_{\mathbf{k-s}}\, \delta_{\mathbf{k+p,r+s}} \to V_{\mathbf{k-s}} \phi_{\mathbf{kprs}}\, \delta_{\mathbf{k+p,r+s}}, \tag{4.1}$$

the existing techniques may be taken over with only minor and obvious changes. We shall summarize the resulting formalism in the present section.[19]

Let us define the temperature-domain propagator $S_{\mathbf{k}}(u, u')$ by

$$S_{\mathbf{k}}(u, u') = -\langle T[q_{\mathbf{k}}(u) q_{\mathbf{k}}^{\dagger}(u')] \rangle \quad (u, u' \text{ real}), \tag{4.2}$$

where

$$q_{\mathbf{k}}(u) = e^{uH} q_{\mathbf{k}} e^{-uH}, \qquad q_{\mathbf{k}}^{\dagger}(u) = e^{uH} q_{\mathbf{k}}^{\dagger} e^{-uH}. \tag{4.3}$$

The ordering operator T is defined by

$$\begin{aligned} T[q_{\mathbf{k}}(u) q_{\mathbf{k}}^{\dagger}(u')] &= q_{\mathbf{k}}(u) q_{\mathbf{k}}^{\dagger}(u') \qquad (u > u'), \\ T[q_{\mathbf{k}}(u) q_{\mathbf{k}}^{\dagger}(u')] &= \mp q_{\mathbf{k}}^{\dagger}(u') q_{\mathbf{k}}(u) \qquad (u \leq u'). \end{aligned} \tag{4.4}$$

In (4.4) and in all subsequent expressions where a plus-minus or minus-plus sign occurs, the upper sign refers to fermions and the lower to bosons. The brackets $\langle\ \rangle$ denote an average over the grand canonical ensemble. For any operator B,

$$\langle B \rangle \equiv \mathrm{Tr}\, \{e^{-\beta(H-\mu N)} B\} / \mathrm{Tr}\, \{e^{-\beta(H-\mu N)}\}, \tag{4.5}$$

where N is defined below (3.14) and μ is the chemical potential.

The propagator has a Fourier expansion of the

[19] Our treatment is based principally upon reference 8, but our notation does not agree completely with that of any of the references cited. (The latter differ substantially among themselves.)

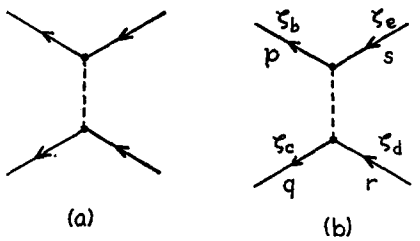

FIG. 2. (a) A vertex. (b) A labeled vertex.

form

$$S_{\mathbf{k}}(u, u') = \beta^{-1} \sum_{a=-\infty}^{\infty} S_{\mathbf{k}}(\zeta_a) \exp\left[\zeta_a(u' - u + \delta)\right], \tag{4.6}$$

where

$$\begin{aligned} \zeta_a &= \mu + i\pi(2a + 1)\beta^{-1} \quad \text{(fermions)}, \\ \zeta_a &= \mu + 2i\pi a\beta^{-1} \qquad\quad \text{(bosons)}, \end{aligned} \tag{4.7}$$

and a takes all integer values. The quantity δ is an infinitesimal real, positive number. We shall call $S_{\mathbf{k}}(\zeta_a)$ a propagator also, and we shall call ζ_a an 'energy.'

The complete thermodynamic behavior of the system can be obtained from $S_{\mathbf{k}}(\zeta_a)$. The mean number of particles at a given temperature and chemical potential is

$$N(\beta, \mu) = \sum_{\mathbf{k}} \bar{N}_{\mathbf{k}},$$

$$\bar{N}_{\mathbf{k}} = \pm\beta^{-1} \sum_{a} S_{\mathbf{k}}(\zeta_a) \exp(\zeta_a \delta), \tag{4.8}$$

where the $\bar{N}_{\mathbf{k}} \equiv \langle N_{\mathbf{k}} \rangle$ are the mean occupation numbers. The mean energy also has a direct expression. Using (3.1), (3.3), (3.4), and (4.3), we find

$$\pm \sum_{\mathbf{k}} \left[\partial S_{\mathbf{k}}(u, u')/\partial u'\right]_{u'=u} = \langle H_0 \rangle + 2\langle H_i \rangle, \tag{4.9}$$

and we note that $\langle H_0 \rangle = \pm\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} S_{\mathbf{k}}(u, u)$. Then it follows from (4.6) that the mean energy $E(\beta, \mu)$ is given by[20]

$$E(\beta, \mu) = \pm\tfrac{1}{2}\beta^{-1} \sum_{\mathbf{k},a} (\epsilon_{\mathbf{k}} + \zeta_a) S_{\mathbf{k}}(\zeta_a) \exp(\zeta_a \delta). \tag{4.10}$$

The entropy, pressure, and other thermodynamic quantities can be found from $N(\beta, \mu)$ and $E(\beta, \mu)$. [Alternatively, the thermodynamic potential may be obtained from $S_{\mathbf{k}}(\zeta_a)$ by an integration over an interaction strength parameter.[8]]

The propagator for free particles is

$$S_{\mathbf{k}}^{(0)}(\zeta_a) = (\zeta_a - \epsilon_{\mathbf{k}})^{-1}. \tag{4.11}$$

[20] See N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).

The coupled-particle propagator $S_{\mathbf{k}}(\zeta_a)$ may be expressed in terms of $S_{\mathbf{k}}^{(0)}(\zeta_a)$ by a linked-diagram expansion constructed according to the following rules:

1. Call the diagram part shown in Fig. 2(a) a vertex. A vertex consists of two solid-line junctions connected by a dashed line. 'Line' hereafter will mean solid line except where noted.

2. For each positive integer n, take n vertices and join incoming with outgoing lines in pairs so as to form, just once, all possible distinct, linked diagrams with just one incoming and one outgoing external line. Linked diagrams are those which do not consist of disconnected parts. External lines are those which leave or enter the diagram. In reckoning distinctness, the n original vertices are considered indistinguishable and the two solid-line junctions in any vertex are considered indistinguishable. However, incoming lines are distinct from outgoing lines. Examples: Figs. 6(a) and 8(a) are distinct, but Figs. 6(a) and 9(a) are not.[21]

3. Label the external lines with momentum $\mathbf{k}$. Label the internal lines with momenta $\mathbf{k}'$, $\mathbf{k}''$, $\cdots$. In addition, associate the 'energy' ζ_a with the external lines, and 'energies' $\zeta_{a'}$, $\zeta_{a''}$, $\cdots$ with the internal lines.

4. With each line, external or internal, associate a factor $S_{\mathbf{p}}^{(0)}(\zeta_b)$, where $\mathbf{p}$ is the momentum labeling the line and ζ_b is the associated 'energy.' Special case: Include an additional factor $\exp(\zeta_b\delta)$ if the beginning and termination of the line are in the same vertex.

5. With each vertex, at which are joined lines with momentum labels $\mathbf{p}$, $\mathbf{q}$, $\mathbf{r}$, $\mathbf{s}$ and respective 'energies' ζ_b, ζ_c, ζ_d, ζ_e as shown in Fig. 2(b), associate a factor

$$-\beta^{-1}\phi_{\mathbf{pqrs}} V_{\mathbf{p}-\mathbf{s}}\, \delta_{\mathbf{p}+\mathbf{q},\mathbf{r}+\mathbf{s}}\, \delta_{b+c,d+e}.$$

Note: This rule is ambiguous with respect to the exchange $(\mathbf{p}, \mathbf{s}) \rightleftharpoons (\mathbf{q}, \mathbf{r})$. By (2.3) and (3.5), however, the factor called for by the rule is invariant in value under the exchange.

6. For fermions only: Associate with each diagram a factor $(-1)^l$, where l is the number of closed solid-line loops in the diagram.

7. To form the contribution of a given diagram, multiply together all the factors introduced by rules 4, 5, and 6 and then sum over all the momenta $\mathbf{k}'$, $\mathbf{k}''$, $\cdots$ and 'energies' $\zeta_{a'}$, $\zeta_{a''}$, $\cdots$ associated with the internal lines.

8. To form $S_{\mathbf{k}}(\zeta_a)$, first sum the contributions given by rule 7 for all the diagrams admitted by rule 2. Then add the contribution $S_{\mathbf{k}}^{(0)}(\zeta_a)$, which is associated with the zeroth order ($n = 0$) diagram Fig. 3(a).

We shall call the expansion for $S_{\mathbf{k}}(\zeta_a)$ generated by rules 1–8 the *primitive linked-diagram expansion*. A more compact expansion, which we shall call the *irreducible linked-diagram* expansion, may be con-

[21] If the vertices and junctions were considered distinguishable, one would obtain, for each of our distinct diagrams, a total of $2^n n!$ diagrams, all of which would give identical contributions to $S_{\mathbf{k}}(\zeta_a)$. If one counts these diagrams separately, which we do not do, the contribution per diagram obtained by our rules 1–7 must be multiplied by $1/2^n n!$ The latter procedure is adopted in reference 8.

structed by replacing rules 2 and 4 with the following altered rules:

2′. Retain only those diagrams admitted by rule 2 which do not contain self-energy parts. We shall call these irreducible diagrams. (A self-energy part is a part of a diagram which contains at least one but not all the vertices and which is connected to the rest of the diagram by just one outgoing and one incoming line.)

4′. In rule 4, replace each factor $S_{\mathbf{p}}^{(0)}(\zeta_b)$ by a factor $S_{\mathbf{p}}(\zeta_b)$. Exception: With the outgoing external line associate the factor $S_{\mathbf{k}}^{(0)}(\zeta_a)$ as before.

The primitive diagram expansion gives $S_{\mathbf{k}}(\zeta_a)$ as an infinite sum of integrals (we consider the case $\Omega \to \infty$) over the known quantities $S_{\mathbf{k}}^{(0)}(\zeta_a)$. In contrast, the irreducible expansion is really an infinite-series integral equation for $S_{\mathbf{k}}(\zeta_a)$. A convenient way to express the irreducible expansion is as follows: We define $M_{\mathbf{k}}(\zeta_a)$ by

$$S_{\mathbf{k}}(\zeta_a) = [\zeta_a - \epsilon_{\mathbf{k}} - M_{\mathbf{k}}(\zeta_a)]^{-1}. \qquad (4.12)$$

Then the irreducible linked-diagram expansion for $M_{\mathbf{k}}(\zeta_a)$ is the same as that for $S_{\mathbf{k}}(\zeta_a)$ except for the changes expressed by the following further rule alterations:

4″. In rule 4′, omit entirely the factors for the two external lines.

8′. In rule 8, omit the contribution of the zeroth-order diagram.

The use of the rules will be illustrated by the examples treated in Sec. 5. If we take $\phi_{\mathbf{kprs}} = 1$ for all $\mathbf{k}, \mathbf{p}, \mathbf{r}, \mathbf{s}$, then the rules we have given yield the established propagator expansions for the true problem.

5. PROPAGATOR EQUATIONS FOR THE MODELS

5.1. Underlying Assumptions

We shall now show that our fermion and boson models lead to closed integral equations for $S_{\mathbf{k}}(\zeta_a)$ in the limit $\Omega \to \infty$ with fixed μ or ρ. We wish first to state clearly the assumptions which underlie the analysis:

1. As in Sec. 2, we restrict $V(\mathbf{x})$ to be a smooth, bounded function such that $|V_{\mathbf{k}}| \leq O(k^{-2})$, $k \to \infty$.

2. We assume that all the sums over intermediate momenta which occur in any given order of the primitive linked-diagram expansion converge at infinity. More precisely, we assume that, for given $\mathbf{k}$ and a, the contributions to $S_{\mathbf{k}}(\zeta_a)$ which involve intermediate momenta higher than some given momentum $k_{\max}$ vanish as $k_{\max} \to \infty$. Moreover, we assume that they vanish in a manner independent of Ω as $\Omega \to \infty$. We believe that this assumption actually follows from assumption 1, but we shall not try to prove this here.

3. As in Sec. 2, we assume that $V_{\mathbf{k}} = O(\Omega^{-1})$ for all $\mathbf{k}$ as $\Omega \to \infty$. This means that for long-range potentials a cutoff length l must be employed as in (2.24). We take the limit $l \to \infty$ only after the limit $\Omega \to \infty$ has been performed.

4. For every $\mathbf{k}$ and a we assume that $S_{\mathbf{k}}^{(0)}(\zeta_a)$ approaches a limit independent of Ω as $\Omega \to \infty$ with ρ constant. This excludes from our present considerations boson systems below the Einstein-Bose condensation temperature.

5. The final assumption involves a deep-lying convergence question corresponding to that which arose in Sec. 2. We shall see, for each of the models, that large classes of diagrams give a vanishing contribution to $S_{\mathbf{k}}(\zeta_a)$ in the limit $\Omega \to \infty$, up to any given order of diagram. On this basis, we shall assume that these classes do not contribute when summed to *all* orders. It will not follow from our analysis that this is actually so. The reason is that the diagrams of order $N(=\rho\Omega)$ and higher are enormous in number for large Ω, and it will not be clear that cancellations due to the randomness of the $\phi_{\mathbf{kprs}}$ will suppress the contribution of these diagrams as they do contributions of finite order.

The necessity for assumptions 3 and 4 will be eliminated by the generalized treatment given in the following paper. There we construct models for systems of any size and obtain closed propagator equations without taking the limit $\Omega \to \infty$. The final equations are identical with those to be derived here, and they justify the latter in cases where assumptions 3 and 4 are not satisfied. In particular, they establish the closed model equations for condensed boson systems. The generalized treatment provides much neater derivations of all the results to be obtained in Sec. 5. We do not employ it at the outset because it requires an unfamiliar and more elaborate formalism.

Assumption 5 also is best examined by the methods of the following paper. The approach to this question adopted there is to consider the propagators in the real-time domain, rather than the temperature domain, and to regard them as the limits of more general quantities (correlation and Green's functions) which are defined for non-equilibrium as well as equilibrium. Linked-diagram expansions exist which give the evolution of the correlation and Green's functions forward in time from a given initial statistical state. As in the present case, these expansions can be formally

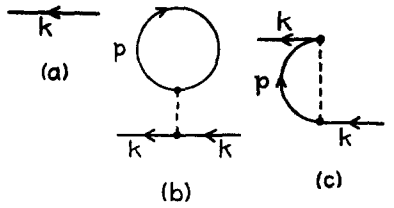

FIG. 3. The zeroth and first-order diagrams for $S_k(\zeta_a)$.

summed and expressed by closed equations for each of our models.

A new feature, however, is that the evolution in time can also be examined by an alternate method which seems genuinely independent of perturbation expansions. One can replace the exact differential equations of evolution by corresponding difference equations involving small time increments. In contrast to a perturbation expansion (which is akin to a Taylor series) such a procedure should converge, as the increment size is decreased to zero, whenever the differential equations themselves are meaningful. This permits an examination of assumption 5 from a new point of view. Although the analysis we shall present in the following paper is not rigorous, we feel that it provides substantial support for the validity of our closed model equations.

5.2. Hartree-Fock and Random-Coupling Models

The derivation of closed propagator equations is simplest for the Hartree-Fock model. Consider the primitive linked-diagram expansion for $S_k(\zeta_a)$. There are two distinct first-order diagrams, and they are shown in Figs. 3(b) and 3(c). By the rules of Sec. 4, the contributions of these diagrams involve the factors ϕ_{kpkp} and ϕ_{kpkp}, respectively, but no other ϕ factors. Therefore, by (3.18), their contributions are identical in the Hartree-Fock model and in the true problem.

However, consider Fig. 4(a). The contribution of this second-order diagram to the primitive expansion for $S_k(\zeta_a)$ is

$$\mp\beta^{-2}\sum_{ps}\phi_{kprs}\phi_{srpk}V_{k-s}V_{s-k}\sum_{bc}S_k^{(0)}(\zeta_a)S_p^{(0)}(\zeta_b) \times S_s^{(0)}(\zeta_c)S_r^{(0)}(\zeta_d)S_k^{(0)}(\zeta_a), \qquad (5.1)$$

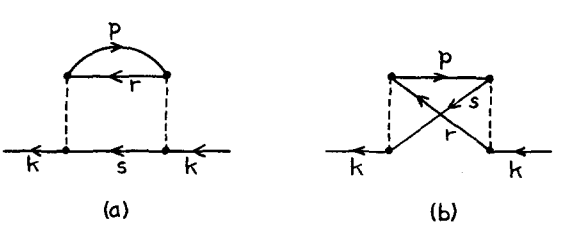

FIG. 4. The second-order irreducible diagrams for $S_k(\zeta_a)$.

where $\mathbf{r} = \mathbf{k} + \mathbf{p} - \mathbf{s}$, $d = a + b - c$, by momentum and 'energy' conservation. By (3.18), the only surviving terms in the sum are those for which either $\mathbf{s} = \mathbf{k}$, $\mathbf{r} = \mathbf{p}$ or $\mathbf{r} = \mathbf{k}$, $\mathbf{s} = \mathbf{p}$. Thus, there is only one free intermediate momentum, which we may take as $\mathbf{p}$. Now as $\Omega \to \infty$, the number of allowed momenta $\mathbf{p}$ in any given volume of momentum space is $\propto\Omega$. It then follows from assumptions 2, 3, and 4 of Sec. 5.1 that the contribution (5.1) vanishes as Ω^{-1}.

If similar considerations are applied to the rest of the primitive linked diagrams, it is possible to verify the following result: The only diagrams which survive in the limit $\Omega \to \infty$ are those for which momentum conservation alone assures that the ϕ product given by the rules of Sec. 4 consists wholly of factors of the form ϕ_{pqqp} or ϕ_{pqpq}. Such diagrams give the same contribution as they do in the true problem. For every other diagram of finite order, (3.18) so restricts the summations over intermediate momenta that the result vanishes as some positive integral power of Ω^{-1}.

It is easy to see from the rules of Sec. 4 that the higher surviving primitive diagrams, which we have just specified, are simply those which can be obtained from Figs. 3(b) and 3(c) by repeatedly inserting these first-order diagrams into themselves and into each other as self-energy parts. An example is shown in Fig. 5. Now let us invoke assumption 5 of Sec. 5.1. It then follows that Figs. 3(b) and 3(c) are the *only* diagrams which survive in the *irreducible* expansion for $S_k(\zeta_a)$ in the limit $\Omega \to \infty$. We may see this by noting that the primitive expansion can be recovered from the irreducible expansion by taking every factor S which occurs in the latter and replacing it by its own primitive expansion. If diagrams other than Figs. 3(b) and 3(c) occurred in the irreducible expansion, then it is clear that the primitive expansion for $S_k(\zeta_a)$ thus recovered would contain diagrams other than those we have specified.

Using the rules of Sec. 4 to evaluate the contribution to $M_k(\zeta_a)$ of the two surviving irreducible diagrams, we find

$$M_k(\zeta_a) = \beta^{-1}\sum_{pb}(\pm V_0 - V_{k-p})S_p(\zeta_b)\exp(\zeta_b\,\delta), \qquad (5.2)$$

where we have noted (2.3). The first term on the right side of (5.2) arises from Fig. 3(b) and the second from Fig. 3(c). Upon inserting (5.2) into (4.12), we obtain a closed integral equation for $S_k(\zeta_a)$ for the Hartree-Fock model. Equation (5.2)

may be rewritten in the form

$$M_{\mathbf{k}}(\zeta_a) = \sum_{\mathbf{p}} (V_0 \mp V_{\mathbf{k}-\mathbf{p}})\bar{N}_{\mathbf{p}}, \qquad (5.3)$$

where we use (4.8). The parts of this result involving V_0 and $V_{\mathbf{k}-\mathbf{p}}$ are, respectively, the direct and exchange parts of the effective potential which is obtained in the usual Hartree-Fock approximation to the true problem.

Let us consider next the random-coupling model. By (3.16) and (3.17), we find

$$\phi_{\mathbf{kppk}} = 1, \quad \phi_{\mathbf{kpkp}} = 1, \quad \phi_{\mathbf{kprs}}\phi_{\mathbf{srpk}} = 1, \quad \phi_{\mathbf{kprs}}\phi_{\mathbf{srkp}} = 1. \qquad (5.4)$$

It then follows from the rules of Sec. 4 that Figs. 3(b), 3(c), 4(a), and 4(b) all survive in the primitive expansion for $S_{\mathbf{k}}(\zeta_a)$ and give the same contributions as in the true problem.

However, consider Fig. 6(a). The contribution which it makes to the primitive expansion for $S_{\mathbf{k}}(\zeta_a)$ is of the form

$$\pm\beta^{-3} \sum_{\mathbf{prsr's'}} \phi_{\mathbf{kprs}}\phi_{\mathbf{srr's'}}\phi_{\mathbf{s'r'pk}}\, \delta_{\mathbf{k+p,r+s}} \times \delta_{\mathbf{r+s,r'+s'}}\, \delta_{\mathbf{r'+s',p+k}} \times V_{\mathbf{k-s}}V_{\mathbf{s-s'}}V_{\mathbf{s'-k}} \sum_{\text{(energies)}} (\text{product of } S^{(0)} \text{ factors}). \qquad (5.5)$$

There is an identity among the conservation conditions given by the three Kronecker symbols. Consequently there are three independent intermediate momenta, which we may take as **p**, **s**, and **s**′. For special values of these momenta, the ϕ product is unity by (5.4). However, in correspondence to the result noted above for the Hartree-Fock model, it is easy to see that these special values give a vanishing contribution to $S_{\mathbf{k}}(\zeta_a)$ when $\Omega \to \infty$. Except for these restricted momentum values, the ϕ product will have a phase which, by (3.16) *et seq.*, fluctuates at random with change of **p**, **s**, and **s**′.

Now let us divide the momentum space into small regions, of 'volume' Δ, such that $S_{\mathbf{p}}^{(0)}(\zeta_b)$ exhibits negligible change if **p** varies within a given region. By assumption 4 of Sec. 5.1, this should be possible in the limit $\Omega \to \infty$. Now as $\Omega \to \infty$, the density of allowed modes in momentum space is $\sim \Omega$. Hence, in the summation over momenta in (5.5), the number of terms for **p**, **s**, and **s**′ within given small regions will be $\sim (\Omega\Delta)^3$. Let us consider the contribution from those terms in which the phase of the ϕ product fluctuates at random with change of **p**, **s**, and **s**′. As we have just noted, these constitute all but a negligible fraction of the terms. Because of the phase-fluctuation, the total contribution of these terms will be down by a factor $\sim (\Omega\Delta)^{-\frac{1}{2}}$ from the value it would have in the true problem. Since this factor vanishes as $\Omega \to \infty$, it follows from assumptions 2 and 3 of Sec. 5.1 that the contribution to $S_{\mathbf{k}}(\zeta_a)$ from Fig. 6(a) vanishes in the limit. Our argument, of course, assumes a typical assignment of values to the randomly chosen parameters $\theta_{\mathbf{kprs}}$ (cf. the discussion in Sec. 2.2).

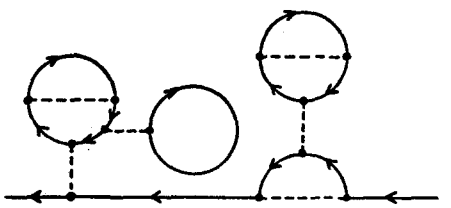

FIG. 5. A primitive diagram which survives in the Hartree-Fock model.

Similar analysis may be applied to the higher diagrams in the primitive expansion for $S_{\mathbf{k}}(\zeta_a)$. The result is that the only diagrams which survive are those for which momentum conservation alone assures that the ϕ product consists entirely of factors and/or factor-pairs of the forms shown in (5.4). Any other diagram gives a contribution which vanishes as some negative power of Ω as $\Omega \to \infty$. The surviving diagrams can be seen to be those which can be constructed from Figs. 3(b), 3(c), 4(a), and 4(b) by inserting these same four diagrams repeatedly as self-energy parts, in correspondence to the situation for the Hartree-Fock model. It follows from this that the only surviving diagrams in the irreducible expansion for $S_{\mathbf{k}}(\zeta_a)$ are Figs.

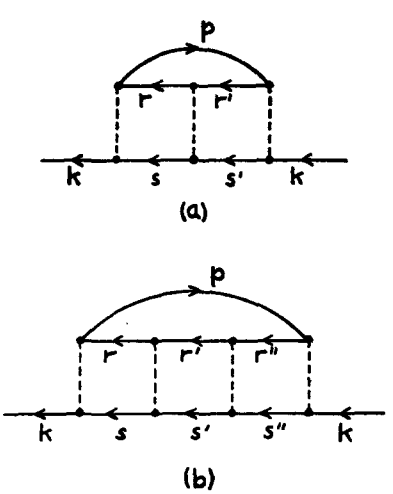

FIG. 6. The third-order and fourth-order ladder diagrams.

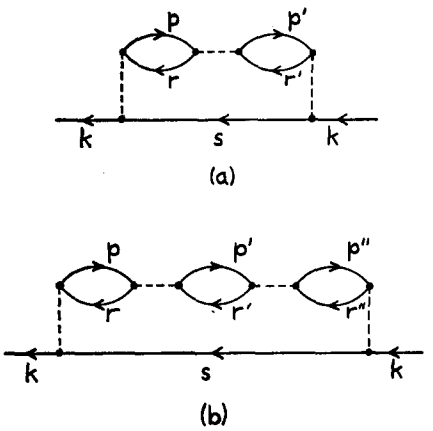

FIG. 7. The third-order and fourth-order ring diagrams.

3(b), 3(c), 4(a), and 4(b). Again, assumption 5 of Sec. 5.1 is implicit in the argument.

Combining the contributions of the four surviving irreducible diagrams according to the rules of Sec. 4, we find

$$M_{\mathbf{k}}(\zeta_a) = \sum_{\mathbf{p}} (V_0 \mp V_{\mathbf{k}-\mathbf{p}})\bar{N}_{\mathbf{p}} \mp \beta^{-2} \sum_{\mathbf{p}\mathbf{s}bc} V_{\mathbf{k}-\mathbf{s}}(V_{\mathbf{k}-\mathbf{s}} \mp V_{\mathbf{p}-\mathbf{s}}) S_{\mathbf{p}}(\zeta_b) S_{\mathbf{s}}(\zeta_c) S_{\mathbf{k}+\mathbf{p}-\mathbf{s}}(\zeta_{a+b-c}), \quad (5.6)$$

where, again, we note (4.8).

If the third of constraints (3.17) were relaxed in assigning random values to the $\theta_{\mathbf{k}\mathbf{p}\mathbf{r}\mathbf{s}}$, we would obtain a version of the random-coupling model in which the exchange diagram Fig. 4(b) did not survive. The corresponding expression for $M_{\mathbf{k}}(\zeta_a)$ would not include the term in (5.6) which involves $V_{\mathbf{p}-\mathbf{s}}$.

5.3. Ring and Ladder Models

The results described above for the Hartree-Fock and random-coupling models may be summarized very simply: The only diagrams which survive in the irreducible expansion for $M_{\mathbf{k}}(\zeta_a)$ are those for which the associated ϕ product has the value one for all values of the intermediate momenta allowed by momentum conservation. The contributions of the surviving diagrams have precisely the same form in the models as in the true problem. This general result is also true for the ring and ladder models under the assumptions of Sec. 5.1. Analysis similar to that we have described shows that the irreducible diagrams in which the ϕ product can exhibit a randomly fluctuating phase give vanishing contributions in the limit $\Omega \to \infty$. We shall now identify the surviving irreducible diagrams in the ring and ladder models and construct the corresponding closed expressions for $M_{\mathbf{k}}(\zeta_a)$.

It follows from (3.11) and (3.12) that the first three of relations (5.4) are satisfied in the ring model. Thus the irreducible diagrams Figs. 3(b), 3(c), and 4(a) survive. However, the ϕ product associated with Fig. 4(b) is

$$\phi_{\mathbf{k}\mathbf{p}\mathbf{r}\mathbf{s}}\phi_{\mathbf{s}\mathbf{r}\mathbf{k}\mathbf{p}} = \exp\,[i(\bar{\theta}_{\mathbf{k}\mathbf{s}} + \bar{\theta}_{\mathbf{p}\mathbf{r}}) + i(\bar{\theta}_{\mathbf{s}\mathbf{p}} + \bar{\theta}_{\mathbf{r}\mathbf{k}})]. \quad (5.7)$$

The random phase of this product does not vanish when $\mathbf{p}$, $\mathbf{r}$, and $\mathbf{s}$ are constrained by momentum conservation alone. Consequently, the diagram does not survive. The further irreducible diagrams which do survive in the ring model are the infinite class of *ring* diagrams, whose first two members are shown in Fig. 7. (If the incoming and outgoing external lines are joined together, these diagrams from symmetrical rings.) The ϕ products associated with the successive ring diagrams have the phases

$$[(\bar{\theta}_{\mathbf{k}\mathbf{s}} + \bar{\theta}_{\mathbf{p}\mathbf{r}}) + (\bar{\theta}_{\mathbf{r}\mathbf{p}} + \bar{\theta}_{\mathbf{p}'\mathbf{r}'}) + (\bar{\theta}_{\mathbf{r}'\mathbf{p}'} + \bar{\theta}_{\mathbf{s}\mathbf{k}})],$$
$$[(\bar{\theta}_{\mathbf{k}\mathbf{s}} + \bar{\theta}_{\mathbf{p}\mathbf{r}}) + (\bar{\theta}_{\mathbf{r}\mathbf{p}} + \bar{\theta}_{\mathbf{p}'\mathbf{r}'}) + (\bar{\theta}_{\mathbf{r}'\mathbf{p}'} + \bar{\theta}_{\mathbf{p}''\mathbf{r}''}) + (\bar{\theta}_{\mathbf{r}''\mathbf{p}''} + \bar{\theta}_{\mathbf{s}\mathbf{k}})], \quad (5.8)$$
$$\cdots,$$

which all vanish, by (3.12).

It may be seen from the rules of Sec. 4 that the ring diagrams give a set of contributions to $M_{\mathbf{k}}(\zeta_a)$ which resemble a geometric series. They may be summed easily by the usual methods for such series. If we include also the contributions from Figs. 3(b), 3(c), and 4(a), the final result for $M_{\mathbf{k}}(\zeta_a)$ is

$$M_{\mathbf{k}}(\zeta_a) = V_0\bar{N} - \beta^{-1} \sum_{\mathbf{s}c} V'_{\mathbf{k}-\mathbf{s}}(\zeta_{a-c}) S_{\mathbf{s}}(\zeta_c) \exp\,(\zeta_c\,\delta), \quad (5.9)$$

where $\bar{N} = \sum_{\mathbf{p}} \bar{N}_{\mathbf{p}}$, and $V'_{\mathbf{k}-\mathbf{s}}(\zeta_{a-c})$ is defined by

$$V'_{\mathbf{q}}(\zeta_d) = V_{\mathbf{q}} \pm \beta^{-1} \sum_{\mathbf{p}b} V_{\mathbf{q}} S_{\mathbf{p}}(\zeta_b) S_{\mathbf{p}+\mathbf{q}}(\zeta_{b+d}) V'_{\mathbf{q}}(\zeta_d). \quad (5.10)$$

The term in (5.9) proportional to $\bar{N}$ arises from the Hartree-Fock diagram Fig. 3(b). To verify the remainder of the result, we may solve (5.10) by iteration to yield $V'_{\mathbf{k}-\mathbf{s}}(\zeta_{a-c})$ as a power series in $V_{\mathbf{k}-\mathbf{s}}$ and then substitute into (5.9). The first term $V_{\mathbf{k}-\mathbf{s}}$ in the series gives the contribution of Fig. 3(c), and the higher terms give those of Fig. 4(a) and the successive ring diagrams. [The factor $\exp\,(\zeta_c\delta)$ is superfluous for the second- and higher-order contributions; it does not affect their values.]

Equation (5.10) may be rewritten as

$$V'_{\mathbf{q}}(\zeta_d) = V_{\mathbf{q}}[1 \mp \beta^{-1} \sum_{\mathbf{p}b} V_{\mathbf{q}} S_{\mathbf{p}+\mathbf{q}}(\zeta_{b+d}) S_{\mathbf{p}}(\zeta_b)]^{-1}. \quad (5.11)$$

We note that the potential components for different values of $\mathbf{q}$ are not explicitly mixed in this expression, a fact which recalls the classical ring results obtained in Sec. 2.3. We may call $V'_{\mathbf{q}}(\zeta_d)$ an 'effective potential' for the ring model. In field-theoretic terminology, it is a kind of vertex operator. From a particle viewpoint, we may consider $\mathbf{k} - \mathbf{s}$ and ζ_{a-c} in (5.9) as a momentum and 'energy' which are taken from the incoming particle, transmitted along a chain of intermediate particles, and finally returned to the original particle to complete the ring.

It is of interest to compare the ring summation represented by (5.9) and (5.10) with that given by Montroll and Ward.[3] The latter appears to correspond to a summation over ring diagrams for the *primitive* linked-diagram expansion. It omits the iterated self-energy corrections which our model includes.

It follows from (3.6) and (3.7) that all of the relations (5.4) are satisfied for the ladder model. Hence the irreducible diagrams Figs. 3(b), 3(c), 4(a), and 4(b) all survive. The further irreducible diagrams which survive are the infinite classes of *ladder* diagrams and *exchange ladder* diagrams. The first two members of each class are shown in Figs. 6 and 8, respectively. It follows from (3.6), (3.7), and the rules of Sec. 4 that the ϕ products associated with corresponding diagrams in the two classes have the same value. For the successive diagrams in either class, these products have the phases

$$[(-\theta_{\mathbf{pk}} + \theta_{\mathbf{rs}}) + (-\theta_{\mathbf{rs}} + \theta_{\mathbf{r's'}}) + (-\theta_{\mathbf{r's'}} + \theta_{\mathbf{pk}})],$$
$$[(-\theta_{\mathbf{pk}} + \theta_{\mathbf{rs}}) + (-\theta_{\mathbf{rs}} + \theta_{\mathbf{r's'}}) + (-\theta_{\mathbf{r's'}} + \theta_{\mathbf{r''s''}}) + (-\theta_{\mathbf{r''s''}} + \theta_{\mathbf{pk}})], \quad (5.12)$$
$$\cdots,$$

which vanish identically. The ladder and exchange ladder diagrams exhaust the higher irreducible

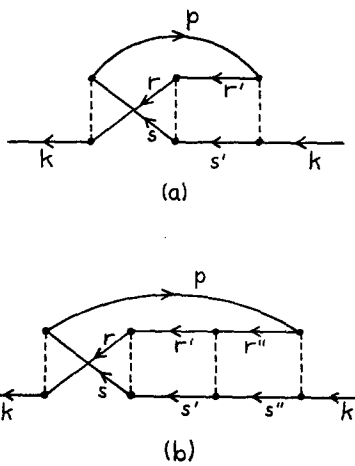

FIG. 8. The third-order and fourth-order exchange ladder diagrams.

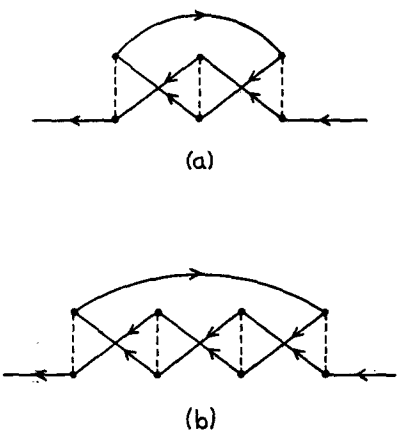

FIG. 9. (a) A diagram redundant with Fig. 6(a). (b) A diagram redundant with Fig. 8(b).

diagrams which survive in the ladder model. [It should be noted that according to the rules of Sec. 4, diagrams like Fig. 9(a) and Fig. 9(b), which are topologically identical with Figs. 6(a) and 8(b), respectively, are not to be counted separately.]

The contributions of the ladder and exchange ladder diagram sequences can easily be summed in closed form, in a similar fashion to the ring diagrams. If we include also the contributions from Figs. 3(b), 3(c), 4(a), and 4(b), the final result for the ladder model is

$$M_{\mathbf{k}}(\zeta_a) = \pm\beta^{-1} \sum_{pb} [V'_{\mathbf{kppk}}(\zeta_{a+b}) \mp V'_{\mathbf{kpkp}}(\zeta_{a+b})] S_{\mathbf{p}}(\zeta_b) \exp(\zeta_b \delta), \quad (5.13)$$

where $V'_{\mathbf{kprs}}(\zeta_{a+b})$ is defined by

$$V'_{\mathbf{kprs}}(\zeta_{a+b}) = V_{\mathbf{k-s}} - \beta^{-1} \sum_{s'c'} V_{\mathbf{k-s'}} V'_{\mathbf{s'r'rs}}(\zeta_{a+b}) \times S_{\mathbf{s'}}(\zeta_{c'}) S_{\mathbf{r'}}(\zeta_{a+b-c'}), \quad (5.14)$$

with $\mathbf{r} = \mathbf{k} + \mathbf{p} - \mathbf{s}$ and $\mathbf{r}' = \mathbf{k} + \mathbf{p} - \mathbf{s}'$. If (5.14) is expanded by iteration and the result for $V'_{\mathbf{kprs}}(\zeta_{a+b})$ is substituted into (5.13), one obtains the explicit contributions from all the diagrams which survive in the ladder model. The nonexchange contributions all arise from the factor $V'_{\mathbf{kppk}}(\zeta_{a+b})$ in (5.13), and the exchange contributions from the factor $V'_{\mathbf{kpkp}}(\zeta_{a+b})$. The quantities $V'_{\mathbf{kprs}}(\zeta_{a+b})$ may be regarded as defining an effective potential for the ladder model. It is easily seen that they satisfy

$$V'_{\mathbf{kprs}}(\zeta_{a+b}) = V'_{\mathbf{pksr}}(\zeta_{a+b}). \quad (5.15)$$

If the symmetry constraint (3.7) is relaxed in assigning random values to the phases $\theta_{\mathbf{kp}}$, an abbreviated ladder model results in which none of the exchange diagrams survive. The abbreviated model violates the second of conditions (3.5), and

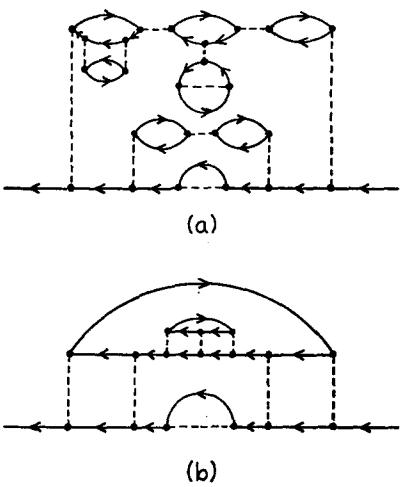

FIG. 10. Examples of higher primitive diagrams contributing in the ring model (a) and the ladder model (b).

n consequence it requires an elaboration of our diagram formalism: The two junctions which make up a vertex must be distinguished. We shall not discuss this model further here.

Equations (4.12), (5.9), and (5.10) constitute a closed set of integral equations which determine $S_{\mathbf{k}}(\zeta_a)$ for the ring model. Similarly, (4.12), (5.13), and (5.14) constitute a closed set for the ladder model. These equations incorporate extensive classes of terms from the primitive diagram expansion for $S_{\mathbf{k}}(\zeta_a)$ in the true problem. They include all primitive diagrams which can be obtained from the surviving irreducible diagrams by repeatedly inserting these irreducible diagrams into themselves and each other as self-energy parts. Examples of complicated primitive diagrams included in the ring and ladder models are shown in Figs. 10(a) and 10(b), respectively.

Note added in proof. The propagator equations obtained above for the Hartree-Fock, ladder, and ring models are equivalent to approximations proposed recently by G. Baym and L. P. Kadanoff [Phys. Rev. **124**, 287 (1961)], who were guided by a requirement that energy, momentum, and angular momentum be conserved under weak coupling to external systems. In the present approach, these properties follow from the fact that a model Hamiltonian is treated with formal exactness. One can see immediately from the generalized formulation in the following paper that the invariance properties of the true Hamiltonian are preserved in the models. When the model Hamiltonians are bounded from below, one expects in addition that the equations yield non-negative one-particle energy and momentum distribution functions.

6. RELATION BETWEEN DISTINGUISHABLE AND INDISTINGUISHABLE PARTICLE MODELS

We wish now to establish a correspondence between the models formulated in Secs. 2 and 3 and thereby verify that the thermodynamic relations obtained in Sec. 2 are at least formal classical limits for the fermion and boson models. The correspondence is already suggested by the identity of the lower bounds on the ring and ladder model Hamiltonians which we found in the two cases. Our procedure here will be to formulate the distinguishable-particle problem in terms of second-quantized fields, one for each particle. Then we shall appeal to two assumptions: the thermodynamic equivalence of canonical and grand canonical ensembles for infinite systems, and the equivalence of distinguishable and indistinguishable particles in in the classical limit.

The Hamiltonian of a system of $\bar{N}$ distinguishable but similar particles interacting through the pair potential $V(\mathbf{x})$ may be written

$$H = \sum_n \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} q^\dagger_{\mathbf{k}(n)} q_{\mathbf{k}(n)} + H_i, \tag{6.1}$$

$$H_i = \tfrac{1}{2} \sum_{nm} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}}\, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q^\dagger_{\mathbf{k}(n)} q^\dagger_{\mathbf{p}(m)} q_{\mathbf{r}(m)} q_{\mathbf{s}(n)}$$

$$(n, m = 1, 2, \cdots, \bar{N}). \tag{6.2}$$

Here we have introduced a separate second-quantized field [labeled (n)] for each particle, and we restrict the system to those states which are eigenstates with eigenvalue one for all the number operators

$$N_{(n)} = \sum_{\mathbf{k}} N_{\mathbf{k}(n)} = \sum_{\mathbf{k}} q^\dagger_{\mathbf{k}(n)} q_{\mathbf{k}(n)}. \tag{6.3}$$

The commutation relations are

$$[q_{\mathbf{k}(n)}, q^\dagger_{\mathbf{p}(m)}]_- = \delta_{nm}\, \delta_{\mathbf{kp}}. \tag{6.4}$$

The restriction of each field to one-particle states makes the choice of plus or minus commutator immaterial.

Let us consider the limit $\bar{N} \to \infty$ with β and $\rho = \bar{N}/\Omega$ constant. We shall assume in this limit that the canonical ensemble for our system gives the same thermodynamics as a grand canonical ensemble in which all states of the second-quantized fields are admitted. The latter ensemble is chosen so that

$$\langle N_{(n)} \rangle = 1, \qquad \langle N \rangle = \sum_n \langle N_{(n)} \rangle = \bar{N}, \tag{6.5}$$

where

$$\langle N_{(n)} \rangle = \mathrm{Tr}\, \{e^{-\beta(H-\mu N)} N_{(n)}\} / \mathrm{Tr}\, \{e^{-\beta(H-\mu N)}\}. \tag{6.6}$$

We should note that (6.5) implies $\mu \to -\infty$ when $\bar{N} \to \infty$ with constant ρ and β, as may readily be verified for free particles. The consequence is that the one-particle distribution function takes the Maxwell-Boltzmann form in the limit, as it must for consistency. We may also note that the variance $\langle (N_{(n)} - 1)^2 \rangle$ vanishes in the limit.

Now let us replace (6.2) with a model H_i,

$$H_i = \tfrac{1}{2} \sum_{nm} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}} \phi_{\mathbf{kprs}} \, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q^{\dagger}_{\mathbf{k}(n)} q^{\dagger}_{\mathbf{p}(m)} q_{\mathbf{r}(m)} q_{\mathbf{s}(n)}, \tag{6.7}$$

where the $\phi_{\mathbf{kprs}}$ are the same parameters as in Sec. 3. The thermodynamics of the model system may be obtained by a propagator formalism very similar to that of Sec. 4. Let us write

$$S_{\mathbf{k}}(u, u') = \sum_n S_{\mathbf{k}(n)}(u, u') = -\sum_n \langle T[q_{\mathbf{k}(n)}(u) q^{\dagger}_{\mathbf{k}(n)}(u')] \rangle, \tag{6.8}$$

and then define $S_{\mathbf{k}}(\zeta_a) = \sum_n S_{\mathbf{k}(n)}(\zeta_a)$ in terms of this $S_{\mathbf{k}}(u, u')$ by (4.6). Again, it will not affect the final results whether the fermion or boson case is taken. With these definitions, we find that (4.8) and (4.10) hold also for the present system, with $N_{\mathbf{k}} \equiv \sum_n N_{\mathbf{k}(n)}$. (Of course, for given ρ and β, the chemical potential μ will be very different in the present case than in Sec. 4, as we have noted above.)

Let us write

$$S^{(0)}_{\mathbf{k}(n)}(\zeta_a) = (\zeta_a - \epsilon_{\mathbf{k}})^{-1}. \tag{6.9}$$

Then the primitive linked-diagram expansion for $S_{\mathbf{k}}(\zeta_a)$ is given by the rules of Sec. 4 provided the following changes are made:

(a) Give each line a *particle* label as well as a momentum label. Associate with each line a factor of the form (6.9).

(b) With each vertex, bearing momentum labels $\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{s}$ and particle labels n, m, m', n' as shown in Fig. 11, associate a factor

$$-\beta^{-1} \phi_{\mathbf{pqrs}} V_{\mathbf{p}-\mathbf{s}} \, \delta_{\mathbf{p}+\mathbf{q},\mathbf{r}+\mathbf{s}} \, \delta_{b+c,d+e} \, \delta_{nn'} \, \delta_{mm'}.$$

(c) Sum the final result over all values of all the particle labels, including those on the external lines.

The principal difference between the results of this expansion and that of Sec. 4 is that now the contributions of all diagrams with particle exchange vanish in the limit $\bar{N} \to \infty$, $\Omega \to \infty$, as we would expect. The formal reason this happens is that the factors of the form $\delta_{nn'}$ severely restrict the summations over particle labels in the exchange diagrams. In the diagrams without exchange, each closed loop represents a separate intermediate particle which interacts with the incoming particle or with another intermediate particle. Examples are shown in Fig. 12.

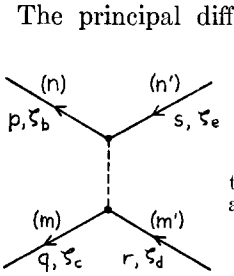

FIG. 11. A labeled vertex for the second-quantized distinguishable particle system.

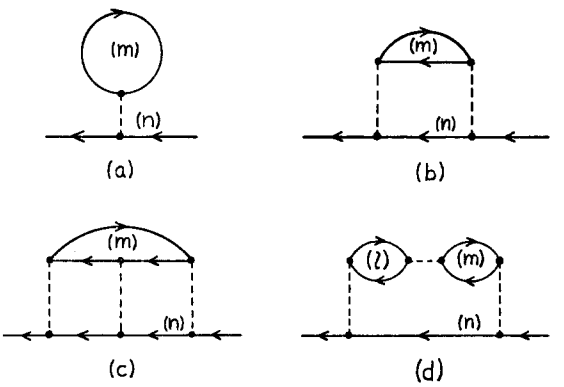

FIG. 12. Some diagrams for the system of distinguishable particles.

Suppose that we now determine the $\phi_{\mathbf{kprs}}$ by (3.6) and (3.7), the conditions for the fermion or boson ladder model. It is clear from Sec. 5.3 that if similar analysis is carried out for the present case, the surviving diagrams will be all those which arise from the irreducible diagrams Figs. 3(b), 4(a), and the ladder sequence illustrated in Fig. 6. As we have just noted, there are no exchange contributions for the present system, and consequently the exchange ladder sequence of Fig. 8 gives nothing.

Let us compare this result with what we get from the distinguishable-particle ladder model of Sec. 2. We replace (6.7) by the interaction Hamiltonian

$$H_i = \tfrac{1}{2} \sum_{nm} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}} \phi_{n,m;\mathbf{k}-\mathbf{s}} \cdot \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q^{\dagger}_{\mathbf{k}(n)} q^{\dagger}_{\mathbf{p}(m)} q_{\mathbf{r}(m)} q_{\mathbf{s}(n)}, \tag{6.10}$$

where the $\phi_{n,m;\mathbf{k}-\mathbf{s}}$ are given by (2.9) *et seq.* It is clear that the only change in the expansion for $S_{\mathbf{k}}(\zeta_a)$ is that the factor $\phi_{\mathbf{pqrs}} V_{\mathbf{p}-\mathbf{s}}$ in rule (b) above must be replaced by the factor $\phi_{n,m;\mathbf{p}-\mathbf{s}} V_{\mathbf{p}-\mathbf{s}}$.[22] We readily find that precisely the same diagrams survive in the present case as for the previous ladder model. We shall illustrate the equivalence by two examples.

[22] We may formally extend the definition of the $\phi_{n,m;\mathbf{k}}$ to include the case $n = m$, as we did in Sec. 2.3. This case represents a vanishing contribution here, in the limit $\bar{N} \to \infty$.

Consider first the diagram of Fig. 12(c) and equip it with momentum labels as in Fig. 6(a). Its contribution contains the factors

$$V_{\mathbf{k}-\mathbf{s}}V_{\mathbf{s}-\mathbf{s}'}V_{\mathbf{s}'-\mathbf{k}}\exp\{-i[(\mathbf{k}-\mathbf{s})+(\mathbf{s}-\mathbf{s}')+(\mathbf{s}'-\mathbf{k})]\cdot\mathbf{d}_{n,m}\}, \quad (6.11)$$

according to our rules and to (2.9). The phase of this expression is identically zero, and consequently the contribution survives when it is summed over the particle labels n and m in accord with rule (c). Next, however, consider the ring diagram Fig. 12(d), with momentum labels as in Fig. 7(a). Its contribution contains the factors

$$V_{\mathbf{q}}V_{\mathbf{q}}V_{\mathbf{q}}\exp[-i\mathbf{q}\cdot(\mathbf{d}_{n,l}+\mathbf{d}_{l,m}+\mathbf{d}_{m,n})], \quad (6.12)$$

where $\mathbf{q}\equiv\mathbf{k}-\mathbf{s}$ and we have used the momentum conservation relations. The phase of this expression fluctuates at random as we sum over all values of n, l, and m, so that the contribution does not survive in the limit $\bar{N}\to\infty$, $\Omega\to\infty$. (The contribution from the special value $\mathbf{q}=0$ also vanishes in the limit.)

The equivalence of the distinguishable and indistinguishable ring, random-coupling, and Hartree-Fock models may be verified in a similar fashion. We shall give one further illustration: Consider again Fig. 12(d), with momentum labels as in Fig. 7(a), but now fix the $\phi_{n,m;\mathbf{k}}$ by relation (2.19) for the ring model. The contribution from this diagram now contains the factors

$$V_{\mathbf{q}}V_{\mathbf{q}}V_{\mathbf{q}}\exp\{i[(\theta_{n;\mathbf{q}}+\theta_{l;-\mathbf{q}})+(\theta_{l;\mathbf{q}}+\theta_{m;-\mathbf{q}})+(\theta_{m;\mathbf{q}}+\theta_{n;-\mathbf{q}})]\}, \quad (6.13)$$

and we see from (2.20) that the phase vanishes.

We have seen that the thermodynamics of our second-quantized distinguishable-particle system is formally the same in the limit $\bar{N}\to\infty$, $\Omega\to\infty$ whether the models of Sec. 2 or those of Sec. 3 are used. Our argument was based on the equivalence of canonical and grand canonical ensembles for the system, and also implicitly made use of assumption 5 of Sec. 5.1, which underlies all our work. Now let us make the further assumption that in the classical limit (sufficiently high temperature and low density) the thermodynamics of fermion, boson, and distinguishable particle systems become identical in the true problem (all ϕ's = 1), provided the same values of ρ and β are taken in each case. We have seen that, except for exchange diagrams, the models of Sec. 3 select precisely the same diagrams from the true-problem expansion for $S_{\mathbf{k}}(\zeta_a)$ in all three cases: fermion, boson, and distinguishable-particle. However, the exchange diagrams do not contribute in any event in the classical limit. It then follows from all this that the models of Sec. 2, applied to a distinguishable particle system, should give the same thermodynamics in the classical limit as the models of Sec. 3, applied to fermions and bosons. It follows that the classical results of Sec. 2 for A should represent classical limits of the ring, ladder, random-coupling, and Hartree-Fock models for fermions or bosons.

It may also be possible to investigate the relation between our two kinds of models by using the formalisms of Montroll and Ward[3] or Lee and Yang,[23] neither of which require second quantization. In the method of Lee and Yang, the thermodynamics of distinguishable (Maxwell-Boltzmann) particles is expressed in terms of a "binary kernel" which is determined from the ordinary two-particle matrix elements

$$\langle\mathbf{k},\mathbf{p}\,|H_i|\,\mathbf{s},\mathbf{r}\rangle = V_{\mathbf{k}-\mathbf{s}}\,\delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}}. \quad (6.14)$$

Then an algorithm is used to obtain results for fermions or bosons. To attempt an expression of our models in this formalism, we would replace (6.14) by the model matrix element

$$\langle\mathbf{k},\mathbf{p}\,|H_i|\,\mathbf{s},\mathbf{r}\rangle_{n,m} = \phi_{n,m;\mathbf{k}-\mathbf{s}}V_{\mathbf{k}-\mathbf{s}}\,\delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} \quad (6.15)$$

for the Sec. 2 models, or by

$$\langle\mathbf{k},\mathbf{p}\,|H_i|\,\mathbf{s},\mathbf{r}\rangle_{n,m} = \phi_{\mathbf{kprs}}V_{\mathbf{k}-\mathbf{s}}\,\delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} \quad (6.16)$$

for the Sec. 3 models. Here n and m denote the pair of particles for which the matrix element is evaluated. We have not explored this procedure.

Recognition of the thermodynamic results of Sec. 2 as classical limits for the fermion and boson models may provide some useful insights into the behavior of the latter. For example, the lack of saturation found in the classical ladder model suggests that a similar lack characterizes the fermion and boson ladder models. However, the correspondence between the Sec. 2 and Sec. 3 models also leads to a rather discouraging general observation. It points out how modest are the presently feasible quantum-mechanical diagram summations compared to known classical ones. Our fermion and boson ladder and ring summations, carried out in Sec. 5.3, are more comprehensive than those usually employed; they include infinite classes of self-energy corrections which usually are omitted. Nevertheless, we have seen that the ladder summation corresponds in the classical limit to just *one term* in the Mayer irreducible cluster expansion. Similarly, our ring summation

[23] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959); **117**, 22 (1960).

represents only a partial contribution from each term of the classical irreducible ring diagram sequence. The familiar Montroll-Mayer summation (2.29) appears to correspond, in the quantum-mechanical case, to retaining both ladder and ring summations, together with the self-energy corrections of all orders obtained by repeatedly inserting the retained irreducible diagrams as self-energy parts.

7. DISCUSSION

In the present paper we have obtained formally exact closed equations which express the statistical mechanics of a class of Hermitian, momentum-conserving model Hamiltonians for infinite many-body systems. The potential value of these equations lies largely in the fact that certain of the models, the ring and ladder models, share important boundedness properties with the true many-body Hamiltonian: The eigenvalues of the ladder-model Hamiltonian are non-negative if the pair potential $V(\mathbf{x})$ is purely repulsive, and those of the ring-model Hamiltonian are bounded from below if $V(\mathbf{x})$ is bounded and has a non-negative Fourier transform.

These properties suggest that the ring and ladder models, with appropriate $V(\mathbf{x})$, should have a meaningful statistical mechanics even in the zero-temperature limit. Moreover, the structure of the models is such that they embody some important qualitative dynamical features of the true many-body system. For example, we may expect that dissipative damping of single-particle excitations survives in the models. This is particularly clear in the distinguishable-particle formulation of the models: each particle interacts individually with every other particle. A similar situation exists for the fermion and boson models, but there it is more natural to think of interaction among individual momentum modes rather than among individual particles.

The remarks just made suggest that the ladder or ring models may be appropriate for investigating whether the sharp Fermi surface of an infinite system of uncoupled fermions at zero temperature persists when the particles are coupled. Similarly, the model solutions may be of aid in deciding whether singular occupancy of the zero-momentum state, which characterizes an infinite free-boson system at very low temperatures, persists when the particles are coupled. (We anticipate here the extension of our analysis to low-temperature boson systems which will be carried out in the following paper.) The natural way in which the effective density components ρ_k appear in the ring model suggests that it may be appropriate for investigating phonon-like excitations and other collective phenomena.

However, any confidence which our rigorously bounded model Hamiltonians may inspire in a given problem does not automatically extend to the closed equations which we have derived for the model propagators. First we must establish that these equations are exact descriptions of the models in actuality, as well as formally. This has not been done in the present paper. As we discussed in Sec. 5.1, a fundamental convergence question relating to extremely high-order diagrams is involved. We shall state this question more precisely in Sec. 4 of the following paper,[11] using generalized stochastic models which yield our formally closed equations for finite as well as infinite systems. In Sec. 7 of that paper, we shall outline what we hope is the basis for a satisfying justification of our closed model propagator equations.

The analysis in the following paper is concerned almost exclusively with the indistinguishable-particle models, and we shall not attempt there to offer explicit justification for the assumptions which underlie the classical results of the present Sec. 2. However, we have already found a degree of support for these results: The closed expressions for the Helmholtz free energy obtained in Sec. 2 reproduced precisely the rigorous lower bounds on the ring and ladder model potential energies.

Our third model, the random-coupling model, exhibited no lower bound on the potential energy per particle in the limit of an infinite system. The results of Sec. 2.4 suggest that this is the case whatever the form of $V(\mathbf{x})$. Consequently, we must expect the random-coupling model not to give sensible statistical-mechanical results at zero temperature in either the classical or the quantum-mechanical case.[24]

The indicated failure of the random-coupling model at zero temperature may point a moral. We have seen in Sec. 5 that this model corresponds to taking just the lowest few diagrams in the irreducible diagram expansion of the propagator for the true many-body Hamiltonian. The failure of the model suggests that a term-by-term treatment of the irreducible diagram expansion for the true problem may not be justified at very low tempera-

[24] This does not necessarily exclude the random-coupling model for condensed boson systems. The classical equation of state (2.33) suggests admissibility at any given ρ and β provided $V(\mathbf{x})$ is weak enough. Thus the model may be admissible quantum-mechanically even below the λ-point, if $V(\mathbf{x})$ is weak enough. We regard this argument with strong suspicion.

tures, and that results obtained from such a treatment should be viewed with caution.

A general question raised by the present paper is whether there exists an infinite sequence of stochastic models which correspond to more and more comprehensive (but summable) classes of terms from the linked diagrams expansion for the true many-body problem. We have so far not succeeded in constructing substantially more elaborate models than those presented here. An obvious next step is to seek a model that combines both ring and ladder summations so as to correspond to the classical Montroll-Mayer ring-diagram summation. On the basis of a preliminary investigation, we offer the following opinion: If such a model can be constructed within the general formal framework of Sec. 3.1, it probably can be achieved only by allowing the parameters ϕ_{kprs} to have stochastically distributed moduli as well as phases. The difficulty is not in writing propagator equations which yield the desired summations but in realizing the corresponding model Hamiltonian.

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APPENDIX

We wish to discuss here two topics which arose in Sec. 2: the derivation of (2.11) for the classical models, and the significance of the condition $(\partial p/\partial\rho)_\beta < 0$ for the models.

Equation (2.11) for the true problem usually is derived on the basis of the grand canonical ensemble and rigid-wall boundary conditions. It then is formally exact in the limit $\Omega \to \infty$. [See, for example, T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), Chap. 5.] However, with our cyclic $V(\mathbf{x})$ the factoring of reducible cluster integrals into irreducible integrals is exact for any Ω. Consequently, (2.11) is formally valid for any Ω, with the grand canonical ensemble. In the limit $N \to \infty$, $\Omega \to \infty$ it is usually considered immaterial whether the grand canonical or canonical distribution is used, and we shall assume that this is so here.

In the case of our models, a grand canonical ensemble can be formed by considering each of the N particles in the canonical ensemble as a separate species and taking an activity such that the mean total number of particles over the grand ensemble is N. [In doing this, we may extend (2.5)–(2.8) to include the case $n = m$, so as to allow interaction among particles of the same species.] The derivation of (2.11) in the limit $N \to \infty$, $\Omega \to \infty$, with B_α interpreted as in the text, then depends upon two facts. First, a reducible cluster integral involving any given $\alpha + 1$ particles factors exactly into irreducible cluster integrals. As in the true problem, this is true for any Ω because $V^{n,m}(\mathbf{x})$ is cyclic. Second, if B_α is averaged over all N choices of the species of any one of the particles in the cluster, then (in the limit $N \to \infty$, $\Omega \to \infty$) the result is the same for all choices of the species of the other particles, except for a set of choices of relative measure zero. This can be seen for each of the models by analysis similar to that used in the text to evaluate the B_α. We shall not give here a detailed derivation of (2.11) for the models. It is straightforward once the two facts just stated are established.

As in the true problem, we assume in the text that the final averages for an infinite system are independent of whether the grand canonical or canonical ensemble is used. The canonical ensemble is taken in Sec. 2 because it makes the discussion simpler. In the quantum-mechanical treatment of Sec. 6, the grand ensemble is employed.

The derivation and analysis of (2.11) for the models takes a much more elegant form if one uses the generalized models described in Appendix A of reference 11. Then, with the grand ensemble, the formulation in terms of averaged irreducible clusters is exact for all N and Ω.

The statement in the text that $(\partial p/\partial\rho)_\beta < 0$ implies instability must be carefully qualified. Actually, the condition $(\partial p/\partial\rho)_\beta < 0$, or even $p < 0$, does not necessarily imply instability for any of our models, if p is defined as $\rho^2(\partial A/\partial\rho)_\beta$. This is because of the peculiar way in which the potentials $V^{n,m}(\mathbf{x})$ are constructed. The simplest illustration is provided by the Hartree-Fock model as described by (2.34) and (2.35). Suppose that we have $V_0 < 0$, so that the potential energy per particle (which is just $A - A_0$ for this model) decreases without limit as ρ increases; that is, as we pack more particles into a fixed volume Ω. By (2.35), we have $p < 0$ and $(\partial p/\partial\rho)_\beta < 0$, if ρ is high enough. However, since each particle moves in a uniform potential, the potential energy is independent of configuration, for given N and Ω, and the system is not unstable. Instability arises only if, as we pack the N particles into a closer configuration, *we decrease correspondingly the volume of the cyclic cube.* Then, since $V_0 \propto \Omega^{-1}$, the potential energy becomes increas-

ingly negative and the system can collapse catastrophically.

It is likely that the relation $(\partial p/\partial \rho)_\beta < 0$ has a similar interpretation for all the models treated in this paper. This condition need not imply instability if Ω is fixed, which it must be as we have defined the models. However, if we were to allow Ω to vary in accordance with the actual gross volume occupied by the particles, there would be instability. Having Ω vary would actually be a physically appropriate procedure, as the Hartree-Fock example suggests. For this reason, we consider $(\partial p/\partial \rho)_\beta < 0$ to be an instability indication in making a physical interpretation of our models.

It should be noted also that the lack of a lower bound on the potential energy of a system does not preclude a stable thermodynamics. If the density-of-states $\sigma(E)$ (where E is the total energy) decreases faster than exponentially as $E \to -\infty$, a stable thermal equilibrium can exist for all finite β. If the decrease is slower than exponential, equilibrium will be impossible at any β, while, if the decrease is exponential, equilibrium can exist only if β is less than a critical value.

We wish finally to note the conclusion of L. Van Hove [Physica **15**, 951 (1949)] that $(\partial p/\partial \rho)_\beta < 0$ cannot be an exact theoretical result for a gas of pairwise-interacting particles. Although it seems assuredly valid for actual physical systems, Van Hove's result does not appear to be applicable here. Our models violate an assumption basic to his analysis: The $V^{n,m}(\mathbf{x})$ are defined in such a way that is is not possible to divide the system into effectively noninteracting macroscopic sub-volumes. (Van Hove's result clearly is not valid for the Hartree-Fock example discussed above.) It should be stressed, however, that the results obtained in Sec. 2 are not rigorously justified by the analysis we have presented. As we have noted, there is a fundamental convergence question involved.

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Stochastic Models for Many-Body Systems. II. Finite Systems and Statistical Nonequilibrium*

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In a preceding paper [J. Math. Phys. **3**, 475 (1962)], some model Hamiltonians were proposed for quantum-mechanical many-body systems with pair forces. For infinite systems in thermal equilibrium, they led to temperature-domain propagator expansions which were formally summable and expressible by closed equations. These expansions were identical with infinite subclasses of terms from the propagator expansion for the true many-body problem. The two principal models corresponded to ring- and ladder-diagram summations from the true propagator expansion, augmented by infinite classes of self-energy corrections. The model Hamiltonians were called stochastic because they contained parameters whose phases were fixed by random choices. In the present paper, more general models are formulated which yield formally summable propagator expansions for finite systems. The analysis is extended to correlation and Green's functions defined for nonequilibrium ensembles. The nonequilibrium treatment is developed in the Heisenberg representation in such a way that unlinked diagrams do not arise. A basic convergence question associated with the formal closed equations for the model propagators and correlation functions is examined by means of finite-difference integration of the Heisenberg equations of motion. This procedure appears to converge independently of whether the perturbation expansions for the propagators and correlation functions converge. It yields substantial support for the validity of the formal closed model equations.

1. INTRODUCTION

IN the preceding paper[1] (cited herein as I), some so-called stochastic-model Hamiltonians were developed for fermion or boson many-body systems with pair forces. The models yielded temperature-domain particle propagators whose linked-diagram expansions could be formally summed and expressed by closed integral equations. The model propagator expansions were identical with infinite classes of terms from the propagator expansion for the true many-body Hamiltonian. The model Hamiltonians were called stochastic because they contained infinite numbers of parameters whose phases were fixed by random choices. Certain of the models, called the ladder and ring models, had important boundedness properties in common with the true many-body Hamiltonian. For this reason, it was felt that they might represent useful approximations to the behavior of the true system, particularly at low temperatures.

The models described in I led to closed propagator equations only in the limit of an infinite system. In the present paper, we develop more general models which yield formally summable propagator expansions for systems of any size. With the new formulation, no special considerations are required to treat boson systems at very low temperatures, a case which was excluded in I. Moreover, the entire procedure of obtaining the closed propagator equations can be carried out in a neater and more satisfactory fashion. In the limit of an infinite system, the final propagator equations obtained from the old and new models are identical.

The models employed in I were constructed by altering, in a stochastic fashion, the true interactions among the momentum modes of a second-quantized fermion or boson field. Corresponding models for distinguishable particles were constructed by altering the interaction among pairs of particles in a way that was different for each pair. In the present paper, we start with a collection of M similar fermion or boson systems, where before we treated a single many-body system. The M systems are assumed to occupy the same space but not to interact. The particles in each system are distinguishable from those in all the other systems. As a preliminary to constructing stochastic models, we introduce a collective description: We define M quantized fields which are linear combinations of the quantized fields of the M many-body systems. Then we alter in a stochastic fashion the true dynamical couplings among the collective fields. As a result of the alteration, the individual systems in the collection, which are independent in the true problem, turn out to be dynamically coupled in the models. The eventual closed equations for particle-propagators are obtained by considering a

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[1] R. H. Kraichnan, J. Math. Phys. **3**, 475 (1962).

grand canonical ensemble of collections and taking the limit $M \to \infty$.

We shall be principally concerned only with fermions and bosons in the present paper. For completeness, however, we shall describe in Appendix A the corresponding models for distinguishable particles.

The derivation of the closed propagator equations for the models, both in I and in the present paper, involves a fundamental convergence question concerning the contribution of classes of infinite-order diagrams. No attempt to resolve this question was made in I. In the second part of the present paper, we investigate the convergence question by extending the analysis to systems not in statistical equilibrium and treating equilibrium as a limiting case. The nonequilibrium formalism which we use is a direct adaptation, to second-quantized fields, of a method previously developed for the theory of turbulence.[2] Instead of the temperature-domain particle propagators, we employ correlation and Green's functions which are defined for time-dependent statistical ensembles where no temperature exists. In the limit of thermal equilibrium, these quantities are related by analytic continuation to the temperature-domain propagators.

As we shall see, there exist both primitive and irreducible linked-diagram expansions which give the evolution of the correlation and Green's functions forward in time from a given initial instant. It is convenient to develop the expansions in the Heisenberg representation. Then, unlinked diagrams do not arise, and therefore need not be eliminated. As in the equilibrium case, the stochastic model Hamiltonians yield irreducible linked-diagram expansions which are formally summable and expressible by closed integral equations.

In the time-dependent treatment, however, the validity of the formally closed equations can be examined by methods which do not involve perturbation analysis. Our procedure is to replace the exact Heisenberg equations of motion by corresponding difference equations involving small time-increments. Evidence is presented that this procedure should yield convergent results for the correlation and Green's functions, as the increment size is decreased to zero, independently of whether the perturbation expansions for these functions converge. The finite-difference approach yields what we regard as substantial support for the validity of the formal closed model equations. It should be stressed at the outset, however, that our analysis is neither complete nor rigorous and therefore is not conclusive.

The nonequilibrium reducible and irreducible linked-diagram expansions apply to the true Hamiltonian as well as to the models considered here. Apart from nonequilibrium situations as such, they may prove to be a useful tool in the equilibrium limit. There, the expansions deal in a consistent fashion with the propagators in the real time or real frequency domains, without the necessity of representing these quantities as analytic continuations of propagators with imaginary time or complex frequency arguments.

2. GENERALIZED STOCHASTIC MODELS FOR FERMIONS AND BOSONS

2.1. Collective Representation of a Collection of Systems

Let us consider a system of fermions or bosons with Hamiltonian

$$H = H_0 + H_i, \qquad H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} q_{\mathbf{k}}^\dagger q_{\mathbf{k}}, \tag{2.1}$$

$$H_i = \tfrac{1}{2} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}}\, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q_{\mathbf{k}}^\dagger q_{\mathbf{p}}^\dagger q_{\mathbf{r}} q_{\mathbf{s}}, \tag{2.2}$$

where $q_{\mathbf{k}}^\dagger$ and $q_{\mathbf{k}}$ are fermion or boson creation and destruction operators for a particle of momentum $\mathbf{k}$, the $\epsilon_{\mathbf{k}}$ are the free-particle energies, $V_{\mathbf{k}}$ is a Fourier component of the pair potential, and the summation is over all momenta allowed by cyclic boundary conditions on the walls of a box of volume $\Omega = L^3$. We take $\hbar = 1$. This is identical with the Hamiltonian I:(3.1), I:(3.2).[3] We shall continue to call it the true Hamiltonian. As in I, the pair potential in x space is given by

$$V(\mathbf{x}) = \sum_{\mathbf{k}} V_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}) \tag{2.3}$$

and obeys

$$V(\mathbf{x}) = V(-\mathbf{x}), \quad V_{\mathbf{k}} = V_{-\mathbf{k}}, \quad V_{\mathbf{k}} = V_{\mathbf{k}}^* \tag{2.4}$$

We require further that $V(\mathbf{x})$ be finite everywhere and that

$$V_{\mathbf{k}} \leq O(k^{-2}) \qquad k \to \infty. \tag{2.5}$$

Now, instead of a single many-body system, let

[2] R. H. Kraichnan, J. Math. Phys. **2**, 124 (1961); Erratum, **3**, 205 (1962). The formalism to be developed in the present paper is less general than in this reference because we shall not discuss cases where the quantized field $\psi(\mathbf{x})$ has nonzero expectation $\langle\psi(\mathbf{x})\rangle$. Adaptation of the more general formalism may prove desirable for treating condensed boson systems.

[3] The notation I: (3.1) denotes Eq. (3.1) of I. Such notation will be used throughout the present paper. Sections and figures in I will be denoted in the forms I: Sec. 3 and I: Fig. 2.

us consider a collection of M similar systems described by the individual second-quantized fields

$$\psi_{[n]}(\mathbf{x}) = \Omega^{-\frac{1}{2}} \sum_{\mathbf{k}} q_{\mathbf{k}[n]} \exp(i\mathbf{k}\cdot\mathbf{x}) \qquad (n = 1, 2, \cdots, M). \tag{2.6}$$

Let the true total Hamiltonian for the collection of systems be

$$\mathcal{H} = \sum_n H_{[n]}, \tag{2.7}$$

$$H_{[n]} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} q^\dagger_{\mathbf{k}[n]} q_{\mathbf{k}[n]} + \tfrac{1}{2} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}}\, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} q^\dagger_{\mathbf{k}[n]} q^\dagger_{\mathbf{p}[n]} q_{\mathbf{r}[n]} q_{\mathbf{s}[n]}.$$

We shall take the commutation rules as

$$[q_{\mathbf{k}[n]}, q_{\mathbf{p}[m]}]_\mp = 0, \quad [q_{\mathbf{k}[n]}, q^\dagger_{\mathbf{p}[m]}]_\mp = \delta_{nm}\, \delta_{\mathbf{kp}}. \tag{2.8}$$

Thus the individual systems exist in the same box but otherwise are entirely independent.[4] In (2.8), and throughout the paper, the upper sign of a double sign refers to fermions, and the lower to bosons.

As a preliminary to constructing stochastic models, we shall express $\mathcal{H}$ in terms of collective fields which are linear combinations of the $\psi_{[n]}(\mathbf{x})$. Let us restrict M to the form $M = 2S + 1$, where S is a positive integer. We define the collective fields $\psi_\alpha(\mathbf{x})$ by

$$\psi_\alpha(\mathbf{x}) = M^{-\frac{1}{2}} \sum_n \exp(i2\pi\alpha n/M)\psi_{[n]}(\mathbf{x}),$$
$$\psi^\dagger_\alpha(\mathbf{x}) = M^{-\frac{1}{2}} \sum_n \exp(-i2\pi\alpha n/M)\psi^\dagger_{[n]}(\mathbf{x}), \tag{2.9}$$

where

$$\alpha = -S, \cdots, -1, 0, 1, \cdots, S.$$

We shall call α a collective index.[5] By using the identities

$$M^{-1} \sum_n \exp[i2\pi(\alpha - \beta)n/M] = \delta_{\alpha\beta},$$
$$M^{-1} \sum_\alpha \exp[i2\pi\alpha(n - m)/M] = \delta_{nm}, \tag{2.10}$$

we may invert (2.9) and obtain

$$\psi_{[n]}(\mathbf{x}) = M^{-\frac{1}{2}} \sum_\alpha \exp(-i2\pi\alpha n/M)\psi_\alpha(\mathbf{x}). \tag{2.11}$$

Collective destruction and creation operators $q_{\mathbf{k}\alpha}$ and $q^\dagger_{\mathbf{k}\alpha}$ may be defined by

$$\psi_\alpha(\mathbf{x}) = \Omega^{-\frac{1}{2}} \sum_{\mathbf{k}} q_{\mathbf{k}\alpha} \exp(i\mathbf{k}\cdot\mathbf{x}), \tag{2.12}$$

with a corresponding relation for $q^\dagger_{\mathbf{k}\alpha}$. These operators satisfy

$$q_{\mathbf{k}\alpha} = M^{-\frac{1}{2}} \sum_n \exp(i2\pi\alpha n/M) q_{\mathbf{k}[n]},$$
$$q_{\mathbf{k}[n]} = M^{-\frac{1}{2}} \sum_\alpha \exp(-i2\pi\alpha n/M) q_{\mathbf{k}\alpha}. \tag{2.13}$$

It is clear from this that the transformation to the collective fields represents a complex rotation in the space of the $q_{\mathbf{k}[n]}$. By (2.8), (2.10), and (2.13), the commutation rules in the collective representation are

$$[q_{\mathbf{k}\alpha}, q_{\mathbf{p}\beta}]_\mp = 0, \qquad [q_{\mathbf{k}\alpha}, q^\dagger_{\mathbf{p}\beta}]_\mp = \delta_{\alpha\beta}\, \delta_{\mathbf{kp}}. \tag{2.14}$$

Let us adopt the cyclic convention

$$\alpha \equiv \alpha + M, \qquad n \equiv n + M \tag{2.15}$$

for collective indices and individual-system labels. This clearly is consistent with (2.9)–(2.11). Then, by using (2.13) and (2.10), we may rewrite $\mathcal{H}$ in the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_i, \qquad \mathcal{H}_0 = \sum_\alpha \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} q^\dagger_{\mathbf{k}\alpha} q_{\mathbf{k}\alpha}, \tag{2.16}$$

$$\mathcal{H}_i = \tfrac{1}{2} M^{-1} \sum_{\alpha\beta\lambda} \sum_{\mathbf{kprs}} V_{\mathbf{k}-\mathbf{s}}\, \delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} \times \delta_{\alpha+\beta,\mu+\lambda} q^\dagger_{\mathbf{k}\alpha} q^\dagger_{\mathbf{p}\beta} q_{\mathbf{r}\mu} q_{\mathbf{s}\lambda}, \tag{2.17}$$

where $\delta_{\alpha+\beta,\mu+\lambda}$ is to be interpreted by the cyclic convention. We see from (2.17) that the collective fields, in contrast to the individual-system fields, are dynamically coupled by the interaction $V(\mathbf{x})$.

It is clear from the definitions, and also from an examination of (2.14) and (2.17), that the momenta $\mathbf{k}$ and the collective indices α have some formal properties in common. In particular, the factor $\delta_{\alpha+\beta,\mu+\lambda}$ in (2.17) gives a conservation property analogous to momentum conservation. The underlying similarity may be expressed as follows. Consider the case where Ω is very large, so that each many-body system, described by a field $\psi_{[n]}(\mathbf{x})$, is effectively composed of many spatially localized subsystems. Then the Fourier components $q_{\mathbf{k}\alpha}$, considered as functions of $\mathbf{k}$, provide a collective description of the sub-systems in x space. On the other hand, suppose we take M large instead of Ω large. Then the $q_{\mathbf{k}\alpha}$, considered as functions of α, provide a collective description in "n space."[6]

[4] The present procedure should not be confused with that used in I: Sec. 6. There, each second-quantized field represented a single particle instead of a whole many-body system.

[5] In order to minimize confusion in expressions with multiple indices, we shall denote individual-system quantities by square-bracketed italic indices and collective-field quantities by unbracketed Greek indices throughout this paper. Momenta and 'energies' will be denoted by unbracketed Latin indices, as in I.

[6] See Sec. 3 of reference 2 for a discussion of the physical significance of this similarity in a classical context.

2.2. Formulation of Models

In order to construct stochastic models, we replace (2.17) by the more general form

$$\mathcal{H}_i = \tfrac{1}{2}M^{-1} \sum_{\alpha\beta\mu\lambda} \sum_{\mathbf{kprs}} V_{\mathbf{k-s}} \phi_{\alpha\beta\mu\lambda} \times \delta_{\mathbf{k+p,r+s}}\, \delta_{\alpha+\beta,\mu+\lambda} q^\dagger_{\mathbf{k}\alpha} q^\dagger_{\mathbf{p}\beta} q_{\mathbf{r}\mu} q_{\mathbf{s}\lambda}. \quad (2.18)$$

The c number coefficients $\phi_{\alpha\beta\mu\lambda}$ play a role analogous to that of the $\phi_{\mathbf{kprs}}$ in I:(3.4). We impose upon these coefficients the Hermiticity and symmetry constraints

$$\phi_{\alpha\beta\mu\lambda} = \phi^*_{\lambda\mu\beta\alpha}, \qquad \phi_{\alpha\beta\mu\lambda} = \phi_{\beta\alpha\lambda\mu}. \quad (2.19)$$

Then we make stochastic assignments of values to the $\phi_{\alpha\beta\mu\lambda}$ so as to obtain the several stochastic models. We give below the prescriptions which yield the present analogs of the ladder, ring, random-coupling, and Hartree-Fock models defined and discussed in I. In each model, the form of $\phi_{\alpha\beta\mu\lambda}$ is identical with that of $\phi_{\mathbf{kprs}}$ in I:Sec.3.

Ladder Model

Take

$$\phi_{\alpha\beta\mu\lambda} = \exp\,[i(-\theta_{\beta\alpha} + \theta_{\mu\lambda})], \quad (2.20)$$

$$\theta_{\alpha\beta} = \theta_{\beta\alpha}. \quad (2.21)$$

Determine the real phases $\theta_{\alpha\beta}$ by independent random choices in the interval $(0, 2\pi)$, subject only to (2.21).

Ring Model

Take

$$\phi_{\alpha\beta\mu\lambda} = \exp\,[i(\bar{\theta}_{\alpha\lambda} + \bar{\theta}_{\beta\mu})], \quad (2.22)$$

$$\bar{\theta}_{\alpha\lambda} = -\bar{\theta}_{\lambda\alpha}. \quad (2.23)$$

Determine the phases $\bar{\theta}_{\alpha\lambda}$ by independent random choices subject only to (2.23).

Random-Coupling Model

Take

$$\phi_{\alpha\beta\mu\lambda} = \exp\,(i\theta_{\alpha\beta\mu\lambda}), \quad (2.24)$$

$$\theta_{\alpha\beta\mu\lambda} = -\theta_{\lambda\mu\beta\alpha},\ \theta_{\alpha\beta\mu\lambda} = \theta_{\beta\alpha\lambda\mu},\ \theta_{\alpha\beta\mu\lambda} = \theta_{\beta\alpha\mu\lambda}. \quad (2.25)$$

Determine the phases $\theta_{\alpha\beta\mu\lambda}$ by independent random choices subject only to (2.25).

Hartree-Fock Model

Take

$$\phi_{\alpha\beta\beta\alpha} = \phi_{\alpha\beta\alpha\beta} = 1, \qquad \phi_{\alpha\beta\mu\lambda} = 0 \quad (\alpha \neq \mu \text{ or } \lambda). \quad (2.26)$$

There are no random parameters.

The models obtained by the prescriptions just given are stochastic in the same sense as discussed in I:Sec.2.2. The values of the $\phi_{\alpha\beta\mu\lambda}$ are determined by random choices. Once obtained, however, the values are fixed, and we work thereafter with the definite Hamiltonian embodying these values. To obtain an insight as to the physical interpretation of the present models, it is of value to transform (2.18) back to the individual-system representation. We find

$$\mathcal{H}_i = \tfrac{1}{2} \sum_{nmn'm'} \sum_{\mathbf{kprs}} V_{\mathbf{k-s}} A_{[nmm'n']} \times \delta_{\mathbf{k+p,r+s}} q^\dagger_{\mathbf{k}[n]} q^\dagger_{\mathbf{p}[m]} q_{\mathbf{r}[m']} q_{\mathbf{s}[n']}, \quad (2.27)$$

where

$$A_{[nmm'n']} = M^{-3} \sum_{\alpha\beta\mu\lambda} \delta_{\alpha+\beta,\mu+\lambda} \phi_{\alpha\beta\mu\lambda} \times \exp\,[i2\pi(-n\alpha - m\beta + m'\mu + n'\lambda)/M]. \quad (2.28)$$

When all the $\phi_{\alpha\beta\mu\lambda} = 1$, it follows from (2.10) that

$$A_{[nmm'n']} = \delta_{nn'}\, \delta_{mm'}\, \delta_{nm}.$$

Then $\mathcal{H}$ reduces to (2.7), giving us back the true problem in which the individual systems are dynamically independent. In the models, however, $A_{[nmm'n']}$ is not diagonal, and the systems in the collection are coupled. They exchange particles as well as energy and momentum. We see from (2.27) that the elementary interaction is a collision in which a pair of particles from systems n' and m' are destroyed and a pair in systems n and m created.

2.3. Bounds on the Ladder and Ring Model Hamiltonians

Bounds on the eigenvalues of $\mathcal{H}$ for the ladder and ring models may be derived in close analogy to I:Sec.3. In the case of the ladder model, let us define the effective two-body amplitudes

$$\chi_\epsilon(\mathbf{x}', \mathbf{x}) = M^{-\frac{1}{2}} \sum_{\mu\lambda} \delta_{\mu+\lambda,\epsilon} \psi_\mu(\mathbf{x}') \psi_\lambda(\mathbf{x}) \exp\,(i\theta_{\mu\lambda}), \quad (2.29)$$

where (2.15) is to be used in interpreting $\delta_{\mu+\lambda,\epsilon}$. Then, noting (2.12), we may write (2.18) for the ladder model in the form

$$\mathcal{H}_i = \tfrac{1}{2} \sum_\epsilon \times \iint V(\mathbf{x} - \mathbf{x}') \chi^\dagger_\epsilon(\mathbf{x}', \mathbf{x}) \chi_\epsilon(\mathbf{x}', \mathbf{x})\, d^3x\, d^3x'. \quad (2.30)$$

It is clear from (2.30) that $\mathcal{H}_i$ is a non-negative operator if $V(\mathbf{x}) = |V(\mathbf{x})|$ everywhere. It then follows that the eigenvalues of $\mathcal{H}$ are all non-negative in this case.

In the case of the ring model, we define the effective density components $\rho_{\mathbf{k}\epsilon}$ by

$$\rho_\epsilon(\mathbf{x}) = \sum_{\mathbf{k}} \rho_{\mathbf{k}\epsilon} \exp(i\mathbf{k}\cdot\mathbf{x}), \tag{2.31}$$

$$\rho_\epsilon(\mathbf{x}) = M^{-\frac{1}{2}} \sum_{\alpha} \psi^\dagger_\alpha(\mathbf{x})\psi_{\alpha+\epsilon}(\mathbf{x}) \exp(i\bar{\theta}_{\alpha,\alpha+\epsilon}). \tag{2.32}$$

Then, using (2.14) and (2.23), we find

$$\mathfrak{IC}_i = \tfrac{1}{2} \sum_{\epsilon} \sum_{\mathbf{k}} V_{\mathbf{k}} \rho^\dagger_{\mathbf{k}\epsilon}\rho_{\mathbf{k}\epsilon} - \tfrac{1}{2}V(0)\mathfrak{N}, \tag{2.33}$$

where $\mathfrak{N}$, the operator for the total number of particles in the collection, is defined by

$$\begin{aligned} \mathfrak{N} &= \sum_\alpha N_\alpha = \sum_n N_{[n]}, \\ N_\alpha &= \sum_{\mathbf{k}} q^\dagger_{\mathbf{k}\alpha} q_{\mathbf{k}\alpha}, \\ N_{[n]} &= \sum_{\mathbf{k}} q^\dagger_{\mathbf{k}[n]} q_{\mathbf{k}[n]}. \end{aligned} \tag{2.34}$$

If $V_{\mathbf{k}} = |V_{\mathbf{k}}|$ for all $\mathbf{k}$, then the first term on the the right side of (2.33) is a non-negative operator, and the energy per particle in any eigenstate of $\mathfrak{N}$ is bounded from below by $-\frac{1}{2}V(0)$.

3. PROPAGATOR EXPANSIONS FOR THE MODELS

In analogy to I:Sec. 4, let us define the temperature-domain propagator $S_{\mathbf{k}[nm]}(u, u')$ by

$$S_{\mathbf{k}[nm]}(u, u') = -\langle T q_{\mathbf{k}[n]}(u) q^\dagger_{\mathbf{k}[m]}(u')\rangle, \tag{3.1}$$

where, for any operator B,

$$\begin{aligned} B(u) &= \exp(u\mathfrak{IC})B \exp(-u\mathfrak{IC}), \\ B^\dagger(u) &= \exp(u\mathfrak{IC})B^\dagger \exp(-u\mathfrak{IC}). \end{aligned} \tag{3.2}$$

The ordering operator T is the same as in I, and the brackets denote an average over a grand canonical ensemble of collections of systems: For any B,

$$\langle B\rangle = \mathrm{Tr}\{\exp[-\beta(\mathfrak{IC} - \mu\mathfrak{N})]B\} / \mathrm{Tr}\{\exp[-\beta(\mathfrak{IC} - \mu\mathfrak{N})]\}. \tag{3.3}$$

Let us also define the propagator in the collective representation by

$$S_{\mathbf{k}\alpha\beta}(u, u') = -\langle T q_{\mathbf{k}\alpha}(u) q^\dagger_{\mathbf{k}\beta}(u')\rangle. \tag{3.4}$$

'Energy'-domain propagators $S_{\mathbf{k}[nm]}(\zeta_a)$ and $S_{\mathbf{k}\alpha\beta}(\zeta_a)$ may be defined in terms of $S_{\mathbf{k}[nm]}(u, u')$ and $S_{\mathbf{k}\alpha\beta}(u, u')$ by means of relations of the form I:(4.6).

For free particles ($\mathfrak{IC}_i = 0$), it follows from (2.8), (2.14), and (2.16) that

$$\begin{aligned} S_{\mathbf{k}[nm]}(\zeta_a) &= \delta_{nm} S^{(0)}_{\mathbf{k}}(\zeta_a), \\ S_{\mathbf{k}\alpha\beta}(\zeta_a) &= \delta_{\alpha\beta} S^{(0)}_{\mathbf{k}}(\zeta_a), \end{aligned} \tag{3.5}$$

where $S^{(0)}_{\mathbf{k}}(\zeta_a)$ is given by I:(4.11). For the true Hamiltonian (all $\phi_{\alpha\beta\mu\lambda} = 1$), we have

$$S_{\mathbf{k}[nm]}(\zeta_a) = \delta_{nm} S_{\mathbf{k}}(\zeta_a), \tag{3.6}$$

where $S_{\mathbf{k}}(\zeta_a)$ is the true propagator, as defined in I, for any one of the systems in the collection. This follows immediately from the independence of the individual systems. In this case, we find

$$S_{\mathbf{k}\alpha\beta}(\zeta_a) = \delta_{\alpha\beta} S_{\mathbf{k}}(\zeta_a), \tag{3.7}$$

where we have used (2.13) and (2.10).

In correspondence to I:(4.8) and I:(4.10), the mean number of particles and the mean energy in the collection may be expressed for the models in the forms

$$\begin{aligned} \mathfrak{N}(\beta, \mu) &= \pm\beta^{-1} \sum_{\alpha\mathbf{k}a} S_{\mathbf{k}\alpha\alpha}(\zeta_a) \exp(\zeta_a \delta) \\ &= \pm\beta^{-1} \sum_{n\mathbf{k}a} S_{\mathbf{k}[nn]}(\zeta_a) \exp(\zeta_a \delta) \end{aligned} \tag{3.8}$$

and

$$\begin{aligned} \mathcal{E}(\beta, \mu) &= \pm\tfrac{1}{2}\beta^{-1} \sum_{\alpha\mathbf{k}a} (\epsilon_{\mathbf{k}} + \zeta_a) S_{\mathbf{k}\alpha\alpha}(\zeta_a) \exp(\zeta_a \delta) \\ &= \pm\tfrac{1}{2}\beta^{-1} \sum_{n\mathbf{k}a} (\epsilon_{\mathbf{k}} + \zeta_a) S_{\mathbf{k}[nn]}(\zeta_a) \exp(\zeta_a \delta). \end{aligned} \tag{3.9}$$

Equation (3.9) may be derived in the same way as I:(4.10). The mean number of particles per system and the mean energy per system are then given by

$$N(\beta, \mu) = M^{-1}\mathfrak{N}(\beta, \mu), \qquad E(\beta, \mu) = M^{-1}\mathcal{E}(\beta, \mu). \tag{3.10}$$

For the true problem (all $\phi_{\mathbf{kprs}} = 1$ in I and all $\phi_{\alpha\beta\mu\lambda} = 1$ in the present case), $N(\beta, \mu)$ and $E(\beta, \mu)$ are exactly the same functions of β and μ here as in I.

Let us now consider the primitive linked-diagram expansion for the model $S_{\mathbf{k}\alpha\beta}(\zeta_a)$. First of all, it is easy to verify that

$$S_{\mathbf{k}\alpha\beta}(\zeta_a) = \delta_{\alpha\beta} S_{\mathbf{k}\alpha\alpha}(\zeta_a). \tag{3.11}$$

This follows immediately from (3.5) and the presence of the conservation factor $\delta_{\alpha+\beta,\mu+\lambda}$ in (2.18). Because of the similarity of the ways the momenta $\mathbf{k}$ and the collective indices α enter $\mathfrak{IC}$, the primitive linked-diagram expansion for $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$ is given by rules which are obvious generalizations of rules 1–8 of I:Sec.4. We shall state here only the *changes* which are required in the rules of I:

Rule 3. Label the external lines with collective index α as well as momentum $\mathbf{k}$. Label the internal lines with collective indices α', α'', $\cdots$ as well as with momenta $\mathbf{k}'$, $\mathbf{k}''$, $\cdots$.

Rule 5. With each vertex labeled as in Fig. 1 of the present paper, associate a factor

$$-M^{-1}\beta^{-1}\phi_{\beta\gamma\mu\lambda}\, \delta_{\beta+\gamma,\mu+\lambda} V_{\mathbf{p}-\mathbf{s}}\, \delta_{\mathbf{p}+\mathbf{q},\mathbf{r}+\mathbf{s}}\, \delta_{b+c,d+e}.$$

Rule 7. Sum over all the intermediate collective indices $\alpha', \alpha'', \cdots$ as well as over all the intermediate momenta and 'energies.'

According to the present rules, the contribution of any diagram to $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$ has the following form. It consists of a product of V and $S^{(0)}$ factors, summed over momenta and energies, which is multiplied by a product of ϕ's, summed over collective indices. The latter summed product contains the *entire* dependence of the contribution upon the ϕ's and upon α. The summed product of V and $S^{(0)}$ factors is identical with the contribution which the diagram makes to $S_{\mathbf{k}}(\zeta_a)$ in the true problem, where $S_{\mathbf{k}}(\zeta_a)$ is defined as in I. In order to express this result compactly, let us write $S_{\mathbf{k}}(\zeta_a)$ for the true problem in the form

$$S_{\mathbf{k}}(\zeta_a) = S_{\mathbf{k}}^{(0)}(\zeta_a) + \sum_{n=1}^{\infty} \sum_{p} \Gamma_{n;p}(\mathbf{k}, a). \tag{3.12}$$

Here $\Gamma_{n;p}(\mathbf{k}, a)$ is the contribution from a particular distinct linked diagram with n vertices. The index p takes the values $1, 2, \cdots, R(n)$, where $R(n)$ is the number of distinct linked diagrams with n vertices; it labels the $R(n)$ diagrams according to any convenient scheme. We may now write the primitive linked-diagram expansion for the model propagator $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$ as

$$S_{\mathbf{k}\alpha\alpha}(\zeta_a) = S_{\mathbf{k}}^{(0)}(\zeta_a) + \sum_{n=1}^{\infty} \sum_{p} C_{n;p}(\alpha)\Gamma_{n;p}(\mathbf{k}, a), \tag{3.13}$$

where $C_{n;p}(\alpha)$ denotes the summed ϕ product associated with the pth distinct diagram with n vertices. The $\Gamma_{n;p}(\mathbf{k}, a)$ in (3.13) are precisely the same quantities as in (3.12).

We may illustrate the results stated in the last paragraph by considering the contributions to $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$ made by two simple primitive diagrams. Let us assign the value $p = 1$ to the diagram of Fig. 2(a). Then the rules for constructing diagram contributions give

$$\Gamma_{1;1}(\mathbf{k}, a) = \pm\beta^{-1} \sum_{\mathbf{p}b} V_0 S_{\mathbf{k}}^{(0)}(\zeta_a) S_{\mathbf{p}}^{(0)}(\zeta_b) \times \exp(\zeta_b \delta) S_{\mathbf{k}}^{(0)}(\zeta_a), \tag{3.14}$$

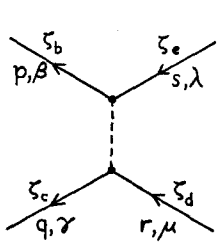

FIG. 1. A labeled vertex.

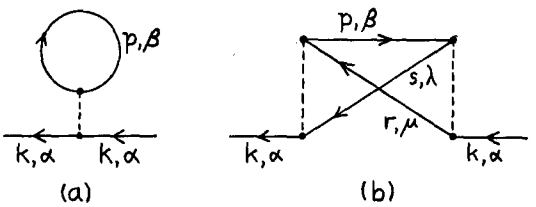

FIG. 2. (a) The diagram associated with $C_{1;1}(\alpha)$; (b) the diagram associated with $C_{2;2}(\alpha)$.

$$C_{1;1}(\alpha) = M^{-1} \sum_{\beta} \phi_{\alpha\beta\beta\alpha}. \tag{3.15}$$

Let us assign the value $p = 2$ to the diagram of Fig. 2(b). Then the rules give

$$\Gamma_{2;2}(\mathbf{k}, a) = \beta^{-2} \sum_{\mathbf{p}\mathbf{s}bc} V_{\mathbf{k}-\mathbf{s}} V_{\mathbf{s}-\mathbf{p}} S_{\mathbf{k}}^{(0)}(\zeta_a) S_{\mathbf{p}}^{(0)}(\zeta_b) \times S_{\mathbf{s}}^{(0)}(\zeta_c) S_{\mathbf{k}+\mathbf{p}-\mathbf{s}}^{(0)}(\zeta_{a+b-c}) S_{\mathbf{k}}^{(0)}(\zeta_a), \tag{3.16}$$

$$C_{2;2}(\alpha) = M^{-2} \sum_{\beta\mu\lambda} \delta_{\alpha+\beta,\mu+\lambda} \phi_{\alpha\beta\mu\lambda} \phi_{\lambda\mu\alpha\beta}. \tag{3.17}$$

Equations (3.15) and (3.17) illustrate a general property of the $C_{n;p}(\alpha)$. The number of M^{-1} factors is always equal to the number of free indices in the summation. Hence in the true problem (all $\phi_{\alpha\beta\mu\lambda} = 1$), we have $C_{n;p}(\alpha) = 1$ for all n and p, as we must for consistency.

Let us now consider the limit $M \to \infty$, which represents an infinite collection of many-body systems. We keep μ fixed as we take the limit. For the true problem, $N(\beta, \mu)$ and $E(\beta, \mu)$ are then independent of M, as we have noted previously. It will appear from what follows that $N(\beta, \mu)$ and $E(\beta, \mu)$ for the models are independent of M in the limit. The present limit $M \to \infty$ plays the same role as the limit $\Omega \to \infty$ (infinite volume) did in I. We found the following general result in I: For any given model, a given diagram survived in the limit $\Omega \to \infty$ if and only if the associated ϕ product had the value one for all values of the intermediate momenta permitted by momentum conservation. The corresponding result in the present case is that a given diagram survives in the limit $M \to \infty$ if and only if the associated ϕ product [i.e., the summand of $C_{n;p}(\alpha)$] has the value one for all values of the intermediate collective indices permitted by collective-index conservation. For each surviving diagram we therefore have $C_{n;p}(\alpha) = 1$, as in the true problem. The demonstration of the present result is neater than that in I because the entire collective-index dependence of each diagram contribution is contained in the ϕ product, whereas in the former treatment the ϕ factors, $S^{(0)}$ factors, and V factors all depended on the intermediate momenta.

The correspondence between the survival of diagrams in the old treatment and the present should become clear upon comparing the following two examples with the corresponding examples in I:Sec.5.3. For the ladder model, we have

$$C_{2;2}(\alpha) = M^{-2} \sum_{\beta\lambda} \exp\,[i(-\theta_{\beta\alpha} + \theta_{\alpha+\beta-\lambda,\lambda}) + i(-\theta_{\alpha+\beta-\lambda,\lambda} + \theta_{\beta\alpha})] = 1, \qquad (3.18)$$

where we have used (2.20) and (2.21). Thus this diagram survives and gives the same contribution as it does in the true problem. For the ring model, however, we have

$$C_{2;2}(\alpha) = M^{-2} \sum_{\beta\lambda} \exp\,[i(\bar{\theta}_{\alpha\lambda} + \bar{\theta}_{\beta,\alpha+\beta-\lambda}) + i(\bar{\theta}_{\lambda\beta} + \bar{\theta}_{\alpha+\beta-\lambda,\alpha})], \qquad (3.19)$$

by (2.22). Except for special values of the indices β and λ, the phase of the summand does not vanish as a result of (2.23). Consequently, for a typical assignment of the phases $\bar{\theta}_{\alpha\beta}$ by random choices, we have $C_{2;2}(\alpha) \to 0$ as $M \to \infty$, and the diagram does not survive. The detailed reasoning follows that in I.

Similar analysis may be applied to any diagram of any finite order. It may thereby be verified that the surviving diagrams for each of our present models, in the limit $M \to \infty$, are precisely the same as those for the model of corresponding name in I:Sec.5, in the limit $\Omega \to \infty$. This is a consequence of the fact that the rules for diagram-contributions in the two cases yield ϕ products with the same structure.

We shall now make a fundamental assumption which corresponds to assumption 5 of I:Sec. 5.1. We assume that diagram classes which do not survive in any finite order make no contribution to $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$, in the limit $M \to \infty$, when they are summed to *all* orders. The implications of this assumption will be discussed in Sec. 4, and in Sec. 7 we shall outline a partial justification.

Since the diagrams we have identified as surviving all have $C_{n;p}(\alpha) = 1$, an immediate consequence of our assumption is that $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$ is independent of α in the limit. Thus we may define $S_{\mathbf{k}}(\zeta_a)$ for the models by

$$S_{\mathbf{k}}(\zeta_a) = S_{\mathbf{k}\alpha\alpha}(\zeta_a) \qquad (M \to \infty). \qquad (3.20)$$

Then, by (2.13), (3.11), and (2.10), we have

$$S_{\mathbf{k}[nm]}(\zeta_a) = \delta_{nm} S_{\mathbf{k}}(\zeta_a) \qquad (M \to \infty). \qquad (3.21)$$

In the true problem, these relations hold for any M.

Let us now consider the irreducible linked-diagram expansions for $S_{\mathbf{k}}(\zeta_a)$, as defined by (3.20), and for $M_{\mathbf{k}}(\zeta_a)$, as defined in terms of this $S_{\mathbf{k}}(\zeta_a)$ by I:(4.12). These expansions are obtained by amending the rules for the primitive diagram expansion with rules 2′, 4′, 4″, and 8′ of I:Sec.4. Since each $S_{\mathbf{k}\alpha\alpha}(\zeta_a)$ is independent of α in the limit $M \to \infty$, it follows that the entire collective-index dependence of any diagram-contribution in the irreducible expansions is contained in the associated ϕ product and therefore is given by the same quantity $C_{n;p}(\alpha)$ associated with that diagram in the primitive expansion. From this it follows that the survival rules for diagrams in the irreducible expansions are precisely those for the primitive expansion: A diagram survives if and only if the summand of $C_{n;p}(\alpha)$ has the value one for all values of the intermediate collective indices permitted by collective-index conservation. This same conclusion may also be reached by reasoning of the kind employed in I:Secs. 5.2 and 5.3 concerning recovery of the primitive expansion from the irreducible expansion.

The results stated in the preceding paragraphs may be combined to give the following conclusion: In the limit $M \to \infty$, only those classes of terms survive, in the irreducible expansions for $S_{\mathbf{k}}(\zeta_a)$ or $M_{\mathbf{k}}(\zeta_a)$, which were identified as surviving for the corresponding models in I:Sec. 5. In each model, the surviving terms are identical in form with the corresponding terms in the irreducible expansion for the true problem. Thus, for each of our present models, we are led to precisely the same final closed equations for $S_{\mathbf{k}}(\zeta_a)$ as we obtained in I:Sec. 5. The essential difference is that now these equations are obtained for finite Ω. Assumptions 3 and 4 of I:Sec. 5.1 have not been made here. An important consequence is that our present results apply to boson systems at low temperatures. A further advantage of the present procedure is that the double limiting process employed in I for long-range potentials is now unnecessary.

4. CONVERGENCE PROPERTIES OF THE MODEL PROPAGATOR EXPANSIONS

For each stochastic model, let us divide all the primitive linked diagrams into two classes, *wanted* and *unwanted*. Wanted diagrams are all those which we identified in Sec. 3 as surviving in the limit $M \to \infty$. The ϕ products associated with them have the value one for all values of the intermediate collective indices permitted by collective index conservation. Consequently, we have $C_{n;p}(\alpha) = 1$ for these diagrams. The unwanted diagrams are all the others. The ϕ products associated with them

have stochastic phases for all but special values of the intermediate collective indices. Consequently, we have $C_{n;p}(\alpha) \to 0$ $(M \to \infty)$ for any given unwanted diagram. We shall examine very soon the strength with which the unwanted $C_{n;p}(\alpha)$ vanish in the limit.

The fundamental assumption made in Sec. 3 concerning the contribution from all unwanted diagrams may be expressed in the form

$$\sum_{n=1}^{\infty} \sum_{p}{}' C_{n;p}(\alpha)\Gamma_{n;p}(\mathbf{k}, a) \to 0 \qquad (M \to \infty), \quad (4.1)$$

where $\sum_p'$ denotes a summation over unwanted diagrams only. The essential point in (4.1) is that we must take the limit $n \to \infty$ before the limit $M \to \infty$. If we did not, we would not be employing the full, formally exact perturbation series for the model, and, consequently, we would be unable to assert that the results embodied the boundedness properties of the model Hamiltonian. We wish to make it clear in the present section that the validity of (4.1) is far from obvious. We shall, in fact, obtain the negative result

$$\sum_{n=1}^{\infty} \sum_{p}{}' |C_{n;p}(\alpha)\Gamma_{n;p}(\mathbf{k}, a)| = \infty \qquad (\text{any } M). \quad (4.2)$$

This result does not mean that (4.1) cannot be true. However, it shows that (4.1) can hold only if there are cancellations among the contributions from different diagrams. We shall not attempt to investigate the latter question directly. Instead, we shall present in Sec. 7 some evidence for the validity of (4.1) which is not based on perturbation theory.

In order to establish (4.2), we must estimate three things: the strength with which the unwanted $C_{n;p}(\alpha)$ vanish for large M, the number $R'(n)$ of distinct unwanted diagrams for large n, and the magnitude of the true-problem diagram contributions $\Gamma_{n;p}(\mathbf{k}, a)$ for large n. Let us consider the $C_{n;p}(\alpha)$ first. In every $C_{n;p}(\alpha)$, the number of independent, summed indices given by index-conservation and the number of M^{-1} factors are both equal to n. The ϕ product which comprises the summand of any $C_{n;p}(\alpha)$ has unit modulus for all of our models but the Hartree-Fock. For that model the ϕ product is either zero or one. It follows that, for all the models, the $C_{n;p}(\alpha)$ all satisfy

$$|C_{n;p}(\alpha)| \leq 1. \quad (4.3)$$

There are two types of contributions to the unwanted $C_{n;p}(\alpha)$. First, in each of the models, there are certain restricted values of the intermediate collective indices for which the ϕ product is identically one (cf. the discussion in I:Sec. 5.2). We may estimate this contribution as follows. In every model we have $\phi_{\alpha\alpha\alpha\alpha} = 1$. Hence the term in the sum with all collective indices $= \alpha$ has the value M^{-n}, which then constitutes a lower bound to the magnitude of the contribution. An upper bound may be given in the form KM^{-1}, corresponding to the restriction of just one of the intermediate indices to K special values.

The second type of contribution comes from the terms in the sum which have stochastic phases. It arises in all the models but the Hartree-Fock. There are M^n terms, each of unit modulus, in the sum which (when multiplied by M^{-n}) comprises $C_{n;p}(\alpha)$. If the phase of each term were fixed by an independent random choice, then, for a typical set of choices, the result would be

$$C_{n;p}(\alpha) = M^{-n}O[\sqrt{(M^n)}] = O(M^{-n/2}).$$

In general, however, the M^n phases are not completely independent. The independent choices are of the $O(M^2)$ linearly independent $\theta_{\alpha\beta}$ or $\bar{\theta}_{\alpha\beta}$ (ladder or ring model) or the $O(M^3)$ linearly independent $\theta_{\alpha\beta\mu\lambda}$ (random-coupling model). In consequence, the contribution to $C_{n;p}(\alpha)$ from the stochastic-phase terms may vanish either more or less strongly than $M^{-n/2}$. Furthermore, if the unwanted primitive diagram contains a wanted diagram as a self-energy part, variation of the intermediate indices corresponding to this self-energy part will not give any change in the phase of the ϕ product. This will result in $C_{n;p}(\alpha)$ vanishing less strongly.

On the basis of the preceding paragraphs, we shall assume the following asymptotic behavior for the unwanted $C_{n;p}(\alpha)$:

$$C_{n;p}(\alpha) \to 0, \qquad M \to \infty, \quad (4.4)$$

$$|C_{n;p}(\alpha)| > M^{-n}, \qquad M \to \infty. \quad (4.5)$$

Two restrictions on the validity of these relations should be noted. We assume a typical assignment of the independent random phase-parameters in asserting (4.4). (Cf. the discussion in I:Sec. 2.2.) In obtaining the lower bound (4.5), we have ignored the contribution to $C_{n;p}(\alpha)$ from the terms with stochastic phases. However, there may be some special combinations of values for n, p, and α such such that the nonstochastic contribution to $C_{n;p}(\alpha)$ is very nearly canceled by the stochastic-phase contribution, with the result that (4.5) is violated. For a typical assignment of phase parameters, these cases constitute a set of relative measure zero in the limit $M \to \infty$. We shall ignore them in discussing (4.2).

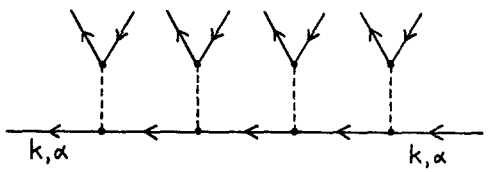

FIG. 3. Incomplete linear diagram with four vertices.

In order to bound $R'(n)$, the number of unwanted, distinct linked diagrams with n vertices, we consider a special class of linked diagrams, which we shall call linear diagrams. Let us form an incomplete diagram with n vertices, as illustrated in Fig. 3 for the case $n = 4$. To form the linear diagrams, we now connect the free outgoing lines with the free incoming lines in all possible ways. There are $n!$ ways of doing this, and each gives a distinct linear diagram. Now we note that the linear diagrams are a very restricted class of all the distinct linked diagrams. Hence, for large n, we have $R(n) \gg n!$. Moreover, we note that the unwanted linked diagrams constitute most of the linked diagrams for large n, no matter which of our models we take. The wanted diagrams in each case are very special classes. Consequently, we may safely assume the bound

$$R'(n) > n! \qquad (n \to \infty). \tag{4.6}$$

We have finally to estimate the $\Gamma_{n;p}(\mathbf{k}, a)$ for large n. On the basis of (2.5), I:(4.11), and I:(4.7), we assume that for any given n and p the summations over intermediate momenta and intermediate 'energies' converge at infinity (cf. assumption 2 of I:Sec. 5.1). It follows that $\Gamma_{n;p}(\mathbf{k}, a)$ can be bounded in the fashion

$$|b(\mathbf{k}, a)|^n < |\Gamma_{n;p}(\mathbf{k}, a)| < |B(\mathbf{k}, a)|^n \ (n \to \infty), \tag{4.7}$$

where $b(\mathbf{k}, a)$ and $B(\mathbf{k}, a)$ are parameters independent of n and p. In general, we will have $|b(\mathbf{k}, a)| > 0$. We shall not attempt to prove (4.7) here.

Equation (4.2) follows immediately from (4.5), (4.6), and (4.7). We have, furthermore,

$$\sum_{n=1}^{\infty} \sum_{p} |\Gamma_{n;p}(\mathbf{k}, a)| = \infty. \tag{4.8}$$

That is to say, the primitive linked-diagram expansion for the true problem is not absolutely convergent when taken diagram by diagram. This result does not preclude the weaker property that

$$\sum_{n=1}^{\infty} |\sum_{p} \Gamma_{n;p}(\mathbf{k}, a)|$$

converge. The latter would correspond to absolute convergence of $S_{\mathbf{k}}(\zeta_a)$ as a power-series in λ if the interaction potential $V(\mathbf{x})$ were replaced by $\lambda V(\mathbf{x})$.

We have already noted that (4.2) does not mean (4.1) cannot be true. However, it certainly indicates that the assumption expressed by (4.1) must be regarded with suspicion in the absence of supporting evidence. We shall attempt to develop such evidence in the remainder of this paper by turning to the more general problem of linked-diagram expansions for nonequilibrium statistical ensembles which evolve in time.

5. NONEQUILIBRIUM CORRELATION AND GREEN'S FUNCTIONS

5.1. Summary of the Method

The formalism we shall outline in Secs. 5 and 6 is an extension, to second-quantized fields, of a nonequilibrium method previously applied to a classical field problem, the evolution of the correlation tensor in turbulence dynamics.[2] The changes required in the present case are due to the different degree of nonlinearity of the equations of motion and to the q-number nature of the fields. Neither characteristic necessitates a drastic modification. We shall develop the formalism here *ab initio*, but not with full proofs or in complete detail. Our interest here is not in nonequilibrium as such but in elucidation of the convergence question which we stated, for equilibrium, in Sec. 4.

The nonequilibrium treatment will be carried out in the Heisenberg representation. Our procedure may be summarized as follows. We define Heisenberg creation and destruction operators which coincide with the Schrödinger operators at an initial time t_0, and we specify an initial statistical ensemble by a weighting operator which is Gaussian in the Schrödinger operators. Then we define correlation functions of the Heisenberg operators, and also Green's functions which give the average response of these operators to infinitesimal external perturbations. The correlation and Green's functions are expressed in terms of the Schrödinger operators by iterative solution of the Heisenberg equations of motion. The results are evaluated by a statistical form of Wick's theorem which is valid for any Gaussian weighting operator. This yields linked-diagram expansions for the correlation and Green's functions. An advantage of working in the Heisenberg representation is that unlinked diagrams do not arise and therefore do not have to be eliminated. Both primitive and irreducible linked-diagram expansions are obtained. The latter yield formally closed equations which give the evolution in time

of the correlation and Green's functions for each of our stochastic models.

5.2. Quantized Nonlinear Oscillator

In order to minimize notational complications, we shall introduce the nonequilibrium treatment in terms of a simple example which yields diagram expansions identical in structure with those for the many-body problem. Consider the true Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_i, \qquad \mathcal{H}_0 = \epsilon \sum_n q^\dagger_{[n]} q_{[n]}, \tag{5.1}$$
$$\mathcal{H}_i = \tfrac{1}{2} V \sum_n q^\dagger_{[n]} q^\dagger_{[n]} q_{[n]} q_{[n]},$$

where V and ϵ are real parameters and the commutation relations are

$$[q_{[n]}, q_{[m]}]_- = 0, \qquad [q_{[n]}, q^\dagger_{[m]}]_- = \delta_{nm}. \tag{5.2}$$

The index $n = 1, 2, \cdots, M$ specifies individual systems in a collection, as before. This Hamiltonian represents a collection of trivially soluble quantized nonlinear oscillators. In the fermion case, $\mathcal{H}_i$ actually vanishes identically, but this will not affect the usefulness of (5.1) for our purposes. In terms of the diagram expansions, the vanishing of $\mathcal{H}_i$ is expressed by the exact cancellation of the contribution of any nonexchange diagram by that of an exchange diagram; the formal structure of the expansion is unaffected.

The general model Hamiltonian corresponding to (5.1) is

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_i, \qquad \mathcal{H}_0 = \epsilon \sum_\alpha q^\dagger_\alpha q_\alpha,$$
$$\mathcal{H}_i = \tfrac{1}{2} M^{-1} V \sum_{\alpha\beta\mu\lambda} \phi_{\alpha\beta\mu\lambda}\, \delta_{\alpha+\beta,\mu+\lambda} q^\dagger_\alpha q^\dagger_\beta q_\mu q_\lambda, \tag{5.3}$$

where the collective operators q_α are defined by

$$q_\alpha = M^{-\frac{1}{2}} \sum_n \exp(i2\pi\alpha n/M) q_{[n]}, \tag{5.4}$$

as in Sec. 2.1, and obey

$$[q_\alpha, q_\beta]_- = 0, \qquad [q_\alpha, q^\dagger_\beta]_- = \delta_{\alpha\beta}. \tag{5.5}$$

For each of our model types (ladder, ring, random-coupling, or Hartree-Fock) the $\phi_{\alpha\beta\mu\lambda}$ are precisely the same parameters as in Sec. 2.2. It may be noted that $\mathcal{H}_i$ in (5.3) bears a close formal resemblance to (2.18).

We define the Heisenberg operators $\mathbf{q}_\alpha$ by

$$\mathbf{q}_\alpha(t) = \exp[i(t - t_0)\mathcal{H}] q_\alpha \exp[-i(t - t_0)\mathcal{H}],$$
$$\mathbf{q}^\dagger_\alpha(t) = \exp[i(t - t_0)\mathcal{H}] q^\dagger_\alpha \exp[-i(t - t_0)\mathcal{H}]. \tag{5.6}$$

The Heisenberg equation of motion for any operator $\mathbf{B}$ is

$$d\mathbf{B}/dt = -i[\mathbf{B}, \mathcal{H}]_-. \tag{5.7}$$

For either the fermion or boson case this yields

$$(d/dt + i\epsilon)\mathbf{q}_\alpha(t) = -iM^{-1}V\mathbf{L}_\alpha(t),$$
$$\mathbf{L}_\alpha(t) \equiv \sum_{\beta\mu\lambda} \phi_{\alpha\beta\mu\lambda}\, \delta_{\alpha+\beta,\mu+\lambda} \mathbf{q}^\dagger_\beta(t)\mathbf{q}_\mu(t)\mathbf{q}_\lambda(t), \tag{5.8}$$

where we have used (5.5) and (2.19).

In addition to the $\mathbf{q}_\alpha$ themselves, we introduce the retarded response or Green's operators $\mathbf{G}_{\alpha\gamma}(t, t')$, defined by

$$\delta\mathbf{q}_\alpha(t) = \int_{t_0}^{t} dt' \sum_\gamma \mathbf{G}_{\alpha\gamma}(t, t')\, \delta f_\gamma(t'),$$
$$\mathbf{G}_{\alpha\gamma}(t, t') = 0 \qquad (t < t'). \tag{5.9}$$

Here δf_γ is an arbitrary infinitesimal forcing operator added to $-iM^{-1}V\mathbf{L}_\gamma$ for times $> t_0$, and $\delta\mathbf{q}_\alpha$ is the increment in $\mathbf{q}_\alpha$ produced by the addition. We restrict $\delta f_\gamma(t)$ to operators which anticommute (commute) with all the $\mathbf{q}_\alpha$ and $\mathbf{q}^\dagger_\alpha$ in the fermion (boson) case.

The δf_γ may be regarded as arising from an infinitesimal modification of $\mathcal{H}$. In this way one obtains the relation[7]

$$\mathbf{G}_{\alpha\gamma}(t, t') = [\mathbf{q}_\alpha(t), \mathbf{q}^\dagger_\gamma(t')]_- \qquad (t \geq t'). \tag{5.10}$$

From (5.6), (5.10), and the stated commutation property of δf_γ, it follows that δf_γ and $\delta f^\dagger_\gamma$ commute with $\mathbf{G}_{\alpha\beta}$ for either the fermion or boson case, whatever the indices or time arguments. Using this property, we obtain

$$(\partial/\partial t + i\epsilon)\mathbf{G}_{\alpha\gamma}(t, t') = -iM^{-1}V\mathbf{M}_{\alpha\gamma}(t, t') \qquad (t \geq t'), \tag{5.11}$$
$$\mathbf{M}_{\alpha\gamma}(t, t') \equiv \sum_{\beta\mu\lambda} \phi_{\alpha\beta\mu\lambda}\, \delta_{\alpha+\beta,\mu+\lambda} [\mathbf{G}^\dagger_{\beta\gamma}(t, t')\mathbf{q}_\mu(t)\mathbf{q}_\lambda(t) \mp \mathbf{q}^\dagger_\beta(t)\mathbf{G}_{\mu\gamma}(t, t')\mathbf{q}_\lambda(t) + \mathbf{q}^\dagger_\beta(t)\mathbf{q}_\mu(t)\mathbf{G}_{\lambda\gamma}(t, t')],$$

with

$$\mathbf{G}_{\alpha\gamma}(t', t') = \delta_{\alpha\gamma}. \tag{5.12}$$

We shall also need (5.8) and (5.11) in the integral forms

$$\mathbf{q}_\alpha(t) = \mathbf{q}^{(0)}_\alpha(t) - iM^{-1}V \int_{t_0}^{t} dt' G^{(0)}(t, t')\mathbf{L}_\alpha(t') \tag{5.13}$$

and

$$\mathbf{G}_{\alpha\gamma}(t, t') = \delta_{\alpha\gamma} G^{(0)}(t, t') - iM^{-1}V \times \int_{t'}^{t} dt'' G^{(0)}(t, t'')\mathbf{M}_{\alpha\gamma}(t'', t'). \tag{5.14}$$

[7] Cf. R. E. Peierls, Proc. Roy. Soc. (London) **A214**, 143 (1952).

Here $\mathbf{q}_\alpha^{(0)}(t)$ and $\delta_{\alpha\gamma}G^{(0)}(t, t')$ are the Heisenberg destruction and Green's operators for the 'unperturbed' case $V = 0$. They are given by

$$\mathbf{q}_\alpha^{(0)}(t) = \exp[-i\epsilon(t - t_0)]q_\alpha \tag{5.15}$$

and

$$\begin{aligned} G^{(0)}(t, t') &= \exp[-i\epsilon(t - t')] \qquad (t \geq t'), \\ &= 0 \qquad\qquad\qquad\quad (t < t'). \end{aligned} \tag{5.16}$$

5.3. Correlation and Green's Functions for the Oscillator Models

Let us now consider ensemble averages of the form

$$\langle \mathbf{B} \rangle \equiv \mathrm{Tr}\,\{\mathfrak{W}\mathbf{B}\}/\mathrm{Tr}\,\{\mathfrak{W}\}, \tag{5.17}$$

where $\mathbf{B}$ is any operator and the weighting operator $\mathfrak{W}$ is a function of the Schrödinger operators $q_\alpha = \mathbf{q}_\alpha(t_0)$. A choice of $\mathfrak{W}$ represents a choice of initial statistical ensemble for the collection of oscillators. For our present purposes, we restrict $\mathfrak{W}$ to the Gaussian form

$$\mathfrak{W} = \exp(-a \sum_\alpha q_\alpha^\dagger q_\alpha), \tag{5.18}$$

where a is a real constant which, for bosons only, must further obey $a > 0$. Since $\mathfrak{W}$ then commutes with $\mathfrak{H}$, such an initial ensemble is actually an equilibrium ensemble. However, we shall not use this fact in developing the time-dependent diagram analysis. The analogous Gaussian weighting operators for the many-body problem, which we shall introduce in Sec. 5.4, do not commute with the Hamiltonian; they represent genuine nonequilibrium ensembles.

We define the correlation functions $Q_\alpha(t, t')$ and Green's functions $G_\alpha(t, t')$ by

$$Q_\alpha(t, t') = \langle \mathbf{q}_\alpha^\dagger(t')\mathbf{q}_\alpha(t) \rangle \tag{5.19}$$

and

$$G_\alpha(t, t') = \langle \mathbf{G}_{\alpha\alpha}(t, t') \rangle. \tag{5.20}$$

We shall also use the auxiliary correlation functions $Q_\alpha^+(t, t')$ defined by

$$Q_\alpha^+(t, t') = \langle \mathbf{q}_\alpha(t)\mathbf{q}_\alpha^\dagger(t') \rangle. \tag{5.21}$$

By (5.10), we have

$$G_\alpha(t, t') = Q_\alpha^+(t, t') \pm Q_\alpha(t, t') \quad (t \geq t'). \tag{5.22}$$

It is easily seen that

$$Q_\alpha(t, t') = Q_\alpha^*(t', t), \quad Q_\alpha^+(t, t') = Q_\alpha^{+*}(t', t), \tag{5.23}$$

and

$$G_\alpha^*(t, t') = \langle \mathbf{G}_{\alpha\alpha}^\dagger(t, t') \rangle, \tag{5.24}$$

where the asterisk denotes complex conjugate. We see that Q_α^+ is wholly determined by Q_α and G_α. It should be noted that the time-ordering operator T has not been used in any of the definitions above. We have not found time ordering to be very useful in the nonequilibrium formalism.

For $V = 0$, the correlation and Green's functions are independent of α for any M. They are given by $Q^{(0)}(t, t')$ and $G^{(0)}(t, t')$, where

$$Q^{(0)}(t, t') = (e^a \pm 1)^{-1} \exp[-i\epsilon(t - t')], \tag{5.25}$$

$$Q^{+(0)}(t, t') = [1 \mp (e^a \pm 1)^{-1}] \exp[-i\epsilon(t - t')], \tag{5.26}$$

and $G^{(0)}(t, t')$ is defined by (5.16).[8]

For $V \neq 0$, $G_\alpha(t, t')$ and $Q_\alpha(t, t')$ satisfy the equations of motion and initial conditions

$$(\partial/\partial t + i\epsilon)G_\alpha(t, t') = J_\alpha(t, t'), \tag{5.27}$$

$$G_\alpha(t', t') = 1, \tag{5.28}$$

$$(\partial/\partial t + i\epsilon)Q_\alpha(t, t') = K_\alpha(t, t'), \tag{5.29}$$

$$Q_\alpha(t_0, t_0) = (e^a \pm 1)^{-1}, \tag{5.30}$$

where

$$\begin{aligned} J_\alpha(t, t') = &-iM^{-1}V \sum_{\beta\mu\lambda} \delta_{\alpha+\beta,\mu+\lambda}\phi_{\alpha\beta\mu\lambda} \\ &\times \langle [\mathbf{G}_{\beta\alpha}^\dagger(t, t')\mathbf{q}_\mu(t)\mathbf{q}_\lambda(t) \mp \mathbf{q}_\beta^\dagger(t)\mathbf{G}_{\mu\alpha}(t, t')\mathbf{q}_\lambda(t) \\ &+ \mathbf{q}_\beta^\dagger(t)\mathbf{q}_\mu(t)\mathbf{G}_{\lambda\alpha}(t, t')] \rangle \end{aligned} \tag{5.31}$$

and

$$\begin{aligned} K_\alpha(t, t') = &-iM^{-1}V \sum_{\beta\mu\lambda} \delta_{\alpha+\beta,\mu+\lambda}\phi_{\alpha\beta\mu\lambda} \\ &\times \langle \mathbf{q}_\alpha^\dagger(t')\mathbf{q}_\beta^\dagger(t)\mathbf{q}_\mu(t)\mathbf{q}_\lambda(t) \rangle. \end{aligned} \tag{5.32}$$

These equations follow directly from (5.8) and (5.11). Because of (5.23), the equation for $\partial Q_\alpha(t, t')/\partial t'$ is redundant with (5.29). The irreducible diagram expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ turn out to have a simpler form than those for $G_\alpha(t, t')$ and $Q_\alpha(t, t')$ themselves, and it is for this reason that we introduce the differential equations (5.27) and (5.29).

5.4. Correlation and Green's Functions for the Many-Body Models

Let us now return to the many-body problem.

[8] For the true problem [Hamiltonian (5.1)], the exact functions are also independent of α for $V \neq 0$. For the fermion case, $\mathfrak{K}_i$ vanishes identically and we have $Q_\alpha(t, t') = Q^{(0)}(t, t')$, etc. For the boson case, we easily find the exact results
$Q_\alpha(t, t') = Q^{(0)}(t, t')\,[(1 - e^{-a})/(1 - e^{-a-i(t-t')V})]^2$,
$Q_\alpha^+(t, t') = Q^{+(0)}(t, t')\,[(1 - e^{-a})/(1 - e^{-a-i(t-t')V})]^2$.
It is of interest to note from these expressions that if $Q_\alpha(t, t')$ is expanded as a power series in V, the radius of convergence is given by $|V| = a/|t - t'|$.

The Heisenberg equation of motion corresponding to the Hamiltonian (2.16), (2.18) is

$$(d/dt + i\epsilon_{\mathbf{k}})\mathbf{q}_{\mathbf{k}\alpha} = -iM^{-1}\sum_{\beta\mu\lambda}\sum_{\mathbf{prs}} V_{\mathbf{k}-\mathbf{s}}\,\delta_{\mathbf{k}+\mathbf{p},\mathbf{r}+\mathbf{s}} \times \delta_{\alpha+\beta,\mu+\lambda}\,\phi_{\alpha\beta\mu\lambda}\mathbf{q}^{\dagger}_{\mathbf{p}\beta}\mathbf{q}_{\mathbf{r}\mu}\mathbf{q}_{\mathbf{s}\lambda}, \quad (5.33)$$

where we have used (2.4) and (2.19). In analogy to the nonlinear oscillator case, we define the Green's operators $\mathbf{G}_{\mathbf{kp}\alpha\beta}(t, t')$ by

$$\delta\mathbf{q}_{\mathbf{k}\alpha}(t) = \int_{t_0}^{t} dt' \sum_{\mathbf{p}\beta} \mathbf{G}_{\mathbf{kp}\alpha\beta}(t, t')\,\delta f_{\mathbf{p}\beta}(t'), \quad (5.34)$$

where $\delta f_{\mathbf{k}\alpha}$ is an infinitesimal forcing operator introduced on the right side of (5.33).

We again consider ensemble averages of the form (5.17), where now the weighting operator has the form

$$\mathfrak{W} = \exp\left[-\sum_{\mathbf{k}\alpha} w(\mathbf{k})N_{\mathbf{k}\alpha}\right], \quad (5.35)$$

with

$$N_{\mathbf{k}\alpha} = q^{\dagger}_{\mathbf{k}\alpha}q_{\mathbf{k}\alpha}.$$ [9]

We restrict the real function $w(\mathbf{k})$ by the condition

$$w(\mathbf{k}) = |w(\mathbf{k})| \propto \epsilon_{\mathbf{k}} \qquad (k \to \infty). \quad (5.36)$$

For bosons only, we further require $w(\mathbf{k}) > 0$ for all $\mathbf{k}$. The correlation and Green's functions for the many-body models may now be defined by

$$Q_{\mathbf{k}\alpha}(t, t') = \langle \mathbf{q}^{\dagger}_{\mathbf{k}\alpha}(t')\mathbf{q}_{\mathbf{k}\alpha}(t)\rangle,$$
$$Q^{+}_{\mathbf{k}\alpha}(t, t') = \langle \mathbf{q}_{\mathbf{k}\alpha}(t)\mathbf{q}^{\dagger}_{\mathbf{k}\alpha}(t')\rangle, \quad (5.37)$$
$$G_{\mathbf{k}\alpha}(t, t') = \langle \mathbf{G}_{\mathbf{kk}\alpha\alpha}(t, t')\rangle. \quad (5.38)$$

For $V(\mathbf{x}) = 0$, the correlation and Green's functions are independent of α for any M, as was the case for the nonlinear oscillator. They are given by

$$Q^{(0)}_{\mathbf{k}}(t, t') = N^{(0)}_{\mathbf{k}} \exp\left[-i\epsilon_{\mathbf{k}}(t - t')\right], \quad (5.39)$$
$$Q^{+(0)}_{\mathbf{k}}(t, t') = (1 \mp N^{(0)}_{\mathbf{k}}) \exp\left[-i\epsilon_{\mathbf{k}}(t - t')\right], \quad (5.40)$$

$$G^{(0)}_{\mathbf{k}}(t, t') = \exp\left[-i\epsilon_{\mathbf{k}}(t - t')\right] \quad (t \geq t'),$$
$$= 0 \quad (t < t'), \quad (5.41)$$

where

$$N^{(0)}_{\mathbf{k}} = (e^{w(\mathbf{k})} \pm 1)^{-1}. \quad (5.42)$$

For $V(\mathbf{x}) \neq 0$, we have

$$(\partial/\partial t + i\epsilon_{\mathbf{k}})G_{\mathbf{k}\alpha}(t, t') = J_{\mathbf{k}\alpha}(t, t'),$$
$$G_{\mathbf{k}\alpha}(t', t') = 1, \quad (5.43)$$

and

$$(\partial/\partial t + i\epsilon_{\mathbf{k}})Q_{\mathbf{k}\alpha}(t, t') = K_{\mathbf{k}\alpha}(t, t'),$$
$$Q_{\mathbf{k}\alpha}(t_0, t_0) = N^{(0)}_{\mathbf{k}}, \quad (5.44)$$

where $J_{\mathbf{k}\alpha}(t, t')$ and $K_{\mathbf{k}\alpha}(t, t')$ are given by obvious modifications of (5.31) and (5.32). The analogs of (5.22)–(5.24) hold also for the many-body case.

The partition of particles and of energy among the momentum modes as a function of time may be expressed directly in terms of $Q_{\mathbf{k}\alpha}(t, t')$. We have, immediately,

$$\langle \mathfrak{N}\rangle = \sum_{\mathbf{k}}\sum_{\alpha} Q_{\mathbf{k}\alpha}(t, t). \quad (5.45)$$

In analogy to I:(4.10), we may easily establish from (5.33) the relation

$$\langle \mathfrak{K}\rangle = \tfrac{1}{2}\sum_{\mathbf{k}}\sum_{\alpha}\left\{\epsilon_{\mathbf{k}}Q_{\mathbf{k}\alpha}(t, t) + i\left[\frac{\partial Q_{\mathbf{k}\alpha}(t, t')}{\partial t}\right]_{t'=t}\right\}. \quad (5.46)$$

5.5. Approach to Equilibrium

Let us consider the case $t_0 \to -\infty$. Then at finite t we anticipate that the ensemble specified by (5.35) will have evolved into a state of statistical stationarity. This need not be so for the random-coupling model, which may be unstable to catastrophic collapse because of the unboundedness of $\mathfrak{K}_i$. However, it seems assured for the ladder and ring models, if $V(\mathbf{x})$ satisfies the conditions which make $\mathfrak{K}_i$ bounded from below. If an approach to equilibrium is granted, we anticipate for any finite t and t' that $Q_{\mathbf{k}\alpha}(t, t')$ and $G_{\mathbf{k}\alpha}(t, t')$ will take the forms

$$Q_{\mathbf{k}\alpha}(t, t') = Q_{\mathbf{k}\alpha}(t - t'),$$
$$G_{\mathbf{k}\alpha}(t, t') = G_{\mathbf{k}\alpha}(t - t'). \quad (5.47)$$

It should be noted that we are not invoking an adiabatic switch-on of $V(\mathbf{x})$. We are simply fixing the initial statistical ensemble by a choice of $\mathfrak{W}$ and then letting the ensemble evolve according to the exact equations of motion.

The equilibrium ensemble which is achieved will in general not be a grand canonical ensemble. The

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[9] The methods to be presented in Secs. 6 and 7 are also applicable to (non-Gaussian) normal ensembles which describe statistically inhomogeneous systems. Such ensembles are specified by weighting operators of the form

$$\mathfrak{W} = \exp\left[-\Sigma_{\mathbf{kp}\alpha} w(\mathbf{k}, \mathbf{p})q_{\mathbf{k}\alpha}{}^{\dagger}q_{\mathbf{p}\alpha}\right],$$

where $w(\mathbf{k}, \mathbf{p})$ is a suitable function. In place of $Q_{\mathbf{k}\alpha}(t, t')$ and $G_{\mathbf{k}\alpha}(t, t')$, one must deal with the more general quantities

$$Q_{\mathbf{kp}\alpha}(t, t') = \langle \mathbf{q}_{\mathbf{p}\alpha}{}^{\dagger}(t')\mathbf{q}_{\mathbf{k}\alpha}(t)\rangle,$$
$$G_{\mathbf{kp}\alpha}(t, t') = \langle G_{\mathbf{kp}\alpha\alpha}(t, t')\rangle.$$

Alternatively, the analysis may be carried out directly in x space by using the fields $\psi_{\alpha}(\mathbf{x})$ and $\psi_{\alpha}{}^{\dagger}(\mathbf{x})$. Such a treatment is illustrated for two classical field problems in Secs. 10 and 11 of reference 2. It is also possible to work with non-normal weighting operators which describe, for example, non-zero initial two-body correlations. This type of generalization is briefly discussed in Sec. 9 of reference 2.

reason is that (5.35) does not in general represent an initial distribution of total energy (kinetic plus potential) and total particle-number corresponding to a grand canonical ensemble. Since $\mathcal{H}$ and $\mathcal{N}$ are constants of motion, the distribution of these quantities can not change with time. Nevertheless, we conjecture that for our models in the limit $M \to \infty$ the equilibrium functions $Q_{\mathbf{k}\alpha}(t - t')$ and $G_{\mathbf{k}\alpha}(t - t')$ will be identical in value with corresponding averages defined over the grand canonical ensemble with the same $\langle \mathcal{H} \rangle$ and $\langle \mathcal{N} \rangle$. In the limit $M \to \infty$, both the grand canonical ensemble and the ensemble specified by (5.35) represent total-energy and total-particle-number distributions which are peaked with infinite sharpness about their means. We have noted previously [cf. (2.27) and (2.28)] that the M systems in the collection are coupled for our models; they exchange both energy and particles. This means that, with respect to the achievement of statistical equilibrium, the models represent infinitely large super systems in the limit $M \to \infty$, even if the mean number of particles per system is small. It is on the basis of these facts that we conjecture the identity of $Q_{\mathbf{k}\alpha}(t - t')$ and $G_{\mathbf{k}\alpha}(t - t')$ for the two kinds of ensemble. The conjecture supposes certain ergodic properties, as does the assumption that ensembles specified by (5.35) will reach equilibrium at all.

If we turn from the models to the true problem (all $\phi_{\alpha\beta\mu\lambda} = 1$), then the M systems in the collection are not coupled, and, if the mean number of particles per system is small, we do not have a large super system in any dynamical sense. In this case, the grand canonical ensemble and the ensemble specified by (5.35) cannot be expected to yield the same averages when $t_0 \to -\infty$. It does not follow that our Gaussian ensembles are physically inappropriate. The grand canonical ensemble is used for equilibrium calculations more because it is mathematically convenient than because it is uniquely appropriate physically. For our present purposes, Gaussian ensembles are the ones which are most convenient mathematically. The real justification for either choice of ensemble is the hope that for a dynamically large system ($M^{-1}\langle \mathcal{N} \rangle \to \infty$ for the true problem; $M \to \infty$ and $M^{-1}\langle \mathcal{N} \rangle$ finite for the models) the values of physically interesting equilibrium averages are insensitive to a substantial range of choices of ensemble. We shall not attempt to go further into this matter here. The questions which arise are not unique to our investigation.

The conjecture made above concerning $Q_{\mathbf{k}\alpha}(t - t')$ and $G_{\mathbf{k}\alpha}(t - t')$ for the models implies that these quantities may be identified with equilibrium correlation and Green's functions of types discussed previously by a number of authors.[10] The temperature-domain propagators $S_{\mathbf{k}\alpha\alpha}(u, u')$ may be expressed in terms of the equilibrium correlation and Green's functions by analytic continuation of the latter. The continuation is given formally by the relations

$$\begin{aligned} S_{\mathbf{k}\alpha\alpha}(u, u') &= -Q^{+}_{\mathbf{k}\alpha}(-iu + iu') \quad (u > u'), \\ &= \pm Q_{\mathbf{k}\alpha}(-iu + iu') \quad (u \leq u'), \end{aligned} \tag{5.48}$$

which follow from (3.4) and (5.37) if $\langle\ \rangle$ is taken throughout as an average over the grand canonical ensemble.

There is a useful general relation between the equilibrium functions $Q_{\mathbf{k}\alpha}(t - t')$ and $G_{\mathbf{k}\alpha}(t - t')$. If we define $G^{S}_{\mathbf{k}\alpha}(t - t')$ by

$$\begin{aligned} G^{S}_{\mathbf{k}\alpha}(t - t') &= G_{\mathbf{k}\alpha}(t - t') \qquad (t \geq t'), \\ &= G^{*}_{\mathbf{k}\alpha}(t' - t) \qquad (t < t'), \end{aligned} \tag{5.49}$$

then the transforms

$$\begin{aligned} \tilde{G}^{S}_{\mathbf{k}\alpha}(\omega) &= (2\pi)^{-1} \int_{-\infty}^{\infty} G^{S}_{\mathbf{k}\alpha}(t) \exp(i\omega t)\, dt, \\ \tilde{Q}_{\mathbf{k}\alpha}(\omega) &= (2\pi)^{-1} \int_{-\infty}^{\infty} Q_{\mathbf{k}\alpha}(t) \exp(i\omega t)\, dt \end{aligned} \tag{5.50}$$

are related by

$$\tilde{Q}_{\mathbf{k}\alpha}(\omega) = (e^{\beta(\omega - \mu)} \pm 1)^{-1} \tilde{G}^{S}_{\mathbf{k}\alpha}(\omega). \tag{5.51}$$

Equation (5.51) has just the form of the free-particle Fermi-Dirac or Einstein-Bose distribution law provided that we interpret $\tilde{G}^{S}_{\mathbf{k}\alpha}(\omega)$ as a density of states for momentum $\mathbf{k}$ and $\tilde{Q}_{\mathbf{k}\alpha}(\omega)$ as a mean occupancy. For the grand canonical ensemble, (5.51) may be obtained directly from the definitions of $\tilde{G}^{S}_{\mathbf{k}\alpha}(\omega)$ and $\tilde{Q}_{\mathbf{k}\alpha}(\omega)$ by using the cyclic properties of the trace.[11,12] However, (5.51) may also be deduced as a necessary condition for equilibrium under coupling to a thermometer, without specifying the precise nature of the equilibrium ensemble. This is clearly preferable for the present application. We hope to present a derivation of this type at another time. The nature of the argument has been stated previously.[13]

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[10] A review discussion is given by D. N. Zubarev, Uspekhi Fiz. Nauk 71, 71 (1960). [Translation: Soviet Phys.—Uspekhi, 3, 320 (1960).] Our $G_{\mathbf{k}}(t - t')$ differs by a factor i from that commonly defined.

[11] R. Kubo, J. Phys. Soc. Japan, 12, 570 (1957).

[12] P. C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959).

[13] R. H. Kraichnan, Phys. Rev. 112, 1054 (1958).

6. DIAGRAM EXPANSIONS FOR THE NONEQUILIBRIUM CORRELATION AND GREEN'S FUNCTIONS

6.1. Primitive Diagram Expansions

The generation of primitive and irreducible linked-diagram expansions for $J_{k\alpha}(t, t')$ and $K_{k\alpha}(t, t')$ is straightforward in principle, but somewhat intricate in practice. We shall introduce the procedure by means of the nonlinear oscillator example discussed in Sec. 5.2. Suppose that we carry out a formal iteration solution of the integral equations (5.13) and (5.14). We thereby obtain $\mathbf{q}_\alpha(t)$ and $\mathbf{G}_{\alpha\gamma}(t, t')$ expressed as power-series in V. The coefficients in these series consist of terms of the following kind: Each term is a multiple integral over a product of Krönecker symbols, of factors of the form $M^{-1}\phi$, and of unperturbed operators of the form $\mathbf{q}^{(0)}_{\alpha'}$, $\mathbf{q}^{\dagger(0)}_{\alpha'}$, $G^{(0)}$, or $G^{(0)*}$. The term is summed over the intermediate indices. If the power-series are substituted into (5.31) and (5.32), we obtain expressions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ as power-series in V. The terms which make up the coefficients in these series involve integrals over ensemble-averages of products of factors $\mathbf{q}^{(0)}_{\alpha'}$, $\mathbf{q}^{\dagger(0)}_{\alpha'}$, $G^{(0)}$, and $G^{(0)*}$.

In order to evaluate the ensemble-averages, we first note that $G^{(0)}(t, t')$, given by (5.16), is a c-number function and may be taken outside the brackets $\langle\ \rangle$. The remaining averages over $\mathbf{q}^{(0)}$ and $\mathbf{q}^{\dagger(0)}$ factors may be evaluated by using a statistical form of Wick's theorem, which follows from the Gaussian form of the weighting operator (5.18).[14] We pair the $\mathbf{q}^{(0)}$ and $\mathbf{q}^{\dagger(0)}$ factors in all possible ways, maintaining always the original left-right order of the two factors in a pair. We replace each pair by its individual ensemble average of the form

$$\langle \mathbf{q}^{\dagger(0)}_\lambda(t')\mathbf{q}^{(0)}_\mu(t)\rangle = \delta_{\mu\lambda}Q^{(0)}(t, t'), \tag{6.1}$$

$$\langle \mathbf{q}^{(0)}_\mu(t)\mathbf{q}^{\dagger(0)}_\lambda(t')\rangle = \delta_{\mu\lambda}Q^{+(0)}(t, t'), \tag{6.2}$$

or

$$\langle \mathbf{q}^{(0)}_\mu(t)\mathbf{q}^{(0)}_\lambda(t')\rangle = \langle \mathbf{q}^{\dagger(0)}_\mu(t)\mathbf{q}^{\dagger(0)}_\lambda(t')\rangle = 0. \tag{6.3}$$

Then we take the product of all the individual averages for each pairing and sum over all the possible pairings. For fermions only, we multiply each product, before summing, by $(-1)^P$, where P is the number of permutations required to obtain the particular pairing.

Let us suppose that we have carried out the procedure just described and have then performed the summation over all the intermediate indices which arise. Each contribution proportional to V^n, in the expansion for either $J_\alpha(t, t')$ or $K_\alpha(t, t')$, then consists of a multiple integral over a product of $Q^{(0)}$, $Q^{+(0)}$, $G^{(0)}$, and $G^{(0)*}$ functions, multiplied by a summed product of Krönecker symbols and n factors $M^{-1}\phi$. The Krönecker symbols express the 'collective-index conservation' which also characterized the equilibrium analysis of Sec. 3. A consequence is that the sums over products of Krönecker symbols and factors $M^{-1}\phi$ turn out to be precisely the quantities $C_{n;p}(\alpha)$ of the equilibrium theory. These quantities contain the entire dependence of the contributions upon the ϕ's and upon α.

As the preceding paragraph suggests, the formal expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ in powers of V have systematic diagram representations which resemble the primitive linked-diagram expansion of the equilibrium theory. It is immediately apparent that only linked diagrams arise. Any intermediate index which occurs arises from an iterative branching of the Heisenberg equations of motion and thus is necessarily linked by a Krönecker symbol to indices which occurred previously in the iteration process.[15]

In order to write the complete contribution to $J_\alpha(t, t')$ or $K_\alpha(t, t')$ which is proportional to V^n, we first write down all the distinct nth-order primitive linked diagrams, just as in the equilibrium treatment. Now, however, it turns out that each diagram [and hence each $C_{n;p}(\alpha)$] above the first order is associated with more than one contribution. The method of forming the diagram contributions is most clearly indicated by giving some examples. Consider the first-order contribution to $K_\alpha(t, t')$ associated with the diagram of Fig. 4. The one vertex in the diagram is associated with the ϕ factor that appears explicitly in (5.32). The contribution is obtained from the product of the zeroth-order terms in the iteration expansions of all the operators in (5.32). This is because a factor V already appears explicitly in (5.32). There are two

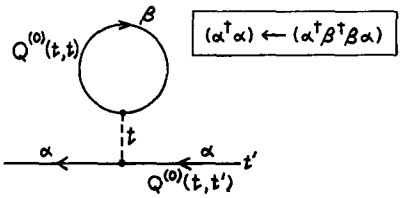

FIG. 4. Representation of the primitive contribution to $K_\alpha(t, t')$ proportional to $C_{1;1}(\alpha)$.

[14] Cf. C. Bloch and C. De Dominicis, Nuclear Phys. 7, 459 (1958).

[15] It is essential here that the Heisenberg equations of motion be taken in the form (5.8). If, instead, the equation

$$d\mathbf{q}_\alpha/dt = i(\mathcal{H}\mathbf{q}_\alpha - \mathbf{q}_\alpha\mathcal{H})$$

is used directly in the iteration procedure, both unlinked and linked diagrams arise, just as in the Schrödinger representation. Thus the elimination of unlinked diagrams in our procedure can be traced to the use of the commutation relations (5.5) in obtaining (5.8).

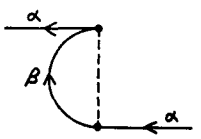

FIG. 5. The diagram associated with $C_{1;2}(\alpha)$.

possible non-vanishing pairings of the creation and destruction operators according to Wick's theorem:

$$(\alpha\lambda)(\beta\mu) \quad \text{and} \quad (\alpha\mu)(\beta\lambda).$$

Only the first pairing corresponds to the present diagram. By (6.1), it yields the contribution

$$-iC_{1;1}(\alpha)VQ^{(0)}(t, t)Q^{(0)}(t, t'), \tag{6.4}$$

where $C_{1;1}(\alpha)$ is given by (3.15). The second pairing corresponds to the exchange diagram Fig. 5, and involves the quantity

$$C_{1;2}(\alpha) = M^{-1}\sum_{\beta}\phi_{\alpha\beta\alpha\beta}. \tag{6.5}$$

We have diagrammed the contribution (6.4) by labeling the vertex in Fig. 4 with time t, labeling the outer end of the incoming external line with time t', and writing the two $Q^{(0)}$ factors along the lines with which they are associated. No factor is associated with the outgoing external line, and this is true of every contribution to the expansions of $K_\alpha(t, t')$ and $J_\alpha(t, t')$. The reason is that we are dealing with the differential equations (5.29) and (5.27) instead of with $Q_\alpha(t, t')$ and $G_\alpha(t, t')$ directly. In the box on the right side of Fig. 4, we have given an alternative symbolic representation of the contribution of this diagram to (5.29).

In Fig. 6, we have diagrammed the contribution to $J_\alpha(t, t')$ associated with $C_{1;1}(\alpha)$. This contribution arises from the third term on the right side of (5.31), and it is obtained by replacing all the operators in that term by their zeroth-order values. By (6.1), the contribution therefore is

$$-iC_{1;1}(\alpha)VQ^{(0)}(t, t)G^{(0)}(t, t'). \tag{6.6}$$

A symbolic representation of the contribution of this diagram to (5.27) is given in the box on the right side of Fig. 6. (The underlined α represents $\mathbf{G}_{\alpha\alpha}$.) The second term on the right side of (5.31) gives rise to the first-order exchange contribution to $J_\alpha(t, t')$, associated with Fig. 5 and $C_{1;2}(\alpha)$. By (6.3), the first term on the right side of (5.31) gives no first-order contribution.

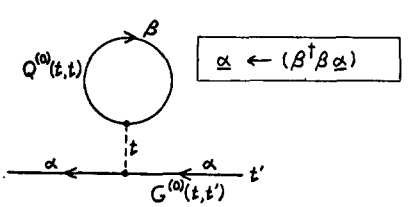

FIG. 6. Representation of the primitive contribution to $J_\alpha(t, t')$ proportional to $C_{1;1}(\alpha)$.

There are three contributions to $J_\alpha(t, t')$ associated with the second-order diagram shown in Fig. 7(a). They are diagrammed in Figs. 7(b), 7(c), and 7(d). In the boxes beside the diagrams we have represented symbolically the particular iteration-substitutions (iterative branchings) and operator pairings associated with the contributions. Below this, we have shown (in square brackets) the left-right ordering of the final set of creation and destruction operators which are produced, in each case, by the iteration

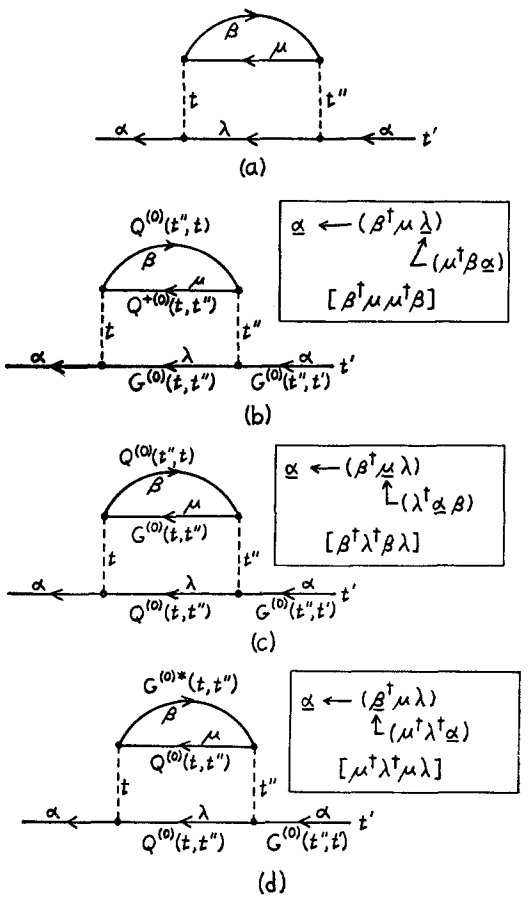

FIG. 7. (a) The diagram associated with $C_{2;1}(\alpha)$; (b), (c), (d) representations of the primitive contributions to $J_\alpha(t, t')$ proportional to $C_{2;1}(\alpha)$.

substitutions. This must be kept account of to determine whether $Q^{(0)}$ or $Q^{+(0)}$ factors are associated with given lines and to determine the sign of the contribution in the fermion case. The total contribution of Fig. 7 to $J_\alpha(t, t')$ is

$$C_{2;1}(\alpha)V^2\int_{t'}^{t}[-Q^{(0)}(t'', t)Q^{+(0)}(t, t'')G^{(0)}(t, t'')$$
$$\pm Q^{(0)}(t'', t)G^{(0)}(t, t'')Q^{(0)}(t, t'') \tag{6.7}$$
$$\mp G^{(0)*}(t, t'')Q^{(0)}(t, t'')Q^{(0)}(t, t'')]G^{(0)}(t'', t')\,dt'',$$

where

$$C_{2;1}(\alpha) = M^{-2} \sum_{\beta\mu\lambda} \delta_{\alpha+\beta,\mu+\lambda}\phi_{\alpha\beta\mu\lambda}\phi_{\lambda\mu\beta\alpha}. \qquad (6.8)$$

The three terms which comprise (6.7) are associated, from left to right, with Figs. 7(b), 7(c), and 7(d), respectively.

The contributions to $K_\alpha(t, t')$ and $J_\alpha(t, t')$ associated with all the primitive diagrams may be determined in the fashion illustrated above. For each diagram, one traces through all the iterative branchings and nonvanishing operator pairings which correspond to the diagram topology. Then one writes down the contributions by using (6.1) and (6.2). The primitive-diagram contributions have the following general characteristics. Each nth-order contribution to $J_\alpha(t, t')$ contains a factor $C_{n;p}(\alpha)$ which multiplies an n-fold integral over n factors $G^{(0)}$ or $G^{(0)*}$ (in some combination) and n factors $Q^{(0)}$ or $Q^{+(0)}$. The contributions to $K_\alpha(t, t')$ are similar except that there are $n - 1$ factors $G^{(0)}$ or $G^{(0)*}$ and $n + 1$ factors $Q^{(0)}$ or $Q^{+(0)}$. In every contribution to $J_\alpha(t, t')$, but in only some of the contributions to $K_\alpha(t, t')$, the factor associated with the incoming external line is a $G^{(0)}$ factor. We have already remarked that no factor is ever associated with the outgoing external line in either the $J_\alpha(t, t')$ or $K_\alpha(t, t')$ expansions.

The primitive linked-diagram expansions for the functions $J_{\mathbf{k}\alpha}(t, t')$ and $K_{\mathbf{k}\alpha}(t, t')$, which appear in (5.43) and (5.44), may be obtained in close analogy to the analysis for the nonlinear oscillator. The only difference is that there is a momentum associated with each line in the diagrams, and the results must be summed over the intermediate momenta, as in the equilibrium analysis. For example, the contributions to $J_{\mathbf{k}\alpha}(t, t')$ which correspond to (6.6) and to the first term in (6.7) are

$$-iC_{1;1}(\alpha) \sum_{\mathbf{p}} V_0 Q_{\mathbf{p}}^{(0)}(t, t) G_{\mathbf{k}}^{(0)}(t, t') \qquad (6.9)$$

and

$$-C_{2;1}(\alpha) \sum_{\mathbf{ps}} V_{\mathbf{k}-\mathbf{s}} V_{\mathbf{s}-\mathbf{k}} \int_{t'}^{t} Q_{\mathbf{p}}^{(0)}(t'', t) Q_{\mathbf{k}+\mathbf{p}-\mathbf{s}}^{+(0)}(t, t'') \times G_{\mathbf{s}}^{(0)}(t, t'') G_{\mathbf{k}}^{(0)}(t'', t')\, dt'', \qquad (6.10)$$

respectively.

Let us now consider the limit $M \to \infty$. As we discussed in Sec. 4, all the primitive linked diagrams may be divided into two classes, 'wanted' and 'unwanted,' for each of the stochastic models. The $C_{n;p}(\alpha)$ for wanted diagrams all have the value one. For any unwanted diagram of finite order n, we have $C_{n;p}(\alpha) \to 0$ as $M \to \infty$. Let us extend to the nonequilibrium case the fundamental assumption made in Sec. 3 about unwanted diagrams. We assume that the total contribution to $J_\alpha(t, t')$, $K_\alpha(t, t')$, $J_{\mathbf{k}\alpha}(t, t')$, and $K_{\mathbf{k}\alpha}(t, t')$ from all unwanted diagrams vanishes in the limit $M \to \infty$. We shall reserve all discussion of the validity of this assumption for Sec. 7. An immediate implication of the assumption is that $J_\alpha(t, t')$, $K_\alpha(t, t')$, $G_\alpha(t, t')$, $Q_\alpha(t, t')$, and the corresponding functions for the many-body problem all become independent of α in the limit. We may therefore omit the index α in these functions. Then, in analogy to (3.21), we find

$$\begin{aligned} \langle \mathbf{q}_{[n]}^{\dagger}(t')\mathbf{q}_{[m]}(t)\rangle &= \delta_{nm} Q(t, t'), \\ \langle \mathbf{q}_{[m]}(t)\mathbf{q}_{[n]}^{\dagger}(t')\rangle &= \delta_{nm} Q^{+}(t, t'), \end{aligned} \qquad (6.11)$$

with corresponding relations for the many-body problem.

6.2. Irreducible Diagram Expansions

Irreducible linked-diagram expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ may be constructed by the following rules: Retain only the irreducible diagrams; that is, those without self-energy parts. (See rule 2′ of I: Sec. 4 for the definition of an irreducible diagram and of a self-energy part.) Then alter the primitive contributions associated with these diagrams by replacing each factor $G^{(0)}$, $G^{(0)*}$, $Q^{(0)}$, or $Q^{+(0)}$ therein with a factor G_σ, G_σ^*, Q_σ, or Q_σ^+ having the same time-arguments. Here σ is the collective index that labels the line associated with the factor. [The external line ($\sigma = \alpha$) does not form an exception to this rule.] Corresponding rules hold for the irreducible expansions for $J_{\mathbf{k}\alpha}(t, t')$ and $K_{\mathbf{k}\alpha}(t, t')$.

The formal validity of these irreducible-diagram expansions may be demonstrated in two ways, neither of which will be carried out here. The first way is to construct directly, by iteration and the use of Wick's theorem, the primitive-diagram expansions for $G_\sigma(t, t')$, $Q_\sigma(t, t')$, etc.[16] One then substitutes these expansions into the irreducible expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ and compares the results with the primitive expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$.

The second method does not require the explicit primitive expansions for $G_\sigma(t, t')$ and $Q_\sigma(t, t')$. It involves calculating the changes in $J_\alpha(t, t')$ and $K_\alpha(t, t')$ produced by small variations in the $\phi_{\alpha\beta\mu\lambda}$, and it gives directly the contribution proportional

[16] In contrast to those for $J_\alpha(t, t')$ and $K_\alpha(t, t')$, the primitive expansions for $G_\alpha(t, t')$ and $Q_\alpha(t, t')$ have factors associated with both external lines.

to each irreducible $C_{n;p}(\alpha)$. The method is illustrated, for another application, in reference 2.[17]

The irreducible expansions are formally exact for any M. In the limit $M \to \infty$, our assumption that unwanted diagrams make no contribution to the primitive expansion implies that these diagrams make no contribution to the irreducible expansions also. The argument is precisely analogous to that given in Sec. 3 for the equilibrium case. Thus, we obtain the formal irreducible expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ in the limit $M \to \infty$ by retaining only the wanted irreducible diagrams. For each of the stochastic models, these expansions can be summed to give closed equations for $G(t, t')$ and $Q(t, t')$, in analogy to the equilibrium case. The results appear substantially more complicated than in the equilibrium case, however. The complete equations for all the models are given in Appendix B, for both the nonlinear oscillator example and the many-body problem.

We have remarked earlier that the irreducible expansions for $J_\alpha(t, t')$ and $K_\alpha(t, t')$ are simpler than those for $G_\alpha(t, t')$ and $Q_\alpha(t, t')$ themselves. The expansion for $G_\alpha(t, t')$ actually may be constructed very easily from that for $J_\alpha(t, t')$ by integrating (5.27). Thus we find

$$G_\alpha(t, t') = G^{(0)}(t, t') + \int_{t'}^{t} G^{(0)}(t, t'')J_\alpha(t'', t')\, dt''. \qquad (6.12)$$

The factor $G^{(0)}(t, t'')$ in the integrand may be considered to be associated with the outgoing external line in each of the irreducible diagrams. [We recall that no factor was associated with this line in any of the diagram-contributions to $J_\alpha(t, t')$.] However, we have not succeeded in finding an equally compact irreducible expansion for $Q_\alpha(t, t')$. Equation (5.29) gives a substantially more complicated result upon integration than does (5.27).

The difficulty in constructing a compact irreducible expansion for $Q_\alpha(t, t')$ is apparent from the structure of the primitive expansion for this quantity. In the primitive expansion for $G_\alpha(t, t')$, the factors associated with the incoming and outgoing external lines are always $G^{(0)}$ factors. This property underlies (6.12) [which is analogous to I:(4.12)]. In the primitive expansion for $Q_\alpha(t, t')$, some contributions have a $G^{(0)}$ factor associated with the outgoing external line and a $G^{(0)*}$ factor associated with the incoming external line. The remaining contributions have a $Q^{(0)}$ factor associated with either the incoming or outgoing external line and a $G^{(0)*}$ or $G^{(0)}$ factor associated with the other external line. This precludes an expression for $Q_\alpha(t, t')$ of the simple form (6.12).

It is clear from what has been presented in this Section that our nonequilibrium primitive and irreducible expansions do not have the simplicity and compactness of the diagram analysis for the equilibrium case, which we discussed in Sec. 3. This may be an unavoidable penalty for abandoning equilibrium, but it may also be that our formulation is unnecessarily awkward.[18]

7. VALIDITY OF THE CLOSED MODEL EQUATIONS

7.1. Description of Method

We wish in Sec. 7 to investigate the basic assumption that the total contribution of the unwanted diagrams vanishes in the limit $M \to \infty$. This assumption was stated for the equilibrium case in Sec. 3 and for nonequilibrium in Sec. 6. It was the essential ingredient in establishing closed equations for the model propagators, correlation functions, and Green's functions. The procedure we shall use here is to integrate the Heisenberg equations of motion by replacing them with a set of difference equations involving the discrete times t_0, $t_0 + \Delta t$, $t_0 + 2\Delta t$, $\cdots$. At each stage of integration, this finite-difference method yields approximations to the nonequilibrium correlation and Green's functions which contain as coefficients the same quantities $C_{n;p}(\alpha)$ that arose in the iteration procedure of Sec. 6. Only $C_{n;p}(\alpha)$ of finite order appear after a finite number of integration steps.

The finite-difference method of integration actually constitutes a definition of the Heisenberg equations of motion. Consequently, we may hope that it converges in the limit $\Delta t \to 0$ to yield the exact correlation and Green's functions, whether or not the iteration solutions of Sec. 6 converge. If, moreover, the convergence as $\Delta t \to 0$ is independent of M for large M, we may conclude immediately that

[17] As it is described in reference 2, the variational method is applicable only in the limit $M \to \infty$. However, it can be extended to finite M by the formal device of introducing a 'collection of collections,' consisting of M' collections each with M systems, and considering the limit $M' \to \infty$.

[18] A nonequilibrium linked-diagram formalism for infinite fermion systems has been described by K. Nishikawa [J. Phys. Soc. Japan 15, 78 (1960)], who uses the interaction representation instead of the Heisenberg representation. The basic quantities are taken as $Q_k(t, t')$ and $Q_k^+(t, t')$, rather than $Q_k(t, t')$ and $G_k(t, t')$. Equivalent complications in the construction of primitive and irreducible expansions arise in that formulation, if the analysis is carried out correctly for a Gaussian initial ensemble and finite $t - t_0$. [The asymptotic irreducible expansion expressed by Fig. 9 of the cited paper is not valid for finite $t - t_0$.]

the unwanted diagrams make zero total contribution to the exact correlation and Green's functions in the limit $M \to \infty$. This is because the unwanted $C_{n;p}(\alpha)$ which appear in any given finite-difference approximation are of finite order and vanish in the limit $M \to \infty$.

In what follows, we do not attempt to prove rigorously the requisite convergence properties of the finite-difference approximations. We make the convergence plausible by showing that the time derivatives of the matrix elements of the $\mathfrak{q}_{\mathbf{k}\alpha}(t)$ have bounds which are independent of M in an appropriate mean-square sense. This is done for all t without any appeal to perturbation expansions. However, it is essential to our analysis that the Hamiltonian be modified by removing all momentum modes above an arbitrarily high but finite cutoff $k_{\max}$. The significance of the momentum cutoff is discussed for the several stochastic models. In the case of the ring and ladder models, it is concluded that the exact functions $G_{\mathbf{k}\alpha}(t, t')$ and $Q_{\mathbf{k}\alpha}(t, t')$ for given $\mathbf{k}$ should be negligibly dependent on $k_{\max}$ if $k_{\max}$ is high enough and if $V(\mathbf{x})$ satisfies the conditions, stated in Sec. 2, which yield lower bounds to the eigenvalues of the model Hamiltonians.

After establishing, to the extent described, that the unwanted diagrams do not contribute to the nonequilibrium correlation and Green's functions, we point out that this does not complete the justification of our formal closed equations for the stochastic models. If the wanted diagrams are sufficiently numerous in high orders that they form nonconverging series, then a uniqueness question arises in the summation of these diagrams. We treat this question by regarding the closed integro-differential equations themselves as limits of finite-difference equations, rather than as summations of infinite classes of perturbation terms. Finally, we examine the conditions under which the nonequilibrium closed model equations imply those for equilibrium.

7.2. Bounds on Matrix Elements and Their Time Derivatives

Let us consider the positive-definite quantities

$$\begin{aligned} {}^{(r)}F_\alpha(t) &\equiv \langle \mathfrak{q}_\alpha^\dagger(t)\mathfrak{q}_\alpha(t)\rangle = Q_\alpha(t, t) \qquad (r = 0), \\ {}^{(r)}F_\alpha(t) &\equiv \left\langle \frac{d^r\mathfrak{q}_\alpha^\dagger(t)}{dt^r}\,\frac{d^r\mathfrak{q}_\alpha(t)}{dt^r}\right\rangle \quad (r = 1, 2, \cdots), \end{aligned} \tag{7.1}$$

where the $\mathfrak{q}_\alpha(t)$ are the Heisenberg operators for the nonlinear oscillator example. We have noted previously that the weighting operator (5.18) commutes with the Hamiltonian. It follows that

$${}^{(r)}F_\alpha(t) = {}^{(r)}F_\alpha(t_0) \qquad (r = 0, 1, 2, \cdots) \tag{7.2}$$

for all t. By (5.30), we then have

$${}^{(0)}F_\alpha(t) = \bar{N}, \tag{7.3}$$

where $\bar{N} = (e^a \pm 1)^{-1}$. Using (7.2), (5.6), (5.8), and Wick's theorem, we find

$$\begin{aligned} {}^{(1)}F_\alpha(t) = {} & \bar{N}\{\epsilon + V\bar{N}[C_{1;1}(\alpha) \mp C_{1;2}(\alpha)]\}^2 \\ & + V^2\bar{N}^2(1 \mp \bar{N})[C_{2;1}(\alpha) \mp C_{2;2}(\alpha)]. \end{aligned} \tag{7.4}$$

The $C_{n;p}(\alpha)$ which appear in (7.4) have been defined by (3.15), (3.17), (6.5), and (6.8). It follows from (2.19) that they are all real.

Expressions similar to (7.4) may be found for the ${}^{(r)}F_\alpha(t)$ of any finite order r. Each ${}^{(r)}F_\alpha(t)$ may be evaluated for all t by repeated differentiation and self-substitution of (5.8) at $t = t_0$, followed by the use of Wick's theorem. The result is a polynomial of finite degree in $\bar{N}$ and the $C_{n;p}(\alpha)$. Only the $C_{n;p}(\alpha)$ of order $n \leq 2r$ appear. It follows from (4.3) that each ${}^{(r)}F_\alpha(t)$ has a finite bound which depends on $\bar{N}$ but is independent of t, α, and M, and is also independent of the choice of model. In particular, this is true in the limit $M \to \infty$.

In order to make clear the significance of this result, let us write the traces which define the ${}^{(r)}F_\alpha(t)$ in the explicit form

$$\begin{aligned} {}^{(0)}F_\alpha(t) &= Z^{-1}\sum_{ss'} \exp\,[-a\mathfrak{N}(s)]\;|\langle s'|\,\mathfrak{q}_\alpha(t)\,|s\rangle|^2, \\ {}^{(r)}F_\alpha(t) &= Z^{-1}\sum_{ss'} \exp\,[-a\mathfrak{N}(s)] \\ &\quad \times |\langle s'|\,d^r\mathfrak{q}_\alpha(t)/dt^r\,|s\rangle|^2 \\ &= Z^{-1}\sum_{ss'} \exp\,[-a\mathfrak{N}(s)] \\ &\quad \times |d^r\langle s'\,|\mathfrak{q}_\alpha(t)|\,s\rangle/dt^r|^2 \qquad (r \geq 1), \end{aligned} \tag{7.5}$$

where

$$Z = \sum_s \exp\,[-a\mathfrak{N}(s)] \tag{7.6}$$

and $\langle s'\,|\mathfrak{q}_\alpha(t)|\,s\rangle$ is the matrix element of $\mathfrak{q}_\alpha(t)$ between the states s and s'. The sums are over the complete set of joint eigenstates s, s' of the Schrödinger number operators $q_\alpha^\dagger q_\alpha$, and

$$\mathfrak{N}(s) = \langle s\,|\sum_\alpha q_\alpha^\dagger q_\alpha|\,s\rangle \tag{7.7}$$

is the total number of quanta in the state s.

The boundedness of ${}^{(r)}F_\alpha(t)$ implies first of all that the sums in (7.5) converge to finite limits. In particular, it implies that the sum over the complete sets of states s which have successively increasing values of $\mathfrak{N}(s)$ converges as $\mathfrak{N}(s) \to \infty$. The density of states in the space of the occupation

numbers is such that the factor $Z^{-1}\exp[-a\mathfrak{N}(s)]$ in (7.5) gives the principal total weight in the sum to states s with $\mathfrak{N}(s) = O(M\bar{N})$. In the limit $M \to \infty$, the sum is in effect sharply confined to states s with $\mathfrak{N}(s)/M = \bar{N}$. Let us consider the complete set of states with a given value of $\mathfrak{N}(s)/M$. The boundedness of ${}^{(r)}F_\alpha(t)$ then implies that the rth time-derivatives of the complete set of matrix elements $\langle s'\,|\mathbf{q}_\alpha(t)|\,s\rangle$ have a mean-square bound which is independent of M in the limit $M \to \infty$ and which is finite if $\mathfrak{N}(s)/M$ is finite. It should be noted that the matrix elements $\langle s'\,|\mathbf{q}_\alpha(t)|\,s\rangle$ are nonvanishing only if $\mathfrak{N}(s') = \mathfrak{N}(s) - 1$. This follows from (5.6) and the fact that $\mathfrak{N}$ commutes with $\mathfrak{IC}$.

We must now extend the analysis to the many-body problem, for which $\mathfrak{IC}$ is given by (2.16) and (2.18). We seek mean-square bounds on the time-derivatives of the matrix elements $\langle s'\,|\mathbf{q}_{\mathbf{k}\alpha}(t)|\,s\rangle$, where s and s' are now joint eigenstates of all the number operators $N_{\mathbf{k}\alpha} = q^\dagger_{\mathbf{k}\alpha}q_{\mathbf{k}\alpha}$. Our previous technique can be applied in the present case only if a momentum cutoff is introduced, as mentioned in Sec. 7.1. We remove from $\mathfrak{IC}$ all terms which contain any q or $q\dagger$ factor whose momentum index exceeds in magnitude some arbitrarily high but finite value $k_{\max}$. It is clear that the cutoff preserves the Hermiticity of $\mathfrak{IC}$. We shall reserve for Sec. 7.5 all discussion of the dynamical significance of the cutoff for the several stochastic models.

Bounds for the many-body matrix elements with the momentum cutoff imposed can be obtained in close analogy to the procedure for the nonlinear oscillator. We introduce the special Gaussian weight operator

$$\mathfrak{W}' = \exp[-\sigma\sum_{\mathbf{k}\alpha}N_{\mathbf{k}\alpha}] = \exp[-\sigma\mathfrak{N}], \tag{7.8}$$

where σ is a real constant. (For bosons only, σ must also be positive.) Unlike the more general form (5.35), this operator commutes with $\mathfrak{IC}$ and therefore corresponds to an equilibrium ensemble. It may be regarded as the infinite-temperature limit ($\beta \to 0$, $-\beta\mu \to \sigma$) of the weighting operator $\exp[-\beta(\mathfrak{IC} - \mu\mathfrak{N})]$ which yields the grand canonical ensemble for the problem with momentum cutoff.

Let $\langle\ \rangle'$ denote a trace weighted by $\mathfrak{W}'$. Then the quantities

$$\begin{aligned} {}^{(r)}F_{\mathbf{k}\alpha}(t) &\equiv \langle \mathbf{q}^\dagger_{\mathbf{k}\alpha}(t)\mathbf{q}_{\mathbf{k}\alpha}(t)\rangle' \qquad (r = 0), \\ {}^{(r)}F_{\mathbf{k}\alpha}(t) &\equiv \left\langle \frac{d^r\mathbf{q}^\dagger_{\mathbf{k}\alpha}(t)}{dt^r}\,\frac{d^r\mathbf{q}_{\mathbf{k}\alpha}(t)}{dt^r}\right\rangle' \quad (r = 1, 2, \cdots) \end{aligned} \tag{7.9}$$

satisfy

$${}^{(r)}F_{\mathbf{k}\alpha}(t) = {}^{(r)}F_{\mathbf{k}\alpha}(t_0). \tag{7.10}$$

The ${}^{(r)}F_{\mathbf{k}\alpha}(t)$ may be evaluated in the same way as the ${}^{(r)}F_\alpha(t)$. We find

$${}^{(0)}F_{\mathbf{k}\alpha}(t) = b, \tag{7.11}$$

$$\begin{aligned} {}^{(1)}F_{\mathbf{k}\alpha}(t) &= b\{\epsilon_{\mathbf{k}} + b\sum_{\mathbf{p}}[V_0C_{1;1}(\alpha) \mp V_{\mathbf{k}-\mathbf{p}}C_{1;2}(\alpha)]\}^2 \\ &\quad + b^2(1 \mp b)\sum_{\mathbf{ps}} V_{\mathbf{k}-\mathbf{s}}[V_{\mathbf{k}-\mathbf{s}}C_{2;1}(\alpha) \mp V_{\mathbf{p}-\mathbf{s}}C_{2;2}(\alpha)], \end{aligned} \tag{7.12}$$

where $b = (e^\sigma \pm 1)^{-1}$. The summations in (7.12) are over all $\mathbf{p}$ and $\mathbf{s}$ such that $|\mathbf{p}|$, $|\mathbf{s}|$, and $|\mathbf{k} + \mathbf{p} - \mathbf{s}|$ are all less than $k_{\max}$. [It should be noted that, since Ω is finite, the problem with momentum cutoff admits only a finite number of momentum modes. Hence, finite b implies a finite mean number of particles per system $\langle\mathfrak{N}\rangle'/M$.] For $r > 1$, we find, as before, that ${}^{(r)}F_{\mathbf{k}\alpha}(t)$ is a finite-degree polynomial in b and in the $C_{n;p}(\alpha)$ of order $n \leq 2r$.

It now follows from (4.3) that ${}^{(r)}F_{\mathbf{k}\alpha}(t)$ has a bound which depends on b and on $\mathbf{k}$ but not on α, t, or M. Let us consider the complete set of states s such that $\mathfrak{N}(s)/M$ has a given value. Here $\mathfrak{N}(s) = \sum_{\mathbf{k}\alpha}N_{\mathbf{k}\alpha}(s)$ is the eigenvalue of the total number of particles. The boundedness of ${}^{(r)}F_{\mathbf{k}\alpha}(t)$ then implies that the rth derivatives of the complete set of matrix elements $\langle s'\,|\mathbf{q}_{\mathbf{k}\alpha}(t)|\,s\rangle$ have a mean-square bound which is independent of M in the limit $M \to \infty$ and which is finite if $\mathfrak{N}(s)/M$ is finite. The argument is the same as for the nonlinear oscillator.

7.3. Integration of the Heisenberg Equations

Let us now consider the evaluation of the nonlinear-oscillator functions $G_\alpha(t, t')$ and $Q_\alpha(t, t')$ by a finite-difference solution of the Heisenberg equations of motion. We seek the solution over some given time-domain $(t_0, t_{\max})$. Let the domain be divided into equal intervals Δt and let (5.8) and (5.11) be replaced by the sets of difference equations

$$\begin{aligned} \mathbf{q}_\alpha(t_{r+1}) &= \mathbf{q}_\alpha(t_r) \\ &\quad - i\,\Delta t[\epsilon\mathbf{q}_\alpha(t_r) + M^{-1}V\mathbf{L}_\alpha(t_r)], \\ \mathbf{q}_\alpha(t_0) &= q_\alpha, \end{aligned} \tag{7.13}$$

and

$$\begin{aligned} \mathbf{G}_{\alpha\gamma}(t_{r+1}, t_m) &= \mathbf{G}_{\alpha\gamma}(t_r, t_m) \\ &\quad - i\,\Delta t[\epsilon\mathbf{G}_{\alpha\gamma}(t_r, t_m) + M^{-1}V\mathbf{M}_{\alpha\gamma}(t_r, t_m)], \\ \mathbf{G}_{\alpha\gamma}(t_m, t_m) &= \delta_{\alpha\gamma}, \end{aligned} \tag{7.14}$$

where $t_r = t_0 + r\,\Delta t$ ($r = 0, 1, 2, \cdots$). We may solve these equations in terms of the Schrödinger operators by recursion, substitute the results into (5.19) and (5.20), use Wick's theorem, and thereby

evaluate the quantities $Q_\alpha(t_r, t_m)$ and $G_\alpha(t_r, t_m)$. Equivalently, we may substitute into (5.31) and (5.32) and evaluate the quantities $J_\alpha(t_r, t_m)$ and $K_\alpha(t_r, t_m)$. The results are related by the equations

$$\begin{aligned} &G_\alpha(t_{r+1}, t_m) - G_\alpha(t_r, t_m) \\ &\quad = \Delta t[-i\epsilon G_\alpha(t_r, t_m) + J_\alpha(t_r, t_m)], \\ &Q_\alpha(t_{r+1}, t_m) - Q_\alpha(t_r, t_m) \\ &\quad = \Delta t[-i\epsilon Q_\alpha(t_r, t_m) + K_\alpha(t_r, t_m)], \end{aligned} \tag{7.15}$$

which are the finite-difference forms of (5.27) and (5.29).

The final expressions obtained by this procedure resemble the results of the iteration expansion carried out in Sec. 6. Each contribution to $Q_\alpha(t_r, t_m)$, or to the other functions, consists of some product of factors $Q^{(0)}(t_0, t_0)$ and $Q^{+(0)}(t_0, t_0)$ multiplied by some power n of V and by a factor $C_{n;p}(\alpha)$. As in the case of the iteration expansion, all the contributions containing a given $C_{n;p}(\alpha)$ may be associated with the pth distinct primitive linked diagram of n vertices. There are two differences, however. The first is that the finite difference results involve only the initial value $Q^{(0)}(t_0, t_0)$, in contrast to the time functions $Q^{(0)}(t, t')$ and $G^{(0)}(t, t')$ which appear in the iteration results. This is because we are taking finite-difference approximations to (5.8) and (5.11) rather than to the integral equations (5.13) and (5.14). The second difference is that the classes of diagrams included by the successive stages of the two procedures are very different. The iteration expansion is a power-series expansion in V; at the rth stage, it yields for $Q_\alpha(t, t')$ an approximation which contains only the $C_{n;p}(\alpha)$ of order $n \leq r$. In contrast, the quantity $Q_\alpha(t_r, t_m)$ obtained by the finite-difference scheme contains some $C_{n;p}(\alpha)$ as high as $n = \frac{1}{2}(3^r + 3^m - 2)$. The finite-difference scheme can be considered a particular kind of consolidation, reordering, and weighting of the iteration (perturbation) expansion.

Let us now consider the convergence properties of the finite-difference approximations in the limit $\Delta t \to 0$. The exact function $Q_\alpha(t, t')$ may be written as the explicit sum

$$\begin{aligned} Q_\alpha(t, t') = Z^{-1} \sum_{ss'} &\exp[-a\mathfrak{N}(s)] \\ &\times \langle s\,|\mathbf{q}_\alpha^\dagger(t')|\,s'\rangle\langle s'\,|\mathbf{q}_\alpha(t)|\,s\rangle. \end{aligned} \tag{7.16}$$

A similar expression for $G_\alpha(t, t')$ may be obtained by using (5.10). The Heisenberg equations (5.8) constitute a coupled set of first-order differential equations for the matrix elements which appear in (7.16). The error in the matrix elements given by the finite-difference integration scheme therefore depends on the magnitude of the second derivatives $d^2\langle s'\,|\mathbf{q}_\alpha(t)|\,s\rangle/dt^2$ over the domain $(t_0, t_{\max})$. These derivatives, however, are not bounded for all s and s'. Certain matrix elements between states in which the total number of quanta is very large oscillate with extreme rapidity. No matter how small Δt may be taken, there will be matrix elements that are poorly approximated. Convergence of the finite-difference approximations for $Q_\alpha(t, t')$ therefore requires that the weighting function $Z^{-1}\exp[-a\mathfrak{N}(s)]$ in (7.16) suppress the contribution of matrix elements with infinitely rapid time variation.

We found in Sec. 7.2 that for each finite r the quantities

$${}^{(r)}F_\alpha(t) = \left[\frac{\partial^{2r}Q_\alpha(t, t')}{\partial t^r\,\partial t'^r}\right]_{t'=t}$$

satisfy finite bounds which are independent of t, α, and M. We note also that the contribution of every matrix element to ${}^{(r)}F_\alpha(t)$ is real and non-negative. It follows from this that matrix elements with infinite time derivatives do not make a finite contribution to $Q_\alpha(t, t)$. By applying Schwarz's inequality to (7.16), we see that the contribution of any matrix element to $Q_\alpha(t, t')$ is bounded by its contributions to $Q_\alpha(t, t)$ and $Q_\alpha(t', t')$. These considerations suggest that in the limit $\Delta t \to 0$ the finite-difference approximations to $Q_\alpha(t, t')$ and $G_\alpha(t, t')$ may converge to give the exact functions over any given domain $(t_0, t_{\max})$.

It should be emphasized that we have not given a proof of convergence. The fact that matrix elements with extremely high oscillation frequencies make a negligible contribution to the exact $Q_\alpha(t, t')$ does not assure that they also make negligible contributions to the finite-difference approximations to $Q_\alpha(t, t')$. The successive approximations to such matrix elements will in general be unstable, and can greatly exceed the exact values after a sufficient number of integration steps. We shall not attempt to resolve this question in the present paper. However, we conjecture that such instability does not destroy the convergence of the finite-difference approximations to $Q_\alpha(t, t')$. The reasoning behind the conjecture is intimately connected with the collective nature of the variables $\mathbf{q}_\alpha(t)$. It is clearest for the true problem, and we shall outline the argument briefly for this case.

The Hamiltonian for the true problem is (5.1). The matrix elements for this case may be evaluated immediately in the representation where the individual-system number operators $q_{[n]}^\dagger q_{[n]}$ are diagonal,

and the $\langle s' \, |\mathbf{q}_\alpha(t)| \, s\rangle$ may then be evaluated by transformation to the representation with the $q_\alpha^\dagger q_\alpha$ diagonal. If one carries this out and takes M very large, the results strongly suggest[19] that, for any given $\bar{N}$, those $\langle s' \, |\mathbf{q}_\alpha(t)| \, s\rangle$ which have significant components with frequencies $\gg (\epsilon + V\bar{N})$ are ones for which $\mathfrak{N}(s)/(M\bar{N}) \gg 1$. However, these matrix elements are very strongly suppressed by the weighting factor $Z^{-1} \exp[-a\mathfrak{N}(s)]$ in (7.16) when M is very large. This makes it plausible that the finite-difference approximations to $Q_\alpha(t, t')$ converge as $\Delta t \to 0$ if we take M infinite.[20] Now we note that the $C_{n;p}(\alpha)$ are independent of M for the true problem and consequently the finite-difference approximations to $Q_\alpha(t, t')$ are independent of M. This then implies, if the previous argument is correct, that the approximations to $Q_\alpha(t, t')$ converge for any M. For small M, however, we conjecture that instabilities arise in such a way that the sum over states s and s' in (7.16) becomes, in effect, a sum over a divergent but formally correct series as we take $\Delta t \to 0$.

The argument just outlined can be extended to the stochastic models by introducing a 'collection of collections' consisting of M' collections each with M systems, taking collective variables in the collection of collections, and considering the case of infinite M'. The extension can also be made without this device. The central part of the argument—that for large M only states with $\mathfrak{N}(s)/(M\bar{N}) \gg 1$ give rise to matrix elements having significant components with frequencies $\gg (\epsilon + V\bar{N})$—appears on qualitative grounds to depend only on the collective nature of the $\mathbf{q}_\alpha(t)$ and to be as valid for the models as for the true problem. A point of consistency which should be noted here is that the explicit expressions for the successive $\langle s' \, |\mathbf{q}_\alpha(t_r)| \, s\rangle$, obtained by recursive solution of (7.13), involve only matrix elements between intermediate states s'' which satisfy $\mathfrak{N}(s'') \leq \mathfrak{N}(s) - 1$.

It now remains to extend our considerations to the many-body problem. In order to clarify the discussion, let the weighting operator (5.35) be taken in the particular form

$$\mathfrak{W} = \exp[-\beta_0(\mathfrak{K}_0 - \mu_0\mathfrak{N})]. \tag{7.17}$$

If $V(\mathbf{x})$ were zero, this would correspond to a grand canonical ensemble at temperature β_0 and chemical potential μ_0. With $V(\mathbf{x})$ nonzero, (7.17) does not correspond to an equilibrium ensemble.

We may now write $Q_{\mathbf{k}\alpha}(t, t')$ as the explicit sum

$$\begin{aligned} Q_{\mathbf{k}\alpha}(t, t') = Z^{-1} \sum_{ss'} & \\ \times \exp\{-\beta_0(\sum_{\mathbf{p}\gamma} \epsilon_{\mathbf{p}} N_{\mathbf{p}\gamma}(s) - \mu_0\mathfrak{N}(s))\} & \\ \times \langle s \, |\mathbf{q}_{\mathbf{k}\alpha}^\dagger(t')| \, s'\rangle\langle s' \, |\mathbf{q}_{\mathbf{k}\alpha}(t)| \, s\rangle. & \end{aligned} \tag{7.18}$$

Here s and s' are members of the complete set of joint eigenstates of the number operators $N_{\mathbf{p}\gamma} = q_{\mathbf{p}\gamma}^\dagger q_{\mathbf{p}\gamma}$, the $N_{\mathbf{p}\gamma}(s)$ are the eigenvalues of these operators, and $\mathfrak{N}(s) = \sum_{\mathbf{p}\gamma} N_{\mathbf{p}\gamma}(s)$ is the eigenvalue of the total number operator $\mathfrak{N}$. The factor Z is now given by

$$Z = \sum_s \exp\{-\beta_0[\sum_{\mathbf{p}\gamma} \epsilon_{\mathbf{p}} N_{\mathbf{p}\gamma}(s) - \mu_0\mathfrak{N}(s)]\}. \tag{7.19}$$

If the term $-\beta_0 \sum_{\mathbf{p}\gamma} \epsilon_{\mathbf{p}} N_{\mathbf{p}\gamma}(s)$ were absent from (7.18), our discussion of the convergence of the finite-difference approximations for the nonlinear oscillator would be immediately applicable to the many-body problem with momentum cutoff. This follows because we found similar mean-square bounds on matrix-element derivatives in the two cases. But it is difficult to see how the presence of the term in question can interfere with convergence. The effect is to weight the sum against states in which there is strong initial excitation of high momenta and, therefore, in which the initial kinetic energy is high. Since the problem is conservative, this implies a discrimination for all t against certain states of high total energy. If we consider large M, then the weighting operator (7.17) effectively confines the sum to states s for which $\mathfrak{N}(s)/(M\bar{N}) \approx 1$, where $\bar{N}$ is determined by β_0 and μ_0. In this respect, it resembles the infinite-temperature weighting operator (7.8) which we used to obtain bounds on matrix elements. But further, it chooses from among the complete set of such states a subset which is weighted in a particular fashion against high total energy eigenvalues. The additional selection may reasonably be expected to increase rather than decrease the suppression of matrix elements with extremely high frequencies of oscillation. We conclude therefore that if the finite-difference scheme converges for the nonlinear oscillator, then it is very plausible that the

[19] We have not proved this rigorously.

[20] It is important here that the Heisenberg equations of motion used in the finite-difference procedure be taken in the form (5.8) and not in the form

$$d\mathbf{q}_\alpha/dt = i(\mathfrak{K}\mathbf{q}_\alpha - \mathbf{q}_\alpha\mathfrak{K}).$$

The latter form yields unlinked- as well as linked-diagram contributions to $Q_\alpha(t, t')$, as we have already noted. It is unsuitable for a finite-difference integration procedure because the eigenvalues of $\mathfrak{K}$ grow with M so that, for large M, $d\mathbf{q}_\alpha/dt$ is expressed as the difference of two operators each with large matrix elements. In this situation, it could not be expected that the convergence of a finite-difference procedure would be independent of M as $M \to \infty$. An equivalent difficulty arises if one attempts finite-difference integration in the Schrödinger representation.

finite-difference approximations to the many-body functions $Q_{\mathbf{k}\alpha}(t, t')$ and $G_{\mathbf{k}\alpha}(t, t')$ also converge, at least for the problem with momentum cutoff.

7.4. Justification of the Formal Model Equations

Let us assume, on the basis of Sec. 7.3, that the finite-difference approximations to $G_{\mathbf{k}\alpha}(t, t')$ and $Q_{\mathbf{k}\alpha}(t, t')$ converge for all M as $\Delta t \to 0$, and that the convergence is independent of M for large M. It follows directly that the total contribution of the unwanted diagrams vanishes for each of the stochastic models in the limit $M \to \infty$. The unwanted $C_{n;p}(\alpha)$ which appear in each approximation are of finite order and vanish in the limit $M \to \infty$. Thus they do not appear in the final functions to which the sequence of finite-difference approximations converges.

The justification of our formal closed model equations for nonequilibrium does not immediately follow from the vanishing of the contribution of the unwanted diagrams. These equations were obtained in Sec. 6 by carrying out formal sums of the primitive- diagram iteration expansions for $Q_{\mathbf{k}\alpha}(t, t')$ and $G_{\mathbf{k}\alpha}(t, t')$ with only the wanted diagrams included. However, it is possible that the expansions are divergent even when they are restricted to wanted diagrams. In this case, it is not assured that the formal closed model equations represent a unique summation of the expansions. This question can be resolved by considering the formal model equations themselves as the limits of finite-difference equations rather than as infinite sums of perturbation terms. The justification of the equations proceeds in several steps, which we shall outline in terms of the nonlinear oscillator example.

It is convenient for the present purpose to carry out a finite-difference solution of the integral equations (5.13) and (5.14) instead of (5.8) and (5.11). Upon substituting the results into (5.19), (5.20), (5.31), and (5.32), one obtains expressions for $G_\alpha(t_r, t_m)$, $Q_\alpha(t_r, t_m)$, $J_\alpha(t_r, t_m)$, and $K_\alpha(t_r, t_m)$ which may be evaluated by Wick's theorem in terms of the quantities $Q^{(0)}(t_{r'}, t_{m'})$, $Q^{+(0)}(t_{r'}, t_{m'})$, $G^{(0)}(t_{r'}, t_{m'})$, and $G^{(0)*}(t_{r'}, t_{m'})$. These expressions are more compact (and also more accurate for finite Δt) than those obtained by the more elementary integration scheme of Sec. 7.3. The results of the present procedure are analogous to the primitive expansions of Sec. 6.1. They contain contributions associated with all the primitive linked diagrams. Only diagrams of finite order contribute to $G_\alpha(t_r, t_m)$, etc. for given r and m.

The expressions for $J_\alpha(t_r, t_m)$ and $K_\alpha(t_r, t_m)$ can be reformulated in terms of contributions associated with irreducible diagrams only. As in Sec. 6.2, one obtains the irreducible forms by retaining only the contributions associated with all the irreducible diagrams, and in them replacing each factor $G^{(0)}(t_{r'}, t_{m'})$, $G^{(0)*}(t_{r'}, t_{m'})$, $Q^{(0)}(t_{r'}, t_{m'})$, or $Q^{+(0)}(t_{r'}, t_{m'})$ with a factor $G_\sigma(t_{r'}, t_{m'})$, $G^*_\sigma(t_{r'}, t_{m'})$, $Q_\sigma(t_{r'}, t_{m'})$, or $Q^+_\sigma(t_{r'}, t_{m'})$, where σ is the collective index which labels the relevant line. The irreducible-diagram expressions for $J_\alpha(t_r, t_m)$ and $K_\alpha(t_r, t_m)$ may be verified, as in Sec. 6.2, by substituting for each factor $G_\sigma(t_{r'}, t_{m'})$, etc., its finite-difference expression in terms of primitive diagrams. In the present case, the expression for each $G_\sigma(t_{r'}, t_{m'})$ is a finite sum over primitive-diagram contributions instead of an infinite series. Alternatively, the irreducible expressions may be obtained by the variational method mentioned in Sec. 6.2.

At this point we may take the limit $M \to \infty$, so that only contributions associated with the wanted irreducible diagrams survive. In the case of the Hartree-Fock and random-coupling models, it may then be verified that if the expressions for $J_\alpha(t_r, t_m)$ and $K_\alpha(t_r, t_m)$ are substituted into (7.15) the results are just the finite-difference forms of the closed integro-differential equations for these models given in Appendix B. In the limit $\Delta t \to 0$, they become identical with these equations. For the ladder and ring models, the further step remains of summing the (finite) series of irreducible diagrams which contribute to each quantity $K_\alpha(t_r, t_m)$ and $J_\alpha(t_r, t_m)$. This can be done by introducing vertex functions defined by difference equations. The final sets of equations thus obtained are again the finite-difference forms of the closed integro-differential equations for the models which are given in Appendix B.

The formal closed model equations may thus be obtained without any use of the perturbation expansions of Sec. 6. Their justification then depends solely upon the validity of our assumption that the finite-difference integration scheme converges in the limit $\Delta t \to 0$.

7.5. Approach to Equilibrium

Let us now consider the extent to which validity of the formal closed model equations for nonequilibrium implies validity of the equilibrium model equations of Sec. 3. On the basis of the preceding discussion, we shall suppose throughout the present section that the nonequilibrium closed equations are valid over any given domain $(t_0, t_{\max})$ for all the stochastic models with momentum cutoff.

Consider first the ladder and ring models when

the conditions stated in Sec. 2 for boundedness of the potential energy per particle are satisfied. It is easy to verify that the imposition of a momentum cutoff does not destroy the boundedness properties. The interaction Hamiltonian for the ladder model may still be written in the form (2.30), which is positive definite if $V(\mathbf{x})$ is non-negative everywhere.[21] When all the $V_{\mathbf{k}}$ are non-negative, the lower bound $-\frac{1}{2}V(0)\mathfrak{N}$, implied by (2.33) for all the total potential energy of the ring model, is replaced by the less negative bound $-\frac{1}{2}\sum_{\alpha\mathbf{k}\mathbf{p}} V_{\mathbf{k}-\mathbf{p}}N_{\mathbf{k}\alpha}$, where the sum over momenta is restricted by $|\mathbf{k}| \leq k_{\max}$, $|\mathbf{p}| \leq k_{\max}$.

Suppose that we take the nonequilibrium ensemble in the form (7.17). For given β_0 and μ_0, momenta $|\mathbf{k}| \sim k_{\max}$ will have negligible initial excitation if $k_{\max}$ is sufficiently high. Since the potential energy per particle is bounded from below and the system is conservative, it then is plausible that such momenta will be negligibly excited at any later time. We anticipate that the behavior of $G_{\mathbf{k}\alpha}(t, t')$ and $Q_{\mathbf{k}\alpha}(t, t')$ will be independent of $k_{\max}$ for all time in the limit $k_{\max} \to \infty$.

The discussion of Sec. 5.5 now suggests that in the limit $t_0 \to -\infty$ the nonequilibrium functions $G_{\mathbf{k}\alpha}(t, t')$ and $Q_{\mathbf{k}\alpha}(t, t')$ should depend only on $t - t'$ and should be related by (5.48) to the temperature-domain equilibrium propagators for some β and μ. (In general, we will have $\beta \neq \beta_0$ and $\mu \neq \mu_0$.) Since the unwanted $C_{n;p}(\alpha)$ do not contribute to the nonequilibrium functions, it follows that they should not contribute to the equilibrium propagators in the limit $M \to \infty$. The closed equations for the model propagators are then justified provided, in addition, that the formal summations of wanted diagrams described in Sec. 3 are justified. The latter supposition is made plausible by the discussion of Sec. 7.4, which validates the corresponding summation of wanted diagrams for the nonequilibrium functions.

The arguments just presented are not conclusive, and they are based in part on ergodic assumptions which are very difficult to investigate. However, it may be feasible to check the correspondence between the equilibrium and nonequilibrium closed-model equations in a direct analytical fashion. If both sets of equations are valid, and if our ergodic assumptions (Sec. 5.5) are valid, then the equations for $S_{\mathbf{k}\alpha}(\zeta_\alpha)$ should be obtainable by analytic continuation from the nonequilibrium equations for $t_0 \to -\infty$. We have not attempted this.

The following point should be noted. Some equilibrium values of β and μ may be unreachable by any choice of β_0 and μ_0 in (7.17). In particular, if $V(\mathbf{x})$ is purely repulsive the initial potential energy will be so high that very low temperatures will be unreachable. The reason is that (7.17) represents zero initial two-body correlations. We may handle this situation by taking a true problem in which the system of interest is coupled by weak forces to a reservoir of otherwise free particles and constructing a stochastic model of the combined system. If enough particles are in the reservoir, and the coupling is weak enough, then any desired equilibrium temperature may be reached by evolution of an ensemble of the form (7.17). In this way we may justify the formal closed equilibrium equations for the propagators of the combined system. Finally, we may let the coupling to the reservoir go to zero and thereby recover the closed propagator equations for the system of interest in isolation.

Now let us consider the random-coupling model, in which there is no lower bound to the potential energy per particle in the limit $M \to \infty$. Our remarks will also apply to the ladder and ring models when $V(\mathbf{x})$ does not satisfy the conditions which give bounds on the eigenvalues of $\mathfrak{K}_i$. In the absence of a momentum cutoff, it is not assured that these models will evolve to equilibrium at all. It is possible that the mean potential energy may grow negatively infinite and the mean kinetic energy positively infinite. With the momentum cutoff, there is a ceiling on the kinetic energy, and in this case we anticipate that an equilibrium will be achieved. The supposition is supported by the existence of the rigorous equilibrium ensembles given by (7.8). However, such an equilibrium may differ very markedly in its properties from a grand canonical ensemble. In particular, it may be unstable under coupling to external systems. Obviously, its properties need not become independent of $k_{\max}$ as $k_{\max} \to \infty$. These considerations lead us to regard the formal closed equations for the temperature-domain propagators with strong suspicion in the case of models with no lower bound on the potential energy per particle. The classical results presented in I perhaps cast some light on the situation.

APPENDIX A. GENERALIZED MODELS FOR DISTINGUISHABLE PARTICLES

Let the true Hamiltonian for a system of N distinguishable particles interacting through the pair

[21] The cutoff does not mean the removal of all $V_{\mathbf{k}}$ from $\mathfrak{K}_i$ for $k > k_{\max}$. Higher $V_{\mathbf{k}}$ are admitted where they connect q and $q^\dagger$ factors admitted by the cutoff. In the x-space representation, the cutoff leaves $V(\mathbf{x})$ unaltered but restricts the fields $\psi_\alpha(\mathbf{x})$ and $\psi_\alpha^\dagger(\mathbf{x})$ to Fourier sums which do not contain the excluded momentum modes.

potential $V(\mathbf{x})$ be

$$H = \tfrac{1}{2}\sum_i \mathbf{p}_i^2 + H_i, \quad H_i = \tfrac{1}{2}\sum_{ij}{}' V(\mathbf{x}_i - \mathbf{x}_j), \tag{A1}$$

as in I:Sec. 2.1. As before, $\sum'_{ij}$ means that $i = j$ is to be omitted in the summation. We consider a collection of M such systems (M odd) with total true Hamiltonian

$$\mathcal{H} = \tfrac{1}{2}\sum_n \sum_i \mathbf{p}_{i[n]}^2 + \mathcal{H}_i,$$
$$\mathcal{H}_i = \tfrac{1}{2}\sum_n \sum_{ij}{}' V(\mathbf{x}_{i[n]} - \mathbf{x}_{j[n]}), \tag{A2}$$

where $\mathbf{x}_{i[n]}$ and $\mathbf{p}_{i[n]}$ are the position and momentum of the ith particle of the nth system. Then we take the general model $\mathcal{H}_i$ in the form

$$\mathcal{H}_i = \tfrac{1}{2}\sum_{nm} \sum_{ij}{}' V_{ij[nm]}(\mathbf{x}_{i[n]} - \mathbf{x}_{j[m]}), \tag{A3}$$

with

$$V_{ij[nm]}(\mathbf{x}) = M^{-1}V(\mathbf{x}) \times \sum_\alpha \exp[-i2\pi(n-m)\alpha/M]\phi_{i,j;\alpha}$$
$$[\alpha = 0, \pm 1, \cdots, \pm \tfrac{1}{2}(M-1)]. \tag{A4}$$

To recover the true problem, we take $\phi_{i,j;\alpha} = 1$ for all i, j, and α, thereby obtaining

$$V_{ij[nm]}(\mathbf{x}) = \delta_{nm}V(\mathbf{x}). \tag{A5}$$

In the stochastic models, the $\phi_{i,j;\alpha}$ have unit modulus but stochastically determined phases. In this case, the individual systems in the collection are dynamically intercoupled. We see from (A4) that $V_{ij[nm]}(\mathbf{x}_{i[n]} - \mathbf{x}_{j[m]})$ depends not only on the displacement $\mathbf{x}_{i[n]} - \mathbf{x}_{j[m]}$ of the pair of particles in space, but also on their 'displacement' $n - m$ in the collection. Moreover, $V_{ij[nm]}(\mathbf{x})$ is different, in general, for each pair i, j.

The distinguishable particle versions of the generalized ladder, ring, random-coupling, and Hartree-Fock models are given by the following prescriptions:

Ladder Model

Take

$$\phi_{i,j;\alpha} = \exp[+i2\pi\alpha\,\Delta_{i,j}/M], \quad \Delta_{i,j} = -\Delta_{j,i}. \tag{A6}$$

For each pair of indices i, j fix the integer $\Delta_{i,j}$ by an independent random choice in the interval $(0 \leq \Delta < M)$, subject only to the antisymmetry constraint in (A6). By (A4) and (2.10), we find

$$V_{ij[nm]}(\mathbf{x}) = \delta_{n-\Delta_{i,j},m}V(\mathbf{x}), \tag{A7}$$

where $\delta_{n-\Delta_{i,j},m}$ is to be interpreted according to the cyclic convention (2.15).

Ring Model

Take

$$\phi_{i,j;\alpha} = \exp[-i2\pi(\Delta_{i;\alpha} + \Delta_{j;-\alpha})/M], \quad \Delta_{i;\alpha} = -\Delta_{i;-\alpha}. \tag{A8}$$

For each pair of indices i, α fix the integer $\Delta_{i;\alpha}$ by an independent random choice in the interval $(0 \leq \Delta < M)$, subject only to the antisymmetry constraint in (A8).

Random-Coupling Model

Take

$$\phi_{i,j;\alpha} = \exp[-i2\pi\,\Delta_{i,j;\alpha}/M], \quad \Delta_{i,j;\alpha} = -\Delta_{j,i;\alpha}, \quad \Delta_{i,j;\alpha} = -\Delta_{i,j;-\alpha}. \tag{A9}$$

For each triad of indices i, j, α, fix the integer $\Delta_{i,j;\alpha}$ by an independent random choice in the interval $(0 \leq \Delta < M)$, subject only to the antisymmetry constraints in (A9).

Hartree-Fock Model

Take

$$\phi_{i,j;0} = 1, \quad \phi_{i,j;\alpha} = 0 \quad (\alpha \neq 0). \tag{A10}$$

There are no random parameters. By (A4) and (2.10), we have

$$V_{ij[nm]} = M^{-1}V(\mathbf{x}_{i[n]} - \mathbf{x}_{j[m]}). \tag{A11}$$

A comparison of the present models with those of I:Sec. 2 shows that 'displacement in collection' $n - m$, and the associated 'Fourier' modes α, now play the roles in constructing the randomized potentials that formerly were played by spatial displacement $\mathbf{x}_i - \mathbf{x}_j$ and the Fourier modes $\mathbf{k}$. In the present models, the shape of the interaction between any pair of particles is always that of $V(\mathbf{x})$; There is no mutilation of the potential as in I:Sec. 2. However, the strength of this interaction can vary with $n - m$, i, and j. In the simplest case, the Hartree-Fock model, we see from (A3) and (A11) that each particle simply moves in the average field of the entire collection of particles.

If one takes a grand canonical ensemble of collections, the present models lead, in the limit $M \to \infty$, to closed expressions for the classical Helmholtz free energy whatever may be the value of $\bar{N}$, the mean number of particles per system. A classical nonequilibrium formalism, analogous to that of Secs. 5 and 6, may be developed for these models. It involves n-body time-displaced distribution functions ($n = 1, 2, \cdots$) and also Green's

functions which give the response of these distributions to small perturbations.

APPENDIX B. NONEQUILIBRIUM MODEL EQUATIONS

We list here the final expressions for $J_{\mathbf{k}\alpha}(t, t')$ and $K_{\mathbf{k}\alpha}(t, t')$ for the four stochastic models in the limit $M \to \infty$. The collective indices α, $\cdots$ are omitted since there is no dependence on these indices in the limit. The equations below, taken together with (5.43) and (5.44), form complete sets which determine the evolution of $G_{\mathbf{k}}(t, t')$, $Q_{\mathbf{k}}(t, t')$, and $Q^{+}_{\mathbf{k}}(t, t') = G_{\mathbf{k}}(t, t') \mp Q_{\mathbf{k}}(t, t')$. (As in the text, the upper and lower signs of a double sign refer to fermions and bosons, respectively.) The equations for the boson random-coupling model (with $t_0 = -\infty$) have been given previously.[13] The equations for the several nonlinear oscillator models may be obtained from those below simply by omitting all the momentum indices and sums over momenta. All integrals in the equations below may be taken from t_0 to $+\infty$; the G functions then automatically restrict the actual ranges of integration according to the defining relation $G_{\mathbf{k}}(t, t') = 0$ $(t < t')$.

Hartree-Fock Model

$$J_{\mathbf{k}}(t, t') = -i \sum_{\mathbf{p}} (V_0 \mp V_{\mathbf{k}-\mathbf{p}}) \bar{N}_{\mathbf{p}}(t) G_{\mathbf{k}}(t, t') \tag{B1}$$

$$K_{\mathbf{k}}(t, t') = -i \sum_{\mathbf{p}} (V_0 \mp V_{\mathbf{k}-\mathbf{p}}) \bar{N}_{\mathbf{p}}(t) Q_{\mathbf{k}}(t, t') \tag{B2}$$

Here

$$\bar{N}_{\mathbf{p}}(t) = Q_{\mathbf{p}}(t, t) \tag{B3}$$

is the mean number of particles per system with momentum $\mathbf{p}$ at time t.

Random Coupling Model

$$\begin{aligned} J_{\mathbf{k}}(t, t') = {} & -i \sum_{\mathbf{p}} (V_0 \mp V_{\mathbf{k}-\mathbf{p}}) \bar{N}_{\mathbf{p}}(t) G_{\mathbf{k}}(t, t') \\ & + \sum_{\mathbf{ps}} V_{\mathbf{k}-\mathbf{s}} (V_{\mathbf{k}-\mathbf{s}} \mp V_{\mathbf{p}-\mathbf{s}}) \\ & \times \int [\mp G^{*}_{\mathbf{p}}(t, t_1) Q_{\mathbf{r}}(t, t_1) Q_{\mathbf{s}}(t, t_1) \\ & \pm Q_{\mathbf{p}}(t_1, t) G_{\mathbf{r}}(t, t_1) Q_{\mathbf{s}}(t, t_1) \\ & - Q_{\mathbf{p}}(t_1, t) Q^{+}_{\mathbf{r}}(t, t_1) G_{\mathbf{s}}(t, t_1)] G_{\mathbf{k}}(t_1, t')\, dt_1 \end{aligned} \tag{B4}$$

$$\begin{aligned} K_{\mathbf{k}}(t, t') = {} & -i \sum_{\mathbf{p}} (V_0 \mp V_{\mathbf{k}-\mathbf{p}}) \bar{N}_{\mathbf{p}}(t) Q_{\mathbf{k}}(t, t') \\ & + \sum_{\mathbf{ps}} V_{\mathbf{k}-\mathbf{s}} (V_{\mathbf{k}-\mathbf{s}} \mp V_{\mathbf{p}-\mathbf{s}}) \\ & \times \int [G^{*}_{\mathbf{k}}(t', t_1) Q^{+}_{\mathbf{p}}(t_1, t) Q_{\mathbf{r}}(t, t_1) Q_{\mathbf{s}}(t, t_1) \\ & \mp Q_{\mathbf{k}}(t_1, t') G^{*}_{\mathbf{p}}(t, t_1) Q_{\mathbf{r}}(t, t_1) Q_{\mathbf{s}}(t, t_1) \\ & \pm Q_{\mathbf{k}}(t_1, t') Q_{\mathbf{p}}(t_1, t) G_{\mathbf{r}}(t, t_1) Q_{\mathbf{s}}(t, t_1) \\ & - Q_{\mathbf{k}}(t_1, t') Q_{\mathbf{p}}(t_1, t) Q^{+}_{\mathbf{r}}(t, t_1) G_{\mathbf{s}}(t, t_1)]\, dt_1. \end{aligned} \tag{B5}$$

In these equations $\mathbf{r} = \mathbf{k} + \mathbf{p} - \mathbf{s}$.

Ring Model

$$\begin{aligned} J_{\mathbf{k}}(t, t') = {} & -i V_0 \bar{N} G_{\mathbf{k}}(t, t') \\ & \pm i \sum_{\mathbf{s}} \int V'_{\mathbf{k}-\mathbf{s}}(t, t_1) Q_{\mathbf{s}}(t, t_1) G_{\mathbf{k}}(t_1, t')\, dt_1 \\ & - \sum_{\mathbf{ps}} \iiint V'_{\mathbf{k}-\mathbf{s}}(t, t_3) V'_{\mathbf{s}-\mathbf{k}}(t_1, t_2) Q_{\mathbf{p}}(t_2, t_3) Q^{+}_{\mathbf{r}}(t_3, t_2) \\ & \times G_{\mathbf{s}}(t, t_1) G_{\mathbf{k}}(t_1, t')\, dt_1\, dt_2\, dt_3 \end{aligned} \tag{B6}$$

$$\begin{aligned} K_{\mathbf{k}}(t, t') = {} & -i V_0 \bar{N} Q_{\mathbf{k}}(t, t') \\ & \pm i \sum_{\mathbf{s}} \int V'_{\mathbf{k}-\mathbf{s}}(t, t_1) Q_{\mathbf{s}}(t, t_1) Q_{\mathbf{k}}(t_1, t')\, dt_1 \\ & + \sum_{\mathbf{ps}} \iiint V'_{\mathbf{k}-\mathbf{s}}(t, t_3) V'_{\mathbf{s}-\mathbf{k}}(t_1, t_2) \\ & \times [G^{*}_{\mathbf{k}}(t', t_1) Q^{+}_{\mathbf{p}}(t_2, t_3) Q_{\mathbf{r}}(t_3, t_2) \\ & \times Q_{\mathbf{s}}(t, t_1) - Q_{\mathbf{k}}(t_1, t') Q_{\mathbf{p}}(t_2, t_3) Q^{+}_{\mathbf{r}}(t_3, t_2) \\ & \times G_{\mathbf{s}}(t, t_1)]\, dt_1\, dt_2\, dt_3. \end{aligned} \tag{B7}$$

Here $\bar{N} = \sum_{\mathbf{p}} \bar{N}_{\mathbf{p}}(t)$ is the (constant) mean number of particles per system, and $\mathbf{r} = \mathbf{k} + \mathbf{p} - \mathbf{s}$. The vertex function $V'_{\mathbf{k}-\mathbf{s}}$ is determined by

$$\begin{aligned} & V'_{\mathbf{q}}(t, t') \\ & = V_{\mathbf{q}} \Big\{ \delta(t - t') + i \sum_{\mathbf{p}'} \int [G^{*}_{\mathbf{p}'}(t, t'') Q_{\mathbf{p}'+\mathbf{q}}(t, t'') \\ & \quad - Q_{\mathbf{p}'}(t'', t) G_{\mathbf{p}'+\mathbf{q}}(t, t'')] V'_{\mathbf{q}}(t'', t')\, dt'' \Big\}. \end{aligned} \tag{B8}$$

It satisfies

$$V'_{\mathbf{q}}(t, t') = V'^{*}_{-\mathbf{q}}(t, t'). \tag{B9}$$

If the initial momentum distribution has reflectional symmetry, $V'_{\mathbf{q}}(t, t')$ is real. The vertex function may be interpreted in terms of a higher-order Green's function, of a kind which is nonvanishing only for nonlinear systems. We have

$$\begin{aligned} & M^{-1} \sum_{\beta\mu\lambda}{}' \delta_{\alpha+\beta,\mu+\lambda} \Phi^{*}_{\alpha\beta\mu\lambda} \\ & \quad \times \langle \delta^3 \mathbf{q}_{\mathbf{k}\alpha}(t) / [\delta f^{\dagger}_{\mathbf{p}\beta}(t_1)\ \delta f_{\mathbf{r}\mu}(t_2)\ \delta f_{\mathbf{s}\lambda}(t_3)] \rangle \\ & = -i \iint G_{\mathbf{k}}(t, t') V'_{\mathbf{k}-\mathbf{s}}(t', t'_1) G^{*}_{\mathbf{p}}(t'_1, t_1) G_{\mathbf{r}}(t'_1, t_2) \\ & \quad \times G_{\mathbf{s}}(t', t_3)\, dt'\, dt'_1. \end{aligned} \tag{B10}$$

Here $\delta f_{\mathbf{k}\alpha}(t)$ is the infinitesimal perturbation operator introduced in Sec. 5, $\sum'_{\beta\mu\lambda}$ means that the values $\mu = \alpha$ and $\lambda = \alpha$ are omitted from the sum, and, again, $\mathbf{r} = \mathbf{k} + \mathbf{p} - \mathbf{s}$. Equation (B10) is valid only for the ring model and for $M \to \infty$.

Ladder Model

$$J_{\mathbf{k}}(t, t') = -i \sum_{\mathbf{p}} \int \bar{V}'_{\mathbf{kppk}}(t, t_1) Q_{\mathbf{p}}(t_1, t) G_{\mathbf{k}}(t_1, t')\, dt_1$$
$$\mp \sum_{\mathbf{ps}} \iiint V_{\mathbf{kprs}}(t, t_3) \bar{V}^*_{\mathbf{pksr}}(t_1, t_2) G^*_{\mathbf{p}}(t, t_1)$$
$$\times Q_{\mathbf{r}}(t_3, t_2) Q_{\mathbf{s}}(t_3, t_2) G_{\mathbf{k}}(t_1, t')\, dt_1\, dt_2\, dt_3 \tag{B11}$$

$$K_{\mathbf{k}}(t, t') = -i \sum_{\mathbf{p}} \int \bar{V}'_{\mathbf{kppk}}(t, t_1) Q_{\mathbf{p}}(t_1, t) Q_{\mathbf{k}}(t_1, t')\, dt_1$$
$$+ \sum_{\mathbf{ps}} \iiint V'_{\mathbf{kprs}}(t, t_3) \bar{V}^*_{\mathbf{kprs}}(t_1, t_2)$$
$$\times [G^*_{\mathbf{k}}(t', t_1) Q^+_{\mathbf{p}}(t_1, t) \mp Q_{\mathbf{k}}(t_1, t') G^*_{\mathbf{p}}(t, t_1)]$$
$$\times Q_{\mathbf{r}}(t_3, t_2) Q_{\mathbf{s}}(t_3, t_2)\, dt_1\, dt_2\, dt_3. \tag{B12}$$

Here $\mathbf{r} = \mathbf{k} + \mathbf{p} - \mathbf{s}$, and

$$\bar{V}'_{\mathbf{kprs}}(t, t') = V'_{\mathbf{kprs}}(t, t') \mp V'_{\mathbf{kpsr}}(t, t'). \tag{B13}$$

The vertex function $V'_{\mathbf{kprs}}$ is determined by

$$V'_{\mathbf{kprs}}(t, t') = V_{\mathbf{k-s}}\, \delta(t - t') - i \sum_{\mathbf{s}'} V_{\mathbf{k-s}'}$$
$$\times \int [\mp G_{\mathbf{r}'}(t, t'') Q_{\mathbf{s}'}(t, t'')\ V'_{\mathbf{r}'\mathbf{s}'\mathbf{sr}}(t'', t')$$
$$+ Q^+_{\mathbf{r}'}(t, t'') G_{\mathbf{s}'}(t, t'') V'_{\mathbf{s}'\mathbf{r}'\mathbf{rs}}(t'', t')]\, dt''. \tag{B14}$$

It satisfies

$$V'_{\mathbf{kprs}}(t, t') = V'_{\mathbf{pksr}}(t, t'), \tag{B15}$$

a fact which has been used in writing (B12). In analogy to the case of the ring model, $V'_{\mathbf{kprs}}$ may be interpreted in terms of a higher-order Green's function. We have

$$M^{-1} \sum'_{\beta\mu\lambda} \delta_{\alpha+\beta,\mu+\lambda} \phi^*_{\alpha\beta\mu\lambda}$$
$$\times \langle \delta^3 \mathbf{q}_{\mathbf{k}\alpha}(t) / [\delta f^\dagger_{\mathbf{p}\beta}(t_1)\ \delta f_{\mathbf{r}\mu}(t_2)\ \delta f_{\mathbf{s}\lambda}(t_3)] \rangle$$
$$= -i \iint G_{\mathbf{k}}(t, t') \bar{V}'_{\mathbf{kprs}}(t', t'_2) G^*_{\mathbf{p}}(t', t_1) G_{\mathbf{r}}(t'_2, t_2)$$
$$\times G_{\mathbf{s}}(t'_2, t_3)\, dt'\, dt'_2, \tag{B16}$$

where $\sum'_{\beta\mu\lambda}$ has the same meaning as in (B10). Equation (B16) is valid only for the ladder model and for $M \to \infty$.

If the vertex functions V' in (B6), (B7), (B11), and (B12) are expanded into infinite series by iteration solution of (B8) and (B14), there result explicitly all the contributions associated with the irreducible diagrams that survive in the ring and ladder models.

The nonequilibrium equations presented above for the several stochastic models should reduce to an equilibrium description in the limit $t_0 \to -\infty$, subject to the reservations expressed in Secs. 5.5 and 7.5. In this case, the equations may be simplified considerably by transformation to the frequency domain and the use of (5.51). The results possibly may prove a useful adjunct to the model equations for the temperature-domain propagators presented in I:Sec. 5. In some applications, the equilibrium quantity of direct interest is $\tilde{Q}_{\mathbf{k}}(\omega)$, defined by (5.50). In principle, $\tilde{Q}_{\mathbf{k}}(\omega)$ may be determined from the temperature-domain propagator $S_{\mathbf{k}}(\zeta_\alpha)$ by analytic continuation, but in practice this may prove very difficult. It is therefore of interest to have equations which directly determine $\tilde{Q}_{\mathbf{k}}(\omega)$.

In this connection, it should be noted that the formalism used for the temperature-domain propagators in I, and in Sec. 3 of the present paper, does not appear to be directly applicable to propagators in the real-time or frequency domain. The reason is that the individual states which make up the unperturbed (free-particle) grand canonical ensemble are not, in general, eigenstates of the adiabatic S matrix; the particles can scatter each other irreversibly while the interaction is switched on. Consequently, it is not clear that the perturbation series for the real-time propagators can be expressed in terms of time-ordered products in the simple way that is possible for the temperature-domain propagators.

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Asymptotic Expansion of the Bardeen-Cooper-Schrieffer Partition Function by Means of the Functional Method*

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The canonical operator $\exp[-\beta(\mathcal{H}-\mu N)]$ associated with the Bardeen-Cooper-Schrieffer (BCS) model Hamiltonian of superconductivity is represented as a functional integral by the use of Feynman's ordering parameter. General properties of the partition function in this representation are discussed. Taking the inverse volume of the system as an expansion parameter, it is possible to calculate the thermodynamic potential including terms independent of the volume. This yields a new proof that the BCS variational value is asymptotically exact. The behavior of the canonical operator for large volume is described and related to the state of free quasiparticles. A study of the terms of the thermodynamic potential which are of smaller order in the volume in the low-temperature limit, shows that the ground state energy is nondegenerate and belongs to a number eigenstate.

I. INTRODUCTION

SINCE Bardeen, Cooper, and Schrieffer[1] (BCS) presented their theory of superconductivity, there has been a rapidly growing interest in the structure of the BCS model Hamiltonian. One of the challenging questions arises from the fact that a lower bound of the partition function $Z=\mathrm{Tr}\exp[-\beta H_{\mathrm{BCS}}]$ is calculated by means of a variational procedure with a particle number nonconserving trial Hamiltonian H_0 (the free quasi-particles) leading to a thermodynamic behavior which, in general, agrees extraordinarily well with experiment. Several investigations of the exactness of the variational solution have been made. Considerations of this kind in the whole temperature range must include, of course, $T = 0$, i.e., the ground-state energy. In the Appendix of the BCS paper, one can find the remark that, for large particle number, the approximative ground state is also the exact one. Later Bogoliubov, Zubarev, and Tserkovnikov[2] claimed that the same is true for the partition function and thus the thermodynamic potential in the full temperature range. Their proof, based on a thermodynamic perturbation calculation, has been criticized by several authors, including Bogoliubov.[3] For temperatures below the transition point, according to this treatment, the partition function of free particles would also be an "exact" solution. A number of authors have treated the limiting case of strong coupling for both zero temperature[4-7] and finite temperature.[5]

Recently, Bogoliubov, Zubarev, and Tserkovnikov[8] (BZT) attacked the problem again by studying the system of differential equations for the thermodynamic Green's functions, associated with the Hamiltonian H_{BCS}. They included an auxiliary term which does not commute with the particle number in the Hamiltonian. Considering the problem in the zero limit of this term, BZT were able to prove that the Green's functions corresponding to free quasi-particles satisfy the full chain of equations in the limit of large volume, and that the trivial free particles solution must be rejected below the transition temperature.

The BZT treatment is an asymptotic expansion performed on an infinite system of differential equations. Usually, in statistical mechanics one transforms the partition function into an integral and applies well-known expansion methods. Studying an integral of the type

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$$I(\Omega) = \int_{-\infty}^{\infty} dx F(x) e^{-\Omega G(x)} \tag{1.1a}$$

asymptotically, is called Laplace's method.[9] For large parameter Ω, the leading term of the integral is

$$I(\Omega) = F(x_0)[2\pi/\Omega G''(x_0)]^{\frac{1}{2}} e^{-\Omega G(x_0)}, \tag{1.1b}$$

provided the G possesses an absolute and isolated minimum x_0.

The purpose of this paper is to bring the BCS partition function into a form suitable for applying an expansion procedure which is similar to the simple Laplace method in one dimension and where the volume of the system plays the role of the large parameter. The method we will use to transform the partition function is not new but will follow the same lines first treated in the work of Stratonowich[10] on distribution functions in a Bose system, and later considered from a more general point of view by Hubbard.[11] Similar ideas were used also by Edwards[12] in calculating the thermal behavior of the classical screened electron gas.

We confine our attention to the BCS Hamiltonian with separable attractive interaction $W_{\mathbf{k}\mathbf{k}'} = -v_{\mathbf{k}} v_{\mathbf{k}'}$,

$$H_{\mathrm{BCS}} = \mathcal{H}_{\mathrm{BCS}} - \mu N = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (n_{\mathbf{k}\uparrow} + n_{\mathbf{k}\downarrow}) - \frac{1}{\Omega} \sum_{\mathbf{k}\neq\mathbf{k}'} v_{\mathbf{k}} v_{\mathbf{k}'} b_{\mathbf{k}}^{+} b_{\mathbf{k}'}, \tag{1.2}$$

$\epsilon_{\mathbf{k}} = \epsilon_{-\mathbf{k}}$ is the single-particle energy relative to the chemical potential; $n_{\mathbf{k}\uparrow} = c_{\mathbf{k}\uparrow}^{+} c_{\mathbf{k}\uparrow}$, $b_{\mathbf{k}\uparrow}^{+} = c_{\mathbf{k}\uparrow}^{+} c_{-\mathbf{k}\downarrow}^{+}$ are the number and pair creation operators for the fermions in the momentum-spin states. The $v_{\mathbf{k}}$ entering in H_{BCS} are independent of the volume Ω. It is very convenient to express H_{BCS} in terms of the operators

$$\begin{aligned} s_1(\mathbf{k}) &= b_{\mathbf{k}}^{+} + b_{\mathbf{k}}, & s_2(\mathbf{k}) &= i(b_{\mathbf{k}}^{+} - b_{\mathbf{k}}) \\ s_3(\mathbf{k}) &= 1 - n_{\mathbf{k}\uparrow} - n_{-\mathbf{k}\downarrow}, & I(\mathbf{k}) &= b_{\mathbf{k}} b_{\mathbf{k}}^{+} + b_{\mathbf{k}}^{+} b_{\mathbf{k}}. \end{aligned} \tag{1.3}$$

For the same $\mathbf{k}$ these Hermitian operators behave like Pauli matrices, $I(\mathbf{k})$ being the unit. They commute for different momenta.[13] The Hamiltonian is

$$\begin{aligned} H_{\mathrm{BCS}} &= H + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} + (1/2\Omega) \sum_{\mathbf{k}} v_{\mathbf{k}}^2 I(\mathbf{k}) \\ H &= -\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} s_3(\mathbf{k}) - \frac{1}{4\Omega}\left[\sum_{\mathbf{k}} v_{\mathbf{k}} s_1(\mathbf{k})\right]^2 \\ &\quad - \frac{1}{4\Omega}\left[\sum_{\mathbf{k}} v_{\mathbf{k}} s_2(\mathbf{k})\right]^2. \end{aligned} \tag{1.4}$$

We consider only H. However, it is quite clear that, apart from $\Sigma\epsilon_{\mathbf{k}}$ the ground states of H_{BCS} and H for equal particle number can differ only by the volume independent term $(2\Omega)^{-1}\Sigma v_{\mathbf{k}}$.[14]

II. OPERATOR INTEGRAL

To illustrate the method we look at the operator $\exp[-\beta(A - \frac{1}{2}B^2/\Omega)]$. First of all, assume the Hermitian quantities A and B commute. Applying the formula

$$e^{\frac{1}{2}\lambda b^2} = \left(\frac{\lambda}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}\lambda x^2 + \lambda b x} \tag{2.1}$$

to the quadratic operator (for instance in the spectral representation of the exponential operator) we get

$$e^{-\beta(A - \frac{1}{2}B^2/\Omega)} = \left(\frac{\beta\Omega}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}\Omega\beta x^2} e^{-\beta(A - xB)}. \tag{2.2}$$

Introducing the integration variable x one achieves a linearization of the exponent; the integration is a Gaussian average.

If A and B do not commute, (2.2) is no longer correct. Nevertheless, it is possible to apply (2.1). One has to introduce Feyman's ordering parameter[15] and to replace

$$\beta\left(A - \frac{1}{2\Omega}B^2\right) \quad \text{by} \quad \sum_{i=1}^{n} \Delta\tau_i \left[A(\tau_i) - \frac{1}{2\Omega}B^2(\tau_i)\right].$$

Here we use a sufficiently fine, but fixed, interval division $0 < \tau_1 < \tau_2 < \cdots < \tau_n = \beta$ with $\sum_i^n \Delta\tau_i = \beta$. The operators $A(\tau)$, $B(\tau)$ can be treated like c numbers; the final elimination of the ordering parameter, the "disentangling" process, must proceed according to the rule $A(\tau_i)B(\tau_j) = B(\tau_j)A(\tau_i) = AB$ for $\tau_i > \tau_j$, $= BA$ for $\tau_i < \tau_j$, respectively. The analog to (2.2) is therefore

$$\begin{aligned} e^{-\beta(A - \frac{1}{2}B^2/\Omega)} &= \prod_i^n \left(\frac{\Delta\tau_i \Omega}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \prod_i^n dx_i \\ &\quad \times \exp\left(-\tfrac{1}{2}\Omega \sum_i^n \Delta\tau_i x_i^2\right) \\ &\quad \times \exp\left\{-\sum_i^n \Delta\tau_i [A(\tau_i) - x_i B(\tau_i)]\right\}. \end{aligned} \tag{2.3}$$

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[9] See A. Erdelyi, *Asymptotic Expansions* (Dover Publications, New York).

[10] R. L. Stratonovich, Soviet Phys.—Doklady **2**, 416 (1958).

[11] J. Hubbard, Phys. Rev. Letters **3**, 77 (1959).

[12] S. F. Edwards, Phil. Mag. **4**, 1171 (1959).

[13] The difference between the $s_i(\mathbf{k})$ and the common Pauli matrices is solely that they act in a four-dimensional space according to the four possibilities of occupying $\mathbf{k}\uparrow$ and $-\mathbf{k}\downarrow$. Here $e^{\alpha\mathbf{n}\cdot\mathbf{s}} = 1 - I + I\cosh\alpha + \mathbf{n}\cdot\mathbf{s}\sinh\alpha$ and $\mathrm{Tr}\, e^{\alpha\mathbf{n}\cdot\mathbf{s}} = 2(1 + \cosh\alpha)$, $\mathbf{n}$ being a unit vector.

[14] The same holds for the thermodynamic potential.

[15] R. P. Feynman, Phys. Rev. **84**, 108 (1951).

Strictly speaking, the equality sign in (2.3) holds only in the limit $n \to \infty$. The right-hand side is nothing but a functional integral with Gaussian measure, the product in front being the normalization factor.[16]

The model Hamiltonian of superconductivity (1.4) has almost the structure discussed above. We have only to introduce an additional set of variables y_i corresponding to the second square getting

$$e^{-\beta H} = \prod_i^n \left(\frac{\Delta\tau_i \Omega}{2\pi}\right) \int_{-\infty}^{\infty} \prod_i^n dx_i\, dy_i \times \exp\left[-\tfrac{1}{2}\Omega \sum_i^n \Delta\tau_i (x_i^2 + y_i^2)\right] \times \exp\left[-\sum_i^n \Delta\tau_i H(\tau_i; x_i y_i)\right], \tag{2.4a}$$

$$H(\tau_i; x_i y_i) = \sum_{\mathbf{k}} h_{\mathbf{k}}(\tau_i; x_i y_i) = -\sum_{\mathbf{k}} \left\{\frac{v_k}{\sqrt{2}} [x_i s_1(\mathbf{k}, \tau_i) + y_i s_2(\mathbf{k}, \tau_i)] + \epsilon_{\mathbf{k}} s_3(\mathbf{k}, \tau_i)\right\}. \tag{2.4b}$$

Eliminating the ordering parameter in the integral of (2.3) means writing the sequence of operators $\exp[-\Delta\tau(A - x_i B)]$ in the order of decreasing i. For a general point $x_1, x_2, \cdots x_n$ in n-dimensional space, the resulting operator is neither Hermitian nor positive as the left side of (2.3) obviously is. This is easily understood because the integral is invariant with respect to the following changes of the variables:

1. $x_i \to x_{n+1-i}$, this inverts the order and guarantees the Hermiticity.
2. $x_i \to -x_i$, this causes the positive definiteness of the integral.

There is in addition another feature of the BCS operator. Whereas $\exp[-\beta H]$ commutes with the number operator $N = \sum_{\mathbf{k}} [1 - s_3(\mathbf{k})]$, the integrand in (2.4) does not. However,

$$N \exp\left[-\sum_i^n \Delta\tau_i H(\tau_i; x_i, y_i)\right] = \exp\left[-\sum_i^n \Delta\tau_i H(\tau_i; -x_i, -y_i)\right] N. \tag{2.5}$$

Therefore the invariance under $x_i \to -x_i$, $y_i \to -y_i$, mentioned above, also yields the particle number conservation of the integral.

Considering a many-particle system with more general interaction, the introduction of a multidimensional integral associated with ordering parameters leads to a linearization of the problem. Because there are infinitely many integration points, the original many-particle problem is replaced by infinitely-many one-particle problems. Whether or not this is an advantage depends, of course, on the special features of the system. In the case of the BCS Hamiltonian the operator (2.4) has two properties which allow a great simplification. First, the exponential in the integrand can be factorized with respect to the momenta $\mathbf{k}$ since the s_l for different $\mathbf{k}$ commute

$$\exp\left[-\sum \Delta\tau_i H(\tau_i; x_i y_i)\right] = \prod_{\mathbf{k}} \exp\left[-\sum \Delta\tau_i h_{\mathbf{k}}(\tau_i; x_i y_i)\right]$$
$$\operatorname{Tr} \exp\left(-\sum \Delta\tau_i H_i\right) = \prod_{\mathbf{k}} \operatorname{Tr} \exp\left(-\sum \Delta\tau_i h_{\mathbf{k}i}\right). \tag{2.6}$$

Here the traces on the right-hand side are evaluated in the 4-dimensional Hilbert space associated with a single $\mathbf{k}$. Second, because the s_l act like Pauli matrices, each factor $\exp[-\sum_i^n \Delta\tau_i h_{\mathbf{k}}(\tau_i; x_i y_i)]$ can be considered as a sequence of infinitesimal imaginary rotations (infinitesimal Lorentz transformations).

III. GENERAL PROPERTIES OF THE PARTITION FUNCTION

Using (2.4) the partition function $Z = \operatorname{Tr} \exp[-\beta H]$ can be written as

$$Z = \prod_i^n \left(\frac{\Delta\tau_i \Omega}{2\pi}\right) \int_{-\infty}^{\infty} \prod_i^n dx_i\, dy_i \times \cos\psi(x_1 \cdots x_n y_1 \cdots y_n) e^{-\Omega G(x_1 \cdots x_n, y_1 \cdots y_n)}. \tag{3.1}$$

ψ is the argument of the complex number

$$\operatorname{Tr} \exp\left[-\sum_i \Delta\tau_i H(\tau_i; x_i y_i)\right]$$

and

$$G = \tfrac{1}{2} \sum_i^n \Delta\tau_i (x_i^2 + y_i^2) - \frac{1}{\Omega} \ln \left|\operatorname{Tr} \exp\left[-\sum_i^n \Delta\tau_i H(\tau_i; x_i y_i)\right]\right|. \tag{3.2}$$

The partition function has been brought into the form mentioned in the introduction by the use of (3.1) To make further statements, one must learn more about the structure of G. For this purpose we

[16] The following could be formulated, of course, in the language of functional analysis, where $x_i \to x(\tau)$ takes the place of the integration point. We will retain, however, the formulation with finite n, because it is more convenient for the asymptotic expansion performed later.

will first construct a lower bound of G for each point (x_i, y_i) in the $2n$-dimensional space. Here the special features of the BCS operator will come into play. It follows from (2.6) that

$$|\mathrm{Tr}\ \exp\,[-\sum_i \Delta\tau_i H(\tau_i; x_i y_i)]|$$
$$= \prod_{\mathbf{k}} |\mathrm{Tr}\ \exp\,[-\sum_i \Delta\tau_i h_{\mathbf{k}}(\tau_i; x_i y_i)]|. \quad (3.3)$$

Furthermore, we take advantage of the analogy to Lorentz rotations by using the following theorem:

Given a product of n imaginary rotations

$$\mathrm{P} = \prod_i^n \exp\,(\alpha_i \mathbf{e}_i \cdot \boldsymbol{\sigma}) = \pi + \mathbf{p}\cdot\boldsymbol{\sigma}, \quad (3.4)$$

where $\alpha_i > 0$ and $\mathbf{e}_i$ are real unit vectors. Then:

$$|\pi| = \tfrac{1}{2}\,|\mathrm{Tr\ P}| \leq \cosh\,(\alpha_1 + \alpha_2 + \cdots + \alpha_n). \quad (3.5)$$

The equality sign applies only if all $\mathbf{e}_i$ are equal (in which case, of course, π is real).

This theorem can easily be proven, e.g., by induction and the use of the fact that P can be split into a product of a single real and a single imaginary rotation.

Applying (3.5), one finds with (2.4b)

$$\left|\mathrm{Tr}\ \exp\left[-\sum_i^n \Delta\tau_i h_{\mathbf{k}}(\tau_i; x_i y_i)\right]\right|$$
$$\leq 2\left\{1 + \cosh\left[\sum_i^n \Delta\tau_i \left(\frac{v_k^2}{2}(x_i^2 + y_i^2) + \epsilon_{\mathbf{k}}^2\right)^{\frac{1}{2}}\right]\right\}. \quad (3.6)$$

Therefore,

$$G(x_1 \cdots x_n y_1 \cdots y_n) \geq G^0(x_1 \cdots x_n y_1 \cdots y_n) \quad (3.7a)$$

where

$$G^0 = \tfrac{1}{2}\sum_i^n \Delta\tau_i (x_i^2 + y_i^2) - \frac{1}{\Omega}\sum_{\mathbf{k}} \ln 2$$
$$\times\left\{1 + \cosh\left[\sum_i^n \Delta\tau_i \left(\frac{v_k^2}{2}(x_i^2 + y_i^2) + \epsilon_{\mathbf{k}}^2\right)^{\frac{1}{2}}\right]\right\}. \quad (3.7b)$$

Points with the same coordinate value

$$x_1 = x_2 = \cdots = x_n = x;$$
$$y_1 = y_2 = \cdots = y_n = y$$

(we call them xy points) correspond to equal unit vectors in (3.4). At these xy points the argument ψ of the trace vanishes and the equality sign applies in (3.7a):

$$G(xy) = G^0(xy) = \tfrac{1}{2}\beta(x^2 + y^2) - \frac{1}{\Omega}\sum_{\mathbf{k}} \ln 2$$
$$\times\left\{1 + \cosh\,\beta\left[\frac{v_k^2}{2}(x^2 + y^2) + \epsilon_{\mathbf{k}}^2\right]^{\frac{1}{2}}\right\}. \quad (3.8)$$

On the other hand, $G^0(x_1 \cdots x_n, y_1 \cdots y_n)$ is a completely symmetrical function of the variables $r_i^2 = x_i^2 + y_i^2$. Thus G^0 takes its extrema only at points with $r_i^2 = r^2$. The condition for the minimum is

$$\left.\frac{\partial G^0}{\partial r_i}\right|_r = \Delta\tau_i\left\{r - \frac{1}{2\Omega}\right.$$
$$\left.\times \sum_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{r}{E_{\mathbf{k}}}[1 - 2f(\beta E_k)]\right\} = 0. \quad (3.9)$$

Here,

$$E_{\mathbf{k}} = [(v_{\mathbf{k}}^2/2)r^2 + \epsilon_{\mathbf{k}}^2]^{\frac{1}{2}} \quad (3.10)$$

and $f(x)$ is the Fermi function. Equation (3.9) is nothing but the well-known gap equation. The nontrivial solution $r_0 \neq 0$ gives the gap parameter

$$\Delta_{\mathbf{k}} = (v_{\mathbf{k}}/\sqrt{2})r_0. \quad (3.11)$$

The absolute minimum $G^0_{\min} = G^0_{x_i^2+y_i^2=r_0^2}$ is the BCS thermodynamic potential per unit volume, divided by kT[17]:

$$G^0_{\min} = \beta F_{\mathrm{BCS}}. \quad (3.12)$$

The behavior of G^0 enables us to say that the function of interest, $G(x_1, \cdots x_n, y_1, \cdots y_n)$ also has the absolute minimum $G^0_{\min}$ and that it reaches this value at all xy points with $x^2 + y^2 = r_0^2$. No direction is specified in the one-dimensional manifold $x_i = r_0 \cos\varphi$, $y_i = r_0 \sin\varphi$ of minimal points. The reason for this is, of course, that the variables x_i, y_i are related to the operators $s_1(\mathbf{k})$ and $s_2(\mathbf{k})$ and the interaction Hamiltonian in (1.4) is symmetrical in these operators.

The fact that it is possible to determine both value and position of the absolute minimum of the complicated function G in an exact manner essentially contains the proof that F_{BCS} must give the leading contribution in a volume expansion of the thermodynamic potential. What remains and what will be done in the next section is a simple Taylor expansion at the minimal points.

IV. ASYMPTOTIC EXPANSION

The derivatives of G at xy points are

$$\frac{\partial G}{\partial x_i} = \Delta\tau_i\left\{x - \frac{1}{\sqrt{2}\,\Omega}\sum_{\mathbf{k}} v_{\mathbf{k}}\langle s_1(\mathbf{k})\rangle\right\}$$
$$\frac{\partial G}{\partial y_i} = \Delta\tau_i\left\{y - \frac{1}{\sqrt{2}\,\Omega}\sum_{\mathbf{k}} v_{\mathbf{k}}\langle s_2(\mathbf{k})\rangle\right\} \quad (4.1)$$

$$\frac{\partial^2 G}{\partial x_i\,\partial x_j} = \Delta\tau_i\left\{\delta_{ij} - \frac{\Delta\tau_j}{2\Omega}\right.$$
$$\left.\times \sum_{\mathbf{k}} v_{\mathbf{k}}^2[\langle s_1(\mathbf{k}\tau_i)s_1(\mathbf{k}\tau_j)\rangle - \langle s_1(\mathbf{k})\rangle^2]\right\} \quad (4.2a)$$

[17] Of course, one has to add the term $\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}$ of (1.4).

$$\frac{\partial^2 G}{\partial y_i\,\partial y_j} = \Delta\tau_i\Big\{\delta_{ij} - \frac{\Delta\tau_j}{2\Omega} \times \sum_{\mathbf{k}} v_{\mathbf{k}}^2[\langle s_2(\mathbf{k}\tau_i)s_2(\mathbf{k}\tau_j)\rangle - \langle s_2(\mathbf{k})\rangle^2]\Big\} \quad (4.2b)$$

$$\frac{\partial^2 G}{\partial x_i\,\partial y_j} = -\frac{1}{2}\frac{\Delta\tau_i\,\Delta\tau_j}{2\Omega}\sum_{\mathbf{k}} v_{\mathbf{k}}^2 \times [\langle s_1(\mathbf{k}\tau_i)s_2(\mathbf{k}\tau_j)\rangle - \langle s_1(\mathbf{k})\rangle\langle s_2(\mathbf{k})\rangle + \text{c.c.}] \quad (4.2c)$$

The averages are taken with respect to

$$\exp\,[-\beta h_k(xy)],$$

where

$$h_{\mathbf{k}}(xy) = -(v_{\mathbf{k}}/\sqrt{2})[xs_1(\mathbf{k}) + ys_2(\mathbf{k})] - \epsilon_{\mathbf{k}}s_3(\mathbf{k}),$$

Further,

$$s_l(\mathbf{k}\tau) = \exp\,[\tau h_{\mathbf{k}}(xy)]s_l(\mathbf{k})\exp\,[-\tau h_{\mathbf{k}}(xy)]. \quad (4.3)$$

In (4.2) the operator with the larger τ always stands to the left. To get the formulas (4.1) and (4.2) from (3.2) one has to use (2.6), the smallness of the $\Delta\tau$, the disentangling rule and the cyclicity of the trace. The expectation value of s_1 becomes

$$\langle s_1(\mathbf{k})\rangle = \frac{v_{\mathbf{k}}}{\sqrt{2}}\frac{x}{E_{\mathbf{k}}}\,[1 - 2f(\beta E_{\mathbf{k}})] \quad (4.4)$$

where $E_{\mathbf{k}}$ is given by Eq. (3.10). Replacing x by y given $\langle s_2\rangle$.

The "correlations," appearing in the second derivatives (4.2), can be easily calculated by means of the simple properties of the s operators. It is convenient to use polar coordinates. Then the derivatives at the minimal points $r_i = r_0$, $\varphi_i, = \varphi$ are given by

$$\partial^2 G/\partial r_i\,\partial r_j = \Delta\tau_i\,\mathrm{R}_{ij} = \Delta\tau_i\Big\{\delta_{ij} - \frac{\Delta\tau_j}{2\Omega}\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{2\cosh^2(\frac{1}{2}\beta E_{\mathbf{k}})} \times \left[\frac{\Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} + \frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}\cosh\,(\beta - 2\,|\tau_i - \tau_j|)E_{\mathbf{k}}\right]\Big\}, \quad (4.5)$$

$$\partial^2 G/\partial\varphi_i\,\partial\varphi_j = \Delta\tau_i r_0^2\Phi_{ij} = \Delta\tau_i r_0^2\Big\{\delta_{ij} - \frac{\Delta\tau_j}{2\Omega} \times \sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{2\cosh^2(\frac{1}{2}\beta E_{\mathbf{k}})}\cosh\,(\beta - 2\,|\tau_i - \tau_j|)E_{\mathbf{k}}\Big\}, \quad (4.6)$$

while the mixed second derivatives vanish. The Taylor expansion of G can be performed at an arbitrary minimal point $r_i = r_0$, $\varphi_i = \varphi$. Remembering that in (3.1) the argument ψ of the trace vanishes at minimal points, we get the following asymptotic expression for the partition function:

$$Z = AB\exp\,(-\beta\Omega F_{\mathrm{BCS}}), \quad (4.7)$$

where,

$$A = \prod_i^n\left(\frac{\Delta\tau_i\Omega}{2\pi}\right)^{\frac{1}{2}}\int_0^\infty\prod_i^n dr_i \times \exp\,[-\tfrac{1}{2}\Omega\sum_{ij}\Delta\tau_i\,\mathrm{R}_{ij}(r_i - r_0)(r_j - r_0)] \quad (4.8)$$

$$B = \prod_i^n\left(\frac{r_0^2\,\Delta\tau_i\Omega}{2\pi}\right)^{\frac{1}{2}}\int_{-\varphi}^{2\pi-\varphi}\prod_i d\varphi_i \times \exp\,[-\tfrac{1}{2}r_0^2\Omega\sum\Delta\tau_i\Phi_{ij}\varphi_i\varphi_j]. \quad (4.9)$$

To proceed, one has to determine the eigenvalues of the matrices R and Φ, defined by Eqs. (4.5) and (4.6). Both matrices have the structure

$$\delta_{ij} - \Delta\tau_j\,\mathrm{K}(|\tau_i - \tau_j|) \quad (4.10)$$

with

$$\mathrm{K}(\tau) = \mathrm{K}(\beta - \tau) > 0. \quad (4.11)$$

Since one is ultimately interested in the limit $n \to \infty$, the eigenvalues λ of (4.10) can be obtained from the integral equation

$$(1 - \lambda)g(\tau) = \int_0^\beta d\tau'\,\mathrm{K}(|\tau - \tau'|)g(\tau'). \quad (4.12)$$

Because of (4.11), it follows for the eigenvalues that

$$\lambda_P = 1 - \int_0^\beta d\tau\,\mathrm{K}(\tau)\cos\frac{2\pi P\tau}{\beta}\,; \qquad P = 0, 1, 2, \cdots. \quad (4.13)$$

The eigenfunctions of (4.12) are trigonometric functions:

$$g_0(\tau) = \beta^{-\frac{1}{2}}; \qquad g_P(\tau) = \begin{cases}\cos\,(2\pi P\tau/\beta)\\ \sin\,(2\pi P\tau/\beta)\end{cases}; \qquad P = 1, 2, \cdots. \quad (4.14)$$

We call $\lambda^{(R)}$ the eigenvalues of R, $\lambda^{(\phi)}$ those of ϕ. The τ integration in (4.13) gives for the (non-degenerate) lowest eigenvalue:

$$\lambda_0^{(\mathrm{R})} = 1 - \frac{1}{2\Omega}\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{E_{\mathbf{k}}} \times \left\{2\beta E_{\mathbf{k}}f_{\mathbf{k}}(1 - f_{\mathbf{k}})\frac{\Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} + (1 - 2f_{\mathbf{k}})\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}\right\}, \quad (4.15)$$

$$\lambda_0^{(\phi)} = 1 - \frac{1}{2\Omega}\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{E_{\mathbf{k}}}(1 - 2f_{\mathbf{k}}), \quad (4.16)$$

where $f_{\mathbf{k}} = f(\beta E_{\mathbf{k}})$. The twofold degenerate higher eigenvalues are ($P = 1, 2, 3, \cdots$):

$$\lambda_P^{(\mathrm{R})} = 1 - \frac{1}{2\Omega}\sum_{\mathbf{k}}\frac{v_{\mathbf{k}}^2}{E_{\mathbf{k}}}(1 - 2f_{\mathbf{k}})\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2 + (\pi P/\beta)^2}, \quad (4.17)$$

$$\lambda_P^{(\phi)} = 1 - \frac{1}{2\Omega}\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}^2}{E_{\mathbf{k}}}(1-2f_{\mathbf{k}})\frac{E_{\mathbf{k}}^2}{E_{\mathbf{k}}^2+(\pi P/\beta)^2}. \quad (4.18)$$

Let us first consider the eigenvalues of the matrix R. By means of $\epsilon_{\mathbf{k}}^2 = E_{\mathbf{k}}^2 - \Delta_{\mathbf{k}}^2$ it follows for the lowest one

$$\lambda_0^{(R)} = \lambda_0^{(\phi)} + \frac{1}{2\Omega}\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}^2\,\Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}^3} \times \{1 - 2f_{\mathbf{k}} - 2\beta E_{\mathbf{k}} f_{\mathbf{k}}(1-f_{\mathbf{k}})\}. \quad (4.19)$$

Taking the nontrivial solution $\Delta_{\mathbf{k}}$ of the gap equation, $\lambda_0^{(\phi)}$ vanishes. The sum on the right-hand side is positive since the factor $1-2f(x)-2xf(x)(1-f(x))$ remains always positive. Therefore, the matrix R is positive definite and the radial part in the asymptotic expansion (4.7) becomes

$$A = (\lambda_0^{(R)})^{-\frac{1}{2}} \prod_{P=1}^{\infty} (\lambda_P^{(R)})^{-1}. \quad (4.20)$$

On the other hand we see easily that (for temperatures below the transition point) the trivial solution of the gap equation ($r = 0$) does not correspond to a minimum of G since in that case $\lambda_0^{(R)} < 0$:

$$\lambda_{0\,\text{trivial}}^{(R)} = 1 - \frac{1}{2\Omega}\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}^2}{|\epsilon_{\mathbf{k}}|}\{1 - 2f(\beta\,|\epsilon_{\mathbf{k}}|)\}.$$

The right-hand side is zero at the transition point $\beta = \beta_c$ and decreases with increasing β.

As already mentioned, the lowest eigenvalue of the matrix ϕ is zero and thus the matrix is positive semidefinite, expressing the fact that no direction in the 1-2 plane is preferred in the problem. In spite of this, it is possible to do the asymptotic expansion of the angular part (4.9). Consider the substitution $\tilde{\varphi}_e = \sum_i U_{ei}\varphi_i$ which diagonalizes the exponent in (4.9), $\tilde{\varphi}_1$ belonging to the eigenvalue zero and therefore not appearing in the exponent. All integrations associated with positive eigenvalues can be performed in the same way as before. In the remaining $\tilde{\varphi}_1$ integration it is important that the region of integration is changed by the transformation from 2π to $\sum_i U_{1i}2\pi = 2\pi\sum_i (\Delta\tau_i/\beta)^{\frac{1}{2}} = 2\pi(\beta/\Delta\tau)^{\frac{1}{2}}$, assuming all elements $\Delta\tau_i$ having the same magnitude. Therefore B takes the form

$$B = (2\pi r_0^2\beta\Omega)^{\frac{1}{2}} \prod_{P=1}^{\infty} (\lambda_P^{(\Phi)})^{-1}. \quad (4.21)$$

Combining (4.7), (4.20), and (4.21) we obtain the following asymptotic expression for the thermodynamic potential below the transition temperature

$$-\frac{1}{\beta}\ln Z = \Omega F_{\text{BCS}} - \frac{1}{2\beta}\ln\left(\frac{2\pi r_0^2\beta\Omega}{\lambda_0^{(R)}}\right) + \frac{1}{\beta}\sum_{P=1}^{\infty}\ln(\lambda_P^{(R)}\lambda_P^{(\phi)}). \quad (4.22)$$

It is easy to get the corresponding expansion for $T > T_c$. In this temperature region the gap equation (3.9) has only the solution $r = 0$. Hence, the function G possesses an isolated minimum at the origin $x_i = y_i = 0$, the minimal value $G_{\min}$ being the thermodynamic potential F_0 of free Fermions divided by kT. Both matrices (4.2a) and (4.2b) are identical, all eigenvalues are positive and given by (4.15)–(4.18), if one puts $\Delta = 0$ in these formulas:

$$\lambda_P = 1 - \frac{1}{2\Omega}\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}^2}{|\epsilon_{\mathbf{k}}|}[1 - 2f(\beta\,|\epsilon_{\mathbf{k}}|)]\frac{\epsilon_{\mathbf{k}}^2}{\epsilon_{\mathbf{k}}^2+(\pi P/\beta)^2}. \quad (4.23)$$

The asymptotic expression above the transition temperature becomes

$$-\frac{1}{\beta}\ln Z = \Omega F_0 + \frac{1}{\beta}\ln\lambda_0 + \frac{2}{\beta}\sum_{P=1}^{\infty}\ln\lambda_P. \quad (4.24)$$

In an expansion of the thermodynamic potential only the leading term which is proportional to the volume is of physical interest. Therefore, the method we used proves that the BCS expression is exact below and above the transition temperature confirming Bogoliubov's result.

The next-order terms in the volume are important insofar as one needs them to decide whether the leading part is stable or not. The phase transition can be determined in approaching T_c either from below or above. In the first case the lowest eigenvalue R (4.15) goes to zero, whereas in the second case λ_0(4.23) changes its sign from positive to negative. It is interesting to note that in the normal phase, the volume independent term $\ln\lambda_0$ in (4.24) blows up for $T \to T_c$.[18] This does not occur in the superconducting phase (4.22), where $\lambda_0^{(R)}$ tends to zero as r_0^2.

As we have seen it is not necessary for an asymptotic expansion of the BCS partition function to introduce a particle nonconserving auxiliary term as did BZT in their Green's function treatment.[8] For the sake of completeness, however, we will include such a mathematical term into the Hamiltonian and sketch the results. They can be obtained with almost no new calculations. Consider the Hamiltonian

$$H - \nu\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{\sqrt{2}}[\cos\varphi_0 s_1(\mathbf{k}) + \sin\varphi_0 s_2(\mathbf{k})] \quad (4.25)$$

where H is given by (1.4) and ν is a small positive parameter. The whole problem now depends on a

[18] This may, perhaps, be related to critical fluctuations as treated by K. Gottfried and L. P. Kadanoff, Bull. Am. Phys. Soc. **6**, 65 (1961).

certain direction φ_0 in the 1-2 plane. All conclusions in Sec. III will remain valid. We merely replace x_i by $x_i + \nu \cos \varphi_0$ and y_i by $y_i + \nu \sin \varphi_0$ under the square root in (3.7b). A consequence of this is that G as a function of the r_i, φ_i now reaches its absolute minimum at a single point in the $2n$-dimensional space determined by $\varphi_i = \varphi_0$ and $r_i = r_0$ where r_0 is a solution of the equation

$$r - \frac{1}{2\Omega} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{r + \nu}{\bar{E}_{\mathbf{k}}} [1 - 2f(\beta \bar{E}_{\mathbf{k}})] = 0 \qquad (4.26)$$

and

$$\bar{E}_{\mathbf{k}} = (\bar{\Delta}_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}}^2)^{\frac{1}{2}}; \qquad \bar{\Delta}_{\mathbf{k}} = (v_{\mathbf{k}}/\sqrt{2})(r_0 + \nu). \qquad (4.27)$$

The eigenvalues which we now call $\bar{\lambda}_P^{(R)}$, $\bar{\lambda}_P^{(\phi)}$ are given by (4.15)–(4.18) if one replaces Δ by $\bar{\Delta}$ and E by $\bar{E}$ in these formulas. The important difference, compared with the previous symmetrical problem, is that the lowest eigenvalue of ϕ takes the form

$$\bar{\lambda}_0^{(\phi)} = \nu/(\nu + r_0) \qquad (4.28)$$

using Eq. (4.26). Therefore, both matrices R and ϕ are positive definite and the asymptotic expansion becomes

$$-\frac{1}{\beta} \ln Z = \Omega \bar{F} + \frac{1}{2\beta} \ln (\bar{\lambda}_0^{(R)} \bar{\lambda}_0^{(\phi)}) + \frac{1}{\beta} \sum_{P=1}^{\infty} \ln (\bar{\lambda}_P^{(R)} \bar{\lambda}_P^{(\phi)}), \qquad (4.29)$$

$\bar{F}$ being the minimal value of G multiplied with kT. Note that the thermodynamic potential does not depend on φ_0. If ν tends to zero as Ω^{-1} $\bar{F}$ will go over in F_{BCS}.

V. THE LIMIT $T \to 0$

The question arises whether an expansion of the partition function allows some conclusions about the behavior of the canonical operator itself. In particular, one may ask whether we can obtain the projector on the ground state wave function by taking the limit $\beta \to \infty$ for the canonical operator. If one includes the very small auxiliary term (4.25) in the Hamiltonian, the leading term (for $\Omega \to \infty$) in the expansion of the functional integral (2.4) for the operator $\exp [-\beta H_{\mathrm{BCS}}]$ will be

$$\exp [\beta \sum_{\mathbf{k}} \{\Delta_{\mathbf{k}} [\cos \varphi_0 s_1(\mathbf{k}) + \sin \varphi_0 s_2(\mathbf{k})] + \epsilon_{\mathbf{k}} s_3(\mathbf{k})\}]. \qquad (5.1)$$

Diagonalization of the exponent leads to the Hamiltonian of free quasi-particles. For $\beta \to \infty$ the normalized operator (5.1) projects out the wave function

$$|\varphi_0\rangle_{\mathrm{BCS}} = \prod_{\mathbf{k}} (u_{\mathbf{k}} + e^{i\varphi_0} v_{\mathbf{k}} b_{\mathbf{k}}^+) |0\rangle \qquad (5.2)$$

where $|0\rangle$ is the vacuum and $u_{\mathbf{k}} = (1 - v_{\mathbf{k}})^{\frac{1}{2}} = (1/\sqrt{2})(1 + \epsilon_{\mathbf{k}}/E_{\mathbf{k}})^{\frac{1}{2}}$.

Similar statements for the original density operator without the BZT auxiliary term cannot be made, simply because, taking $\Omega \to \infty$, there is a whole manifold of terms corresponding to different values of φ_0 which will give a contribution. This is due to the fact that the eigenstates of $\exp [-\beta H_{\mathrm{BCS}}]$ are almost degenerate. We shall see that the level spacing is of order Ω^{-1}.[19] On the other hand the asymptotic expansion performed in Sec. IV is exact only to order Ω^0. Naively taking the limit $\beta \to \infty$ must give a nonsensical result if kT becomes small as Ω^{-1}. Thus we see that without the Bogoliubov trick, the limits $\Omega \to \infty$, $\beta \to \infty$ are not interchangeable. The true eigenstates belong to a definite number as has been emphasized already by BCS. Following Anderson[20] they may be obtained from (5.2) by

$$|N\rangle = C_N \int_0^{2\pi} d\varphi e^{-\frac{1}{2}iN\varphi} |\varphi\rangle_{\mathrm{BCS}}.$$

The part $\ln \Omega^{\frac{1}{2}}$ appearing in the expansion (4.22) of the thermodynamic potential is closely related to the almost degeneracy of H_{BCS}. As we have seen, this term emerged from the fact that the lowest eigenvalue of the matrix ϕ was zero, indicating the symmetry of the problem in the 1-2 plane. To get a better physical understanding of the different terms in the expansion (4.22) for $\beta \to \infty$, we will give a more detailed discussion of the structure of the low-lying levels.

The particle number average and the fluctuation around it, calculated with the BCS state $|\varphi\rangle_{\mathrm{BCS}}$ (5.2) are given by

$$N_0 = \sum_{\mathbf{k}} 2v_{\mathbf{k}}^2 = \sum_{\mathbf{k}} (1 - \epsilon_{\mathbf{k}}/E_{\mathbf{k}}) \qquad (5.3)$$

$$\Delta N^2 = \sum_{\mathbf{k}} 4u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 = \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^2/E_{\mathbf{k}}^2. \qquad (5.4)$$

Expanding $|\varphi\rangle_{\mathrm{BCS}}$ in states of definite particle number:

$$|\varphi\rangle_{\mathrm{BCS}} = \sum_{n=0}^{\infty} e^{in\varphi} a_n |2n\rangle, \qquad (5.5)$$

[19] It should be emphasized that the almost degeneracy applies, of course, only to the operator $H_{\mathrm{BCS}} = \mathcal{H}_{\mathrm{BCS}} - \mu N$ and not to the Hamiltonian itself, the energy difference between the ground states of an $N + 2$- and an N-particle problem being 2μ.

[20] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

we get by (5.2)

$$a_n\,|2n\rangle = \frac{1}{n!}\,(\prod_{\mathbf{k}} u_{\mathbf{k}})\Big(\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\, b_{\mathbf{k}}^{+}\Big)^{n}\,|0\rangle. \tag{5.6}$$

The coefficients of the normalized $2n$ particle states follow

$$a_n^2 = \frac{1}{2\pi i}\oint \frac{dz}{z^{n+1}} \prod_{\mathbf{k}} (u_{\mathbf{k}}^2 + z\,v_{\mathbf{k}}^2). \tag{5.7}$$

A Darwin-Fowler calculation yields

$$a_n^2 = [\pi(\tfrac{1}{2}\,\Delta N)^2]^{-\frac{1}{2}} e^{-(n-\frac{1}{2}N_0)^2/(\frac{1}{2}\Delta N)^2}. \tag{5.8}$$

The very plausible result simply means that in the expansion of the BCS state, only states with the number $N_0 - \Delta N < N < N_0 + \Delta N$ will contribute significantly. One should expect that the expectation values of $\mathcal{H}_{\mathrm{BCS}} - \mu N$ taken with the number eigenstates N_0, $N_0 \pm 2$, $N_0 \pm 4$, $\cdots$ $N_0 \pm \Delta N$ will give a good approximation of the low lying eigenvalues of this operator.[21] Using the same technique as before they are found to be

$$\begin{aligned} \langle N\,|H_{\mathrm{BCS}}|\,N\rangle &= \Omega W_0 + \delta W_N \\ \delta W_N &= -\tfrac{1}{2}\alpha + \alpha(N - N_0)^2/\Delta N^2, \end{aligned} \tag{5.9}$$

where ΩW_0 is the BCS ground-state energy and

$$\alpha = \frac{1}{\Delta N^2}\sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}} \tag{5.10}$$

is an energy independent of Ω. The position of the levels, compared with the energy gap for different coupling strengths in the simplified BCS interaction, is plotted in Fig. 1.

For sufficiently large β the partition function is given by

$$\begin{aligned} Z &= e^{-\beta\Omega W_0} \sum_N e^{-\beta\delta W_N} \\ &= e^{-\beta(\Omega W_0 + \delta W_{N_0})} \sum_N e^{-\beta\alpha(N-N_0)^2/\Delta N^2}. \end{aligned} \tag{5.11}$$

Of course, the sum tends to one as $kT \to 0$. However, if kT remains above the level spacing which is proportional to Ω^{-1}, the sum can be transformed into an integral and the thermodynamic potential becomes

$$-\frac{1}{\beta}\ln Z = \Omega W_0 + \delta W_{N_0} - \frac{1}{2\beta}\ln\Big(\frac{\pi\,\Delta N^2}{4\beta\alpha}\Big). \tag{5.12}$$

The fluctuation square ΔN^2 is proportional to Ω. Hence, the same $\ln \Omega^{\frac{1}{2}}$ term as in the expansion (4.22) appears in formula (5.12). It is clear that this term is not an indication of a "zero-point entropy." It is connected with the almost degeneracy of the lowest eigenvalues of $\mathcal{H}_{\mathrm{BCS}} - \mu N$ and describes the behavior of the thermodynamic potential correctly only if kT remains above the level spacing of this operator.[19]

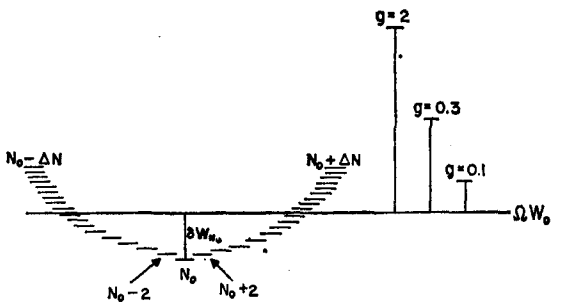

FIG. 1. Ground-state energy of the operator $_{\mathrm{BCS}} - \mu N$ for different particle number compared with the BCS value ΩW_0. On the right, the magnitude of the energy gap is plotted for different coupling strengths.

Let us compare Eqs. (4.22) and (5.12) in more detail for the special case of strong coupling. In this case a constant interaction

$$v_{\mathbf{k}} = \begin{cases} V_0^{\frac{1}{2}} & |\epsilon_{\mathbf{k}}| < \hbar\omega \\ 0 & |\epsilon_{\mathbf{k}}| > \hbar\omega \end{cases} \tag{5.13}$$

near the Fermi surface is so large that one can neglect the kinetic energies $\epsilon_{\mathbf{k}}$ relative to μ and put $E_{\mathbf{k}} = \Delta$. The gap parameter is then $\Delta = g\hbar\omega$ where $g = V_0 D_0$ is the coupling constant and D_0 the density of states per unit volume at the Fermi surface. Equation (5.12) becomes

$$-\frac{1}{\beta}\ln Z = \Omega W_0 - \tfrac{1}{2}\,\Delta - \frac{1}{2\beta}\ln\Big(\frac{\pi\Omega}{2\beta V_0}\Big). \tag{5.14}$$

The volume independent lowering of the BCS ground state energy is the same as in the strong coupling treatment of Baumann *et al.*[7]

On the other hand our original expansion (4.22) will also take a very simple form. All eigenvalues $\lambda_P^{(R)}$ become equal to one. Using (3.11) and (4.18) we get

$$\begin{aligned} -\frac{1}{\beta}\ln Z = \Omega F_{\mathrm{BCS}} &- \frac{1}{2\beta}\ln\Big(\frac{\pi\,\Delta^2\beta\Omega}{V_0}\Big) \\ &- \frac{1}{\beta}\ln\prod_{P=1}^{\infty}\Big[1 + \Big(\frac{\Delta\beta}{\pi P}\Big)^2\Big]. \end{aligned} \tag{5.15}$$

Remembering the product representation

$$\frac{\sinh x}{x} = \prod_{P=1}^{\infty}\Big[1 + \Big(\frac{x}{\pi P}\Big)^2\Big], \tag{5.16}$$

[21] At least as long $\langle N_0 + \Delta N|H_{\mathrm{BCS}}|N_0 + \Delta N\rangle - \langle N_0|H_{\mathrm{BCS}}|N_0\rangle$ does not exceed appreciably the energy gap.

one obtains for $\Delta\beta \gg 1$

$$-\frac{1}{\beta}\ln Z = \Omega F_{\mathrm{BCS}}(T=0) - \Delta - \frac{1}{2\beta}\ln\left(\frac{\pi\Omega}{4\beta V_0}\right). \quad (5.17)$$

Apart from a factor 2, the ln terms in both Eqs. (5.14) and (5.17) coincide. The ground-state energy in both equations is exactly the same if one notices two things. First, the BCS value $\Omega W_0 = \langle\varphi\,|H_{\mathrm{BCS}}|\,\varphi\rangle$ contains, in contrast to $\Omega F_{\mathrm{BCS}}(T=0)$, an Ω independent part which results from the summation restriction $\mathbf{k} \neq \mathbf{k}'$ in Eq. (1.2) and which is quite generally given by

$$\Omega W_0 = \Omega F_{\mathrm{BCS}}(T=0) + \frac{1}{4\Omega}\sum_{\mathbf{k}} V(\mathbf{k},\mathbf{k})\frac{\Delta_{\mathbf{k}}^4}{E_{\mathbf{k}}^4}. \quad (5.18)$$

In the strong-coupling case the second term on the right-hand side is $\frac{1}{2}\Delta$ and therefore cancels $-\frac{1}{2}\Delta$ in (5.14). Second, a similar cancellation will also take place in Eq. (5.17) if one takes into account the term $(2\Omega)^{-1}\sum_{\mathbf{k}} v_{\mathbf{k}}^2$ of Eq. (1.4) which equals Δ for strong coupling and which we have suppressed during the calculations.

Finally, an estimate of the series in Eq. (4.22) for $T = 0$ without restriction of the coupling strength shall be given. We use a relation for the eigenvalues which simply expresses Mercer's theorem for the integral equation (4.12) or the trace invariance of K in (4.10):

$$1 - \lambda_0^{(\mathrm{R})} + \sum_{P=1}^{\infty} 2(1-\lambda_P^{(\mathrm{R})}) = \frac{\beta}{2\Omega}\sum_{\mathbf{k}} v_{\mathbf{k}}^2 \times \left\{2f_{\mathbf{k}}(1-f_{\mathbf{k}})\frac{\Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} + (f_{\mathbf{k}}^2 + (1-f_{\mathbf{k}})^2)\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}\right\}, \quad (5.19)$$

$$1 + \sum_{P=1}^{\infty} 2(1-\lambda_P^{(\phi)}) = \frac{\beta}{2\Omega}\sum_{\mathbf{k}} v_{\mathbf{k}}^2\{f_{\mathbf{k}}^2 + (1-f_{\mathbf{k}})^2\}$$

Taking into account the fact that $\ln\lambda \leq \lambda - 1$, the limit $\beta \to \infty$ will lead to a volume independent lowering of the ground-state energy $\Omega F_{\mathrm{BCS}}(T=0)$ which is at least as large as

$$\delta W = -\frac{1}{2\Omega}\sum_{\mathbf{k}} v_{\mathbf{k}}^2\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}. \quad (5.20)$$

This energy tends to zero with increasing coupling strength in agreement with the treatment above.

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Antisymmetric Functions and Slater Determinants*

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Given a function w completely antisymmetric in n variables, there may exist a set of n functions of one variable such that the given function is a Slater determinant in the latter. The first problem considered is that of obtaining a criterion for this to be the case for a given function. This problem is solved by considering the function w as a mapping of the space of functions in $n-1$ variables onto the space of functions of one variable. A necessary and sufficient condition for the initial function to be a Slater determinant is then shown to be that the image space be n dimensional. This criterion is converted into practical algorithms which can be employed for the determination. The application of one of these yields the theorem that an arbitrary linear combination of the $n+1$ Slater determinants in n variables formed from $n+1$ one-variable functions can always be written as a single Slater determinant. It is further proved that if the image space of the mapping is $m(>n)$ dimensional, the original function can be expressed as a linear combination of $m!/(m-n)!n!$ Slater determinants in n variables formed from m one-variable functions. Playing an important role in the analysis is the product of the mapping described above by its adjoint (the product is simply related to Dirac's density matrix for a quantum mechanical system of identical particles) as well as the eigenvectors and eigenvalues of this Hermitian positive semidefinite mapping. The latter form a basis for a systematic approximation procedure for representing a given function by a single Slater determinant or by sums of Slater determinants formed from a particular number of one-variable functions, which yields results obtained previously by Löwdin. Problems of simultaneous approximation of sets of antisymmetric functions and possible physical applications to many-fermion systems are briefly discussed.

1. INTRODUCTION

THE results described in this paper originated from an attempt to answer the question, How can one determine when a given antisymmetric function is a Slater determinant? Its solution made apparent certain additional applications of the method employed to problems of approximation of antisymmetric functions by single Slater determinants or by linear combinations of them. As the manuscript of this paper was being completed, we were made aware[1] of the existence of some recent work of Löwdin[2] which contain results and ideas related to, and in some cases identical with, some of the content of this paper. Since the present paper begins with a somewhat different approach and contains some results which we have not found in the earlier literature, it was felt for reasons of economy that publication of the manuscript in what is essentially its original form would be justified. In spite of differences in terminology, notation, and normalization, there should be no difficulty for the reader in tracing the connections between the present work and that of Löwdin's. Löwdin's work stems, in part, from a large volume of work on the Hartree-Fock approximation, and some ideas of Slater[3] on extending this approximation, as well as some early work of Dirac[4] on the density matrix. Rather than attempt to document again this earlier work, we refer the reader to the extensive references in the work of Löwdin and Löwdin and Shull.[5]

To those familiar with this earlier work, it may be useful to designate those results of this paper which, to our present knowledge, do not exist in previous work. These are: the initial geometrical approach to the problem including the criterion for a function to be a Slater determinant in geometric form, two algorithms for ascertaining whether a function is a Slater determinant which may in practice be simpler than employing the criterion of Löwdin, the rather interesting Theorem III of Sec. 3 which establishes that an arbitrary linear combination of the $n+1$ Slater determinant for n particles formed from $n+1$ one-particle states can always be written as a single Slater determinant, and some considerations on the

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[1] We are grateful to Dr. M. K. Banerjee for bringing the work of Löwdin to our notice.

[2] P.-O. Löwdin, Phys. Rev. **97**, 1474, 1490, 1509 (1955).

[3] J. C. Slater, Quarterly Progress Report of Solid-State and Molecular Theory Group at Massachusetts Institute of Technology, 6, January 15, 1953 (unpublished); Technical Report No. 3, 39, February 15, 1953 (unpublished); Phys. Rev. **91**, 528 (1953). We have not seen personally the first two of these references which are taken from Löwdin's papers.

[4] P. A. M. Dirac, Proc. Cambridge Phil. Soc. **26**, 376 (1930); **27**, 240 (1931).

[5] P.-O. Löwdin and H. Shull, Phys. Rev. **101**, 1730 (1956); J. Chem. Phys. **30**, 617 (1959).

problem of simultaneously approximating a set of given antisymmetric functions in a limited number of configurations. The relationship between Löwdin's notation and terminology and our own is generally quite transparent, but we have added footnotes to explicitly spell out the connections where this was convenient.

The state of a quantum-mechanical system consisting of n identical particles obeying Fermi statistics is described by a state function $w(q_1, q_2, \cdots q_n)$ which is a completely antisymmetric function of the coordinates q_i, where q_i stands for the collection of coordinates describing the ith particle. All of the variables q_i have the same domain $D(q)$ and the scalar product of two state functions $w_1(q_1 \cdots q_n)$ and $w_2(q_1 \cdots q_n)$ involves an integration (and/or summation) over the domain $D(q)$ for all q variables of the product

$$w_1^*(q_1 \cdots q_n)w_2(q_1 \cdots q_n). \tag{1}$$

It will be convenient to employ an *Einstein convention* for such integrations according to which the repetition of a particular q in any term implies integration over $D(q)$ on this q variable. Thus (1) according to this convention would already indicate that all q variables are integrated over. On the other hand, an expression of the form

$$f(q_1q_2 \cdots q_k \cdots q_n)F(q_1q_2 \cdots q_kq'_{k+1} \cdots q'_m) \tag{2}$$

implies an integration over $q_1q_2 \cdots q_k$ thus yielding a function of the variables $q_{k+1} \cdots q_n$, $q'_{k+1} \cdots q'_m$. All functions of q variables with which we shall deal will be assumed to have the usual properties required of state functions; in particular, a function $f(q_1 \cdots q_n)$ will belong to a Hilbert space of square-integrable functions of n q variables.

A particularly simple antisymmetric function in the variables $q_1 \cdots q_n$ is a Slater determinant of the n functions $u_1(q), \cdots u_n(q)$, which is defined to be

$$S\{u_1 \cdots u_n\} \equiv \begin{vmatrix} u_1(q_1) & u_2(q_1) & \cdots & u_n(q_1) \\ u_1(q_2) & u_2(q_2) & \cdots & u_n(q_2) \\ u_1(q_n) & u_2(q_n) & \cdots & u_n(q_n) \end{vmatrix}. \tag{3}$$

A Slater determinant has the following properties:

(1) It vanishes if the u_i are not linearly independent or if the domain $D(q)$ consists of fewer than n points.

(2) If the functions $v_\alpha(q)$ are related to the functions $u_\beta(q)$ by a linear transformation

$$v_\alpha(q) = \sum_\beta a_{\alpha\beta}u_\beta(q), \tag{4}$$

then

$$S\{v_1 \cdots v_n\} = |a|\, S\{u_1 \cdots u_n\}, \tag{5}$$

where $|a|$ is the determinant of the $a_{\alpha\beta}$. Two Slater determinants will be said to be *equivalent* if one is a nonzero multiple of the other. Thus the two Slater determinants in (5) are equivalent provided $|a| \neq 0$.

(3) Any Slater determinant is equivalent to one in which the functions u_α are orthonormal through a Schmidt orthonormalization process. If the u_i are orthonormal, then the scalar product of the Slater determinant with itself has a value $n!$.

We shall say that an arbitrary nonzero antisymmetric function $w(q_1 \cdots q_n)$ is a Slater determinant if there exists a set of functions $u_1(q), \cdots u_n(q)$ such that w is equivalent to $S\{u_1 \cdots u_n\}$. The primary problem considered in this paper is that of establishing criteria by which it may be determined whether a given antisymmetric function $w(q_1 \cdots q_n)$ is a Slater determinant. Clearly, if it is, the set of functions $u_1, \cdots u_n$ will not be unique, but different solutions will be related by linear transformations.

An approach to the solution of this problem is suggested by the observation that if the Slater determinant (3) is multiplied by an arbitrary function of the variables $q_2 \cdots q_n$, and an integration performed over each of these variables, the result will be a function of the variable q_1 which is a linear combination of the n functions $u_1, \cdots u_n$. In geometrical terms we may thus consider the function $w(q_1 \cdots q_n)$ as giving rise to a mapping of the Hilbert space $[F]$ of functions $F(q_2 \cdots q_n)$ onto the Hilbert space $[f]$ of functions $f(q_1)$ through the correspondence:

$$F(q_2 \cdots q_n) \rightarrow f(q_1) = w(q_1q_2 \cdots q_n)F(q_2 \cdots q_n). \tag{6}$$

In general, this mapping is onto a subspace $[f_w]$ of the space $[f]$, which we may make definite by requiring that it possess no proper subspace onto which all of $[F]$ is mapped by w. Our statement above is then equivalent to the statement that if w is a Slater determinant, then the image space (the subspace $[f_w]$) is n dimensional. What we shall now prove is the converse of this theorem, namely that if w maps $[F]$ onto an *n-dimensional* subspace of $[f]$, then w is a Slater determinant. We will then have the result:

Theorem I. A necessary and sufficient condition that a function $w(q_1 \cdots q_n)$ be a Slater determinant is that the space $[f_w]$ onto which w maps $[F]$ be n dimensional.

It will then be demonstrated how this theorem can be converted into a practical means of determining

whether a function is a Slater determinant. As by-products of the proof we obtain additional results which appear to be quite interesting.

2. SOME RESULTS ON MAPPINGS

Let us call the mapping $[F]$ onto $[f]$ through the agency of the function w the mapping ω so that we write:

$$f(q_1) = \omega F(q_2 \cdots q_n) \tag{7a}$$

as well as $[f_w] = \omega[F]$. We may now define an adjoint mapping of the space $[f]$ onto the space $[F]$. We shall designate this adjoint mapping by ω^+ and define it by

$$\begin{aligned} f(q_1) \rightarrow \omega f(q_1) &= F(q_2 \cdots q_n) \\ &= w^*(q_1 q_2 \cdots q_n) f(q_1). \end{aligned} \tag{7b}$$

Again the mapping is in general onto a subspace $[F_w]$ of $[F]$ which we make specific by requiring that it possess no proper subspace onto which all of $[f]$ is mapped, and we write $[F_w] = \omega^+[f]$. We shall now prove that $[F_w] = \omega^+[f_w]$, $[f_w] = \omega^+[F_w]$, and that these two mappings are each one to one.

To this end we consider the mapping $\Omega \equiv \omega\omega^+$ of the function space $[f]$ onto itself:

$$\begin{aligned} f(q_1) \rightarrow f'(q_1) &= \Omega f(q_1) \\ &= w(q_1 q_2 \cdots q_n) w^*(q_1' q_2 \cdots q_n) f(q_1'). \end{aligned} \tag{8}$$

This is clearly a bounded Hermitian mapping of $[f]$ onto itself and is in addition positive semidefinite. In particular, Ω maps the subspace $[f_w]$ onto itself. Since the mapping is Hermitian it has a complete set of eigenfunctions in the space $[f]$ belonging to non-negative eigenvalues, and these eigenfunctions can always be so chosen as to be orthogonal and normalized. Let a complete set of orthonormal eigenfunctions be denoted $u_1(q)$, $u_2(q)$, $\cdots$ $u_\nu(q)$, $u_{\nu+1}(q)$, $\cdots$ where the order is such that the eigenvalues λ_α^2 associated with these eigenfunctions are in descending order:

$$\lambda_1^2 \geq \lambda_2^2 \geq \cdots \geq \lambda_\nu^2 \geq \cdots, \tag{9}$$

and where λ_ν^2 represent the last *nonzero* eigenvalue in the sequence (we do not exclude the possibility that ν may be infinite). These eigenfunctions and eigenvalues are of course the solutions of the "integral" equation

$$\lambda_\alpha^2 u_\alpha(q) = W(q, q') u_\alpha(q'), \tag{10a}$$

where[6]

$$W(q, q') = w(q, q_2 \cdots q_n) w^*(q' q_2 \cdots q_n). \tag{10b}$$

Under the mapping ω^+ each of these functions is mapped into a function belonging to $[F]$. We define

$$V_\alpha(q_2 \cdots q_n) = w^*(q_1 q_2 \cdots q_n) u_\alpha(q_1). \tag{11}$$

If we form the scalar product of two V_α, we obtain

$$\begin{aligned} &V_\alpha^*(q_2 \cdots q_n) V_\beta(q_2 \cdots q_n) \\ &\quad = u_\alpha^*(q) w(q q_2 \cdots q_n) w^*(q' q_2 \cdots q_n) u_\beta(q') \\ &\quad = \lambda_\beta^2 u_\alpha^*(q) u_\beta(q) = \lambda_\beta^2 \delta_{\alpha\beta}, \end{aligned} \tag{12}$$

where we have used the orthonormality of the u_α. Thus $V_\alpha(q_2 \cdots q_n) = 0$ for $\alpha > \nu$. The $u_\alpha(q_1)$ with $\alpha \leq \nu$ clearly form a basis in $[f_w]$ and the functions $V_\alpha(q_2 \cdots q_n)$ with $\alpha \leq \nu$ clearly form a basis in $[F_w]$. The mapping function $w(q_1 \cdots q_n)$ can then be written as

$$w(q_1 \cdots q_n) = \sum_{\alpha=1} u_\alpha(q_1) V_\alpha^*(q_2 \cdots q_n). \tag{13}$$

To see this we need merely note that (13) performs the same mapping as does w. If the two functions were different, their difference would then map every function of $[F]$ into the zero function in $[f]$. But then the difference could be nonzero only on a set of points of measure zero in the domain of all the variables, and in quantum mechanics as well as in the theory of Hilbert spaces such functions are considered null functions. Thus w has the form given by (13). We note from (12) that the $V_\alpha(q_2 \cdots q_n)$ are not in general normalized; if we define the normalized functions

$$v_\alpha(q_2 \cdots q_n) = (1/\lambda_\alpha) V_\alpha^*(q_2 \cdots q_n), \tag{14}$$

then

$$w(q_1 \cdots q_n) = \sum_{\alpha=1}^{\nu} \lambda_\alpha u_\alpha(q_1) v_\alpha(q_2 \cdots q_n). \tag{15}$$

Of course, the ν functions V_α^* and v_α for $\alpha \leq \nu$ are linearly independent and in fact orthogonal.

An important result following from (15) is that if w is normalized and we form its scalar product with itself and use (12) we obtain

$$\sum_{\alpha=1}^{\nu} \lambda_\alpha^2 = 1. \tag{16}$$

[6] The kernel $W(q, q')$ is identical with the density matrix of Löwdin except for normalization. The eigenvectors of the kernel are called "natural spin orbitals" in the papers of Löwdin[2] and Löwdin and Shull.[5] Löwdin's criterion for w to be a Slater determinant can be written in our notation as $W(q, q'')\, W(q'', q') = nW(q, q')$, $W(q, q) = n$.

We have so far not made use of the antisymmetric properties of $w(q_1 \cdots q_n)$. By the use of these we can obtain the desired converse theorem or actually a generalization of it. We shall establish first the following theorem:

Theorem II. If a completely antisymmetric function $w(q_1 \cdots q_n)$ can be written in the form

$$w(q_1 \cdots q_n) = \sum_{\alpha=1}^{\nu} u_\alpha(q_1) V_\alpha(q_2 \cdots q_n), \qquad (17)$$

where the u_α and the V_α are each sets of linearly independent functions, then

(a) w is not identically zero;
(b) $\nu \geq n$;
(c) if $\nu = n$, then w is a multiple of the Slater determinant $S\{u_1 \cdots u_n\}$;
(d) if $\nu > n$, then w is a linearly combination of the $\nu!/n!(\nu - n)!$ Slater determinant formed by selecting in all possible ways n distinct functions u_α from the ν such functions occurring in (16) but cannot be written as a single Slater determinant.

We lose no generality by assuming that the u_α are orthonormal, since the Schmidt orthonormalization process assures us of the existence of a nonsingular transformation

$$u_\alpha = \sum_{\beta=1}^{\nu} c_{\alpha\beta} u'_\beta$$

such that the u'_β are orthonormal. Under this transformation, (16) becomes

$$w(q_1 \cdots q_n) = \sum_{\beta=1}^{\nu} u'_\beta(q_1) V'_\beta(q_2 \cdots q_n), \qquad (18)$$

with

$$V'_\beta = \sum_\alpha c_{\beta\alpha} V_\alpha \qquad (19)$$

and the V'_β are linearly independent. We shall now proceed under the assumption that the u_α are orthonormal. Then

$$V_\alpha(q_2 \cdots q_n) = u^*_\alpha(q_1) w(q_1 \cdots q_n). \qquad (20)$$

To establish conclusion (a) we now note that if w were identically zero, then by (20) all the V_α would vanish contrary to the hypothesis of their linear independence.

We now use the antisymmetry of w and permute q_1 and q_2 in (16) obtaining

$$\sum_{\alpha=1}^{\nu} u_\alpha(q_1) V_\alpha(q_2 \cdots q_n) = -\sum_{\alpha=1}^{\nu} u_\alpha(q_2) V_\alpha(q_1 q_3 \cdots q_n), \qquad (21)$$

whereupon forming the scalar product of both sides with $u_\beta(q_1)$ we obtain

$$V_\beta(q_2 \cdots q_n) = -\sum_{\alpha=1}^{\nu} u_\alpha(q_2) u^*_\beta(q'_2) V_\alpha(q'_2 q_3 \cdots q_n). \qquad (22)$$

This may be rewritten as

$$V_\alpha(q_2 \cdots q_n) = \sum_{\beta=1}^{\nu} u_\beta(q_2) V_{\alpha\beta}(q_3 \cdots q_n), \qquad (23)$$

where

$$\begin{aligned} V_{\alpha\beta}(q_3 \cdots q_n) &= -u^*_\beta(q'_2) V_\alpha(q'_2 q_3 \cdots q_n) \\ &= -u^*_\beta(q'_2) u^*_\alpha(q'_1) w(q'_1 q'_2 q_3 \cdots q_n) \\ &= u^*_\alpha(q'_1) u^*_\beta(q'_2) w(q'_1 q'_2 q_3 \cdots q_n). \end{aligned} \qquad (24)$$

In obtaining (24) we have used (20) and also interchanged the integration variables q'_1 and q'_2 using the antisymmetry of w. We then have from (23) and (17)

$$w(q_1 \cdots q_n) = \sum_{\alpha=1}^{\nu} \sum_{\beta=1}^{\nu} u_\alpha(q_1) u_\beta(q_2) V_{\alpha\beta}(q_3 \cdots q_n). \qquad (25)$$

We now continue this procedure [at the next step interchanging q_2 and q_3 in (25), etc.] until we obtain finally

$$w(q_1 \cdots q_n) = \sum_{\alpha=1}^{\nu} \sum_{\beta=1}^{\nu} \cdots \sum_{\kappa=1}^{\nu} u_\alpha(q_1) \times u_\beta(q_2) \cdots u_\kappa(q_n) V_{\alpha\beta\cdots\kappa}, \qquad (26)$$

with

$$V_{\alpha\beta\cdots\kappa} = u^*_\alpha(q'_1) u^*_\beta(q'_2) \cdots \times u^*_\kappa(q'_n) w(q'_1 q'_2 \cdots q'_n). \qquad (27)$$

Now $V_{\alpha\beta\cdots\kappa}$ is clearly antisymmetric in all its subscripts and is therefore proportional to the Levi-Civita symbol $\epsilon_{\alpha\beta\cdots\kappa}$; this fact allows us to rewrite (26) as

$$w(q_1 \cdots q_n) = \sum_{\alpha=1}^{\nu} \sum_{\beta=1}^{\nu} \cdots \sum_{\kappa=1}^{\nu} V_{\alpha\beta\cdots\kappa} \times S\{u_\alpha u_\beta \cdots u_\kappa\}, \quad (\alpha < \beta < \cdots < \kappa). \tag{28}$$

For $\nu < n$, (28) clearly vanishes establishing conclusion (b) of our theorem while for $\nu = n$ we clearly have conclusion (c). The first statement of conclusion (d) also follows from (28). The last statement of conclusion (d) follows from the fact that if (17) is considered as a mapping function of $[f]$ onto $[F]$, the functions u_α are mapped into V_α and since these latter are linearly independent, the space onto which w maps must be ν dimensional. On the other hand, if w were a Slater determinant, the space must be n dimensional; since $\nu > n$, w cannot be a Slater determinant.

Combined with our previous results, this theorem then establishes that a necessary and sufficient condition for a function $w(q_1 \cdots q_n)$ to be a Slater determinant is that in the above sense, it generates a mapping onto an n-dimensional subspace of $[f]$. We shall now give several applications of the results obtained above starting with practical algorithms for determining whether a given function can be written as a Slater determinant.

3. IDENTIFICATION OF A SLATER DETERMINANT

To apply Theorem I to determine whether a given function $w(q_1 \cdots q_n)$ is a Slater determinant, we select n linearly independent functions $F(q_2 \cdots q_n)$ from the function space $[F]$ and map them through w into n functions $f(q_1)$ of the function space $[f]$ and then form the Slater determinant of the latter. If this determinant vanishes identically, we know that we have been unfortunate in our selection of our initial n functions and we repeat the process by a new choice of n functions F until we obtain a nonvanishing Slater determinant. The existence of such a choice is guaranteed us by conclusion (a) of Theorem II. In general, by a "random" selection of the initial n functions, there is only a negligible probability that the projection of all of these onto the subspace $[F_w]$ of $[F]$ is onto a proper subspace of $[F_w]$, which is the condition for the vanishing of the determinant so that this will be a rare and purely accidental contingency. In any case, having constructed such a nonvanishing Slater determinant, it is either equivalent or inequivalent to the original function w. In the former case, w is of course a Slater determinant, in the latter case, it cannot be.

Since a direct test of the identity of the function w and the Slater determinant may be rather laborous, an alternative procedure can often be useful. Namely, we select at "random" $n + 1$ functions F from $[F]$, map them into $n + 1$ functions f in $[f]$, and then form the Slater determinant of these $n + 1$ functions. If this determinant is nonvanishing, that is, if the $n + 1$ image functions are linearly independent, then clearly by our theorems, w cannot be a Slater determinant. On the other hand, if the determinant vanishes, but one of its minors is nonvanishing, then w is a Slater determinant. If all of its minors vanish, we have been unlucky in our choice of initial functions and must repeat the procedure, but again this will be a rare contingency.

As an illustration of this method, we shall prove a simple but interesting theorem which was discovered by these procedures. Suppose that we are given $n + 1$ linearly independent one particle functions $u_\alpha(q)$. From these we can form $n + 1$ linearly independent Slater determinants in n-particles by choosing in all possible ways n functions from the set. We now prove:

Theorem III. An arbitrary linear combination of the $n + 1$ Slater determinants in n particles formed from $n + 1$ linearly independent single-particle functions is a Slater determinant.

The proof employs the second of the procedures outlined above. We write

$$w(q_1 \cdots q_n) = a_1 S\{u_2 \cdots u_{n+1}\} + a_2 S\{u_3 \cdots u_{n+1} u_1\} + \cdots + a_{n+1} S\{u_1 \cdots u_n\} \tag{29}$$

and choose our $n + 1$ test functions F to be

$$F_i(q_2 \cdots q_n) = u_{i+2}(q_2) u_{i+3}(q_3) \cdots u_{i+n}(q_n), \tag{30}$$

where i runs from 1 to $n + 1$, and the subscripts on the u's are to be interpreted *modulo* $n + 1$. One can then readily calculate the $n + 1$ image functions f_i to be

$$f_i(q_1) = a_i u_{i+1}(q_1) - a_{i+1} u_i(q_1). \tag{31}$$

That these $n + 1$ functions are not linearly independent can be seen from the fact that if each f_i is multiplied by the product of all the a's with the exception of a_i and a_{i+1}, then the sum of the resultant terms vanishes identically. On the other hand, any n of the f_i are linearly independent and their

Slater determinant is equivalent to w thus establishing the theorem.[7]

While the theorem just established obviously may have some useful applications in shell model calculations, we have not explored the possibilities thereby suggested.

Combining Theorem III with Theorem II tells us that the image space $[f_w]$ can never be of dimensionality $n + 1$. Construction of simple examples shows that a dimensionality $n + 2$ is not excluded. Whether there exist other excluded dimensionalities than $n + 1$, we do not know, but it appears unlikely.

4. RELATION TO A PROBLEM IN CLUSTER-MODEL THEORY

Suppose that one had the exact wave function (or a good approximation to it) for the ground state of a system of n identical fermions and that this function is $w(q_1 \cdots q_n)$. The problem of obtaining the ground state wave function for the system with $n + 1$ fermions is often approached in the following approximation: One assumes a variation wave function of the form

$$\psi(q_1 \cdots q_{n+1}) = Aw(q_1 \cdots q_n)y(q_{n+1}), \qquad (32)$$

where A is an operator which completely antisymmetrizes the function which follows in the $n + 1$ q-variables. Entering with this trial function in the variational theorem one then derives an integro-differential equation for the one particle function y. Now there may exist a number of functions y such that the right-hand side of Eq. (32) is identically zero; in such a case one can readily show that a linear combination of such functions always satisfies the integro-differential equation for any value of the energy eigenvalue.[8] For example, if w itself is a Slater determinant in the functions $u_1, \cdots u_n$, then any linear combination of these u's is a function of the type described. These functions represent states which are forbidden by the exclusion principle. While these "spurious" solutions can never really cause trouble since they do not contribute to the state function ψ, it may sometimes be convenient to know whether such solutions exist and to find them. We shall now show how our work is related to finding the solutions of the equation

$$Aw(q_1 \cdots q_n)y(q_{n+1}) = 0. \qquad (33)$$

To this end we multiply the above equation by $w^*(q_1 \cdots q_n)$ and integrate over the variables $q_1 \cdots 1_n$. To determine the result we note first that the above equation can be rewritten as

$$\begin{aligned} w(q_1 \cdots q_n)y(q_{n+1}) = {} & w(q_{n+1}q_2 \cdots q_n)y(q_1) \\ & + w(q_1q_{n+1}q_3 \cdots q_n)y(q_2) \\ & + \cdots + w(q_1 \cdots q_{n-1}q_{n+1})y(q_n). \end{aligned} \qquad (34)$$

Then, if we assume w is normalized to

$$w(q_1 \cdots q_n)w^*(q_1 \cdots q_n) = 1, \qquad (35)$$

we see that the result of the indicated operation is that we obtain

$$y(q_{n+1}) = nw(q_{n+1}q_2 \cdots q_n)w^*(q_1q_2 \cdots q_n)y(q_1), \qquad (36)$$

or, in the notation introduced earlier,

$$(1/n)y(q) = W(q, q')y(q'), \qquad (37)$$

with $W(q, q')$ defined by Eq. (10). Hence, any solution of (33) is an eigenvector of the mapping Ω belonging to the eigenvalue $1/n$. The converse is not generally true, however. Thus if the manifold of solutions of Eq. (37) can be obtained, among them will be found all the solutions of Eq. (33). In the particular case where w is itself a Slater determinant, one sees immediately that any linear combination of the functions $u_1, \cdots u_n$ is an eigenfunction of W belonging to the eigenvalue $1/n$.

5. BEST APPROXIMATIONS BY A SLATER DETERMINANT

In actual applications of the cluster model, it is not uncommon to mutilate the integro-differential

[7] An alternate proof of this theorem based on a second-quantized representation of the many-particle system has been communicated to the author by F. Coester. [In this connection the following papers are of interest: F. Coester, Nuclear Phys. 7, 421 (1958); 17, 477 (1960).] The theorem can also be proved by elementary methods based on the addition formula for two determinants.

An interesting combinatorial problem arises in an attempt at an extension of Theorem III, to which we have not found a solution. Suppose that one considers an arbitrary linear combination of the $m!/n!(n - m)!$ Slater determinants in n particles formed from m independent single-particle functions and asks what is the smallest number of Slater determinants in which the linear combination can be re-expressed. The following combinatorial problem then arises: Consider all combinations of n objects drawn from a set of m objects. Divide these combinations into classes in which each class is characterized by the fact that all combinations in the class have $n - 1$ objects in common. Such a decomposition into classes is not unique, but we have found in some simple examples that carrying out the division into classes in all possible ways suggests the theorem that the number of classes obtained is always the same and that the numbers of combinations occurring in the various classes for different divisions is also always the same. We have so far not proved that this theorem is generally true, but if it is true and we identify Slater determinants with the combinations, then all Slater determinants belonging to one class can be simply added to yield a single Slater determinant. We further do not know the number of such classes for given m, n, nor whether the resultant Slater determinants associated with different classes may still be further combined to give a smaller total number of Slater determinants.

[8] In this connection, see, P. Swan, Proc. Roy. Soc. (London) **228**, 10 (1955).

equation obtained strictly from the variation principle. In fact one sometimes neglects the integral (nonlocal) terms in the equation or replaces them by (in some sense) equivalent local-interaction terms.[9] In this case the resultant equation may possess spurious solutions which on a reasonable interpretation should be excluded, but there is now no unambiguous way of identifying which of the solutions are the spurious ones and which are the valid ones. The difficulty arises from the fact that unless w is a Slater determinant, there do not exist n one-particle states which are forbidden to the $(n + 1)$th particle. A possible approximate solution to this difficulty is suggested below.

The difficulties attendant when w is not a Slater determinant could be avoided if w were replaced by its "best" Slater determinant approximation, and we may ask whether there is a procedure for securing this. One such procedure would consist in asking for that Slater determinant of n one-particle functions on which w has the largest projection in Hilbert space. It is easy to show that the solution to this problem may be obtained in the following way. One constructs the mapping function $W(q, q')$ from w by the use of Eq. (10) and then determines the n eigenvectors of this function corresponding to the n largest eigenvalues λ^2 as described in Sec. 2. The Slater determinant of these n eigenfunctions will then be the best approximation according to the above criterion. One can then use this Slater determinant in place of the function w in the variational problem. The states forbidden to the $(n + 1)$st particle are then these n eigenfunctions. Since the sum of the squares of all the eigenvalues is unity, the amount by which the sum of the squares of the n largest of these falls short of unity is a measure of the goodness of the approximation. If, after the substitution of the Slater determinant for the function w, a mutilation of the integro-differential equation is performed, or if one persists in employing the mutilated form of the original integro-differential equation, one can solve the resultant equation variationally under the additional condition that the solutions be orthogonal to the one-particle states of the Slater determinant. Alternatively, any solutions of the mutilated integro-differential equation which have large projections on these one-particle states may be rejected. How satisfactory a resolution of the difficulties these suggestions provide is not clear however.

[9] An example of this type of procedure is contained in some recent work of Wackman and Austern on Li^6 (to be published): P. H. Wackman, Ph.D. thesis, University of Pittsburgh (1960).

6. BEST APPROXIMATION BY LIMITED CONFIGURATIONS

The idea involved in the preceding section of finding the "best" Slater determinant approximation to a given antisymmetric function has a natural extension which we here consider. A Slater determinant describes a state of an n-particle system in which there is one particle in each of n one-particle states or "orbitals."[10] Such an assignment of n orbitals for a system of n particles we shall call a "configuration."[11] If there is given a complete set of one-particle states, then the totality of configurations constitutes a complete set of functions for the entire system, and hence an arbitrary state of the system can be described by a linear combination of configurations. It may sometimes be convenient, however, to approximate a function by writing it as a linear combination of configurations formed from a limited number of orbitals, say m where $m > n$. The total number of such configurations is of course $m!/n!(m - n)!$. One can now ask the question: Given the number m, what is the best choice of the one-particle states from which the configurations are to be constructed? Before attacking this problem, we introduce some ideas which are convenient for the discussion.

Let us define a "primitive" of a given completely antisymmetric function as any function which when antisymmetrized yields the given function. Every antisymmetric function has of course many primitives, but we shall now define a specific manner in which a primitive of a given antisymmetric function can be constructed. Let $u_\alpha(q)$ be a complete *ordered* set of orthonormal one-particle functions. The totality of products of n such functions with arguments $q_1 \cdots q_n$, respectively, then form a complete set of functions in which any function $w(q_1 \cdots q_n)$ can be expanded:

$$w(q_1 \cdots q_n) = \sum_{\alpha\beta\cdots\kappa} c_{\alpha\beta\ldots\kappa} u_\alpha(q_1) u_\beta(q_2) \cdots u_\kappa(q_n), \qquad (38)$$

where the sum is taken over all values of $\alpha, \beta, \cdots \kappa$. If w is a completely antisymmetric function, then

[10] These correspond to Löwdin's "spin orbitals."

[11] Note that there is a slight difference from the ordinary usage of the term "configuration." In ordinary usage (with a central field) the magnetic quantum numbers (projection of angular momentum on z axis) of the occupied one-particle states are not specified when a configuration is given, while in the present usage all quantum numbers defining a one-particle state must be specified. It would perhaps be useful to borrow a term from classical statistical mechanics and to call a configuration in our sense a "constellation" since it is the direct quantum analog of the classical meaning of this term. Löwdin also uses the term "configuration" in the new sense.

the coefficients c are completely antisymmetric in their n indices. If one now limits the sum on the right side of (38) so that the sum is taken only over all values of $\alpha, \beta, \cdots \kappa$ such that $\alpha < \beta < \cdots < \kappa$, then the resultant function will be a primitive of w. A primitive of this type can be constructed by the use of any complete ordered set of orthonormal one-particle states. If w is a Slater determinant and the states from which this determinant is constructed are included in the complete set of one-particle states, the primitive obtained will consist of only one term. If these states are the first n states of the ordered set, then the coefficient of this one term will be $c_{123\cdots n} = 1/n!$ and all other c's will then be zero. In the more general case, where w is not a Slater determinant, it would be convenient to select the ordering of the functions u_α such that the absolute magnitudes of the c's form a non-increasing sequence when the c's are arranged in dictionary order with respect to their subscripts; that is, $c_{\alpha\beta\cdots\kappa}$ stands before $c_{\alpha'\beta'\cdots\kappa'}$ if $\alpha < \alpha'$, or if $\alpha = \alpha'$, provided $\beta < \beta'$, $\cdots$ etc. An approximation to the primitive can then be obtained by dropping those terms in the sum which involve one-particle states later in the sequence that the mth. Antisymmetrizing (and renormalizing) the resultant function gives us the best approximation to the original antisymmetric function in terms of the configurations generated from these m orbitals. If we now ask how to choose the m one-particle states such that after truncation we have the best approximation to the original function, the answer is clear. We choose these to be the m eigenfunctions of the kernel $W(q, q')$, formed from w in accordance with Eq. (10), which correspond to the m largest eigenvalues λ^2. Indeed, since the sum of the λ^2 is unity, we again obtain a fairly precise idea as to how good the approximation will be by seeing how far the sum of the m largest λ^2 falls short of unity. Alternatively, one could discover how many orbitals would be required to give a satisfactory approximation to a given antisymmetric function by seeing how far in the sequence of eigenvalues one must go in order that the sum of their squares be sufficiently close to unity.

A generalization of the above problem would consist in attempting to simultaneously approximate two or more antisymmetric functions by configurations derived from a common set of one-particle orbitals. Since in general the kernels derived from each such function will not commute,[12] the kernels will have different eigenvectors. We do not propose a general procedure for the solution of this problem but content ourselves with pointing out that the methods indicated above can still be helpful. For example, suppose that the functions which are to be approximated are $w_1, w_2, \cdots w_k$ and they are to be approximated by configurations derived from m orbitals. Corresponding to each of the functions $w_1, w_2 \cdots w_k$, one can construct the positive semidefinite kernels $W_1, W_2, \cdots W_k$ using (10). The fact that these are positive semidefinite suggests forming the new kernel $W = W_1 + W_2 + \cdots + W_k$, determining the m eigenvectors of W associated with its m largest eigenvalues, and then employing these as the orbitals for the approximation. The expressions for $w_1, w_2, \cdots$ can be explicitly obtained in terms of these orbitals then by replacing each kernel W_i by PW_iP where P is the projection operator on the subspace spanned by the m orbitals. Depending on other considerations which may enter the problem, it may sometimes be more advantageous to employ a weighted sum of the W_i (with positive weight factors) for W in place of the simple sum.

An alternative approximation procedure, useful when no definite bound on the number of orbitals m is envisaged, but only an adequate representation of each of the original functions w is desired, is to find a sequence of eigenvectors for the kernel of each function separately which by the $\sum \lambda^2$ criterion yields an adequate approximation and then to form the union of the subspaces spanned by each of these sets of eigenvectors. Finally one introduces an orthonormal basis in the union of these subspaces. Variations of these procedures can be constructed to take care of special situations.

Our discussion in the present section and the preceding one has been rather abstract in that we have not indicated in practical situations how the initial antisymmetric function or functions w are obtained. We therefore conclude this section by describing an example of the type of situation in which the procedures suggested above may have application.[13] Suppose that one is engaged in a shell-model calculation without configurational mixing (in the usual sense) in which the number of orbitals in the unclosed shell is greater than the number of particles in this shell. One might then calculate the wave function for the lowest state in this approximation by conventional methods yielding a state function w. It is possible that by using the methods

[12] We mean here, of course, that $W_1(q, q'')\, W_2(q'', q') \neq W_2(q, q'')\, W_1(q'', q')$.

[13] For further discussion see also references 2 and 5.

outlined above one finds that w can be represented reasonably accurately by a single Slater determinant in a new set of one-particle states determined by the use of the eigenvectors of the kernel W associated with the function w. One might then usefully introduce the set of eigenfunctions of W as a new set of one-particle basis states in proceeding to find the eigenfunctions of the higher states, and hopefully, in this new representation, the off-diagonal matrix elements of the interaction might be sufficiently smaller than those in the original representation that perturbation methods could be employed where they could not be employed before.

The problems involved in determining the eigenfunctions of the kernel W may be very formidable ones indeed. There is one aspect of this problem which may be favorable, however. One would be interested in determining the eigenfunctions belonging to the largest eigenvalues primarily. For these, certain well-known iterations methods are particularly well adapted and hence may substantially reduce the actual labor involved. Beyond this, little can be said concerning the practical feasibility of employing the methods of this paper without testing them in specific calculations.

7. GENERALIZATIONS OF THE MAPPING PROBLEM

For the purpose of determining if a given antisymmetric function is a Slater determinant, it was convenient to regard the function $w(q_1 \cdots q_n)$ as a mapping of the space of functions of $n-1$ q variables onto the space of functions of a single q variable. There is an obvious generalization of this procedure, namely, regarding w as a mapping of a space of functions of $n-k$ q variables onto a space of k q-variables through the identification:

$$F(q_{k+1} \cdots q_n) \to f(q_1 \cdots q_k) = w(q_1 \cdots q_k q_{k+1} \cdots q_n) F(q_{k+1} \cdots q_n). \quad (39)$$

The procedures we have employed in dealing with the simpler case can be employed here, many with little change.[14] However, we have not pursued this aspect of the problem except in an exploratory way. It is clear that if w is a Slater determinant then the subspace $[f_w]$ of $[f]$ onto which $[F]$ is mapped in this case will have a dimensionality $n!/k!(n-k)!$, and it is likely that this is the minimum dimensionality for any function w, but we have not given a rigorous proof of this nor do we know whether the fact that the image space has this dimensionality is sufficient to establish that w is a Slater determinant. Analyses of these other mapping situations would probably be most valuable when many-body systems with strong correlations are subjected to serious study.

[14] Obviously the adjoint mapping can be defined in an analogous manner to the earlier case, and the kernel $W(q_1 \cdots q_k; q_1' \cdots q_k') = w(q_1 \cdots q_k q_{k+1}'' \cdots q_n'') w^*(q_1' \cdots q_k' q_{k+1}'' \cdots q_n'')$ constructed which gives rise to a Hermitian positive semi-definite mapping of $[f]$ on itself. The kernal W is identical, apart from a normalization and transposition, with the density matrix of order k of Löwdin.

Excitation Spectrum of a Fermion System*

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By the method of "modes" introduced by Sawada, the excitation spectra of a fermion system with singular interactions have been obtained in three cases; (1) with one additional particle above and and one hole below the Fermi surface, (2) with one additional particle above the Fermi surface, and (3) with two particles above the Fermi surface. The argument holds not only for the system of low density (nuclear matter with a hard-core repulsion), but also for the case of the interacting electron gas in the high-density region. The results have been compared with the Brueckner-Goldstone perturbation-expansion formulas, by using diagrams in the second- and third-order of the expansion in interaction strength. We show that in the approximation of our treatment, the occupation probability function at temperature T has the same form as the Fermi distribution function.

INTRODUCTION

CONSIDERING that the operators a^*b^* and ba (which represent a simple excitation "mode" for a many-fermion system) play essential roles in the calculation of ring (or cluster) diagrams in high-density electron gas, Sawada investigated[1] the equation of motion of these operators and succeeded in obtaining knowledge about the ground-state energy without a perturbation expansion in the coupling constant λ. Recently this idea of mode was developed further and the so-called scattering eigenmodes α^* and β were introduced to show that the singular two-body interaction can be consistently replaced by the reaction matrix in the equations of motion and in the expressions for the energies of states.[2] However, the details of the pair-scattering mode (particle-hole correlation) were not given. The pair-scattering mode is essentially important to the present problem, in which shall be evaluated an excitation energy spectrum of a system of fermions (nuclear matter) with one particle above and one hole below the Fermi surface. We shall investigate this mode using Sawada's procedure and obtain knowledge about the approximate excitation spectrum without a perturbation expansion. We shall also evaluate the energies of one particle and two particles when they are put above the Fermi surface. These energies will correspond to the differences of the binding energy of states of nuclei of $N + 1$ and $N + 2$ particles from the ground state of the nucleus of N particles, respectively.

When the two-body interaction is of a Coulomb type, we can also apply our results, since the pair-scattering mode is taken into account. We also discuss the continuity at the Fermi surface in the occupation probability function in our approximation. Finally in Appendix we give a extended prescription of our procedure appling to a finite system (real nuclei such as Ca^{41} and Ca^{42}).

PAIR-SCATTERING MODE

For the details of the procedure for constructing and evaluating modes, we refer the reader to the papers of Sawada.[1,2] For our purpose the following outline will be sufficient. Consider the total Hamiltonian written in the notation of second quantization

$$H = \sum_i \epsilon_i C_i^* C_i + \sum_{i,j,l,m} C_i^* C_j^* \tfrac{1}{2} V_{i,j;l,m} C_m C_l, \qquad (1)$$

where $\epsilon_i = k_i^2/2m$ is the kinetic energy and C_i^* represents a creation operator of a particle in a large volume with momentum, spin, etc., described by k_i. C_i^* is separated into a creation operator of a particle and a destruction operator of a hole by the following definition[3];

$$\begin{aligned} C_i^* &= a_i^*, \qquad \omega_i > \mu, \\ C_i^* &= b_i, \qquad \omega_i < \mu, \end{aligned} \qquad (2)$$

where ω_i is the "true" one-particle energy which is defined to be compatible self-consistently with the equation of the eigenvalue problem, [Eq. (22) of (S.)] and $\mu = dE_N/dN$. (E_N = the ground state energy of the N-particle system and N = total number of particles.)

By this definition the Hamiltonian (1) can be split into the following parts:

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[1] K. Sawada, Phys. Rev. **106**, 372 (1957).
[2] K. Sawada, Phys. Rev. **119**, 2090 (1960). We shall refer to this paper as (S.) from now on.
[3] We use the letters $p, q, p', \cdots$ in the case $\omega_p, \omega_q, \cdots > \mu$ and the letters $r, s, r', \cdots$ in the case $\omega_r, \omega_s, \cdots < \mu$.

$$H = H_0 + H_I,$$
$$H_0 = \sum_p \omega_p a_p^* a_p - \sum_r \omega_r b_r^* b_r + \sum_r \epsilon_r,$$
$$H_I = \sum_{i,j,l,m} (a_i^* + b_i)(a_j^* + b_j) \times \tfrac{1}{2} V_{i,j,l,m}(a_m + b_m^*)(a_l + b_l^*) + \sum_p (\epsilon_p - \omega_p) a_p^* a_p - \sum_r (\epsilon_r - \omega_r) b_r^* b_r. \tag{3}$$

The scattering mode operators α_n^*, β_{-n} are defined by

$$\left.\begin{matrix}\alpha_n^* \\ \beta_{-n}\end{matrix}\right\} = \sum_{p,q} \psi_{p,q}^{*n} a_p^* a_q^* + \sum_{r,s} \chi_{r,s}^{*n} b_r b_s + 2 \sum_{p,r} \xi_{p,r}^{*n} a_p^* b_r. \tag{4}$$

In (4), the wave functions ψ, χ, and ξ are determined by the eigenvalue equation which is obtained from the following equation of motion:

$$\left[\begin{pmatrix}\alpha_n^* \\ \beta_{-n}\end{pmatrix}, H\right]_- = -\begin{pmatrix}\omega_n(S)\alpha_n^* \\ \omega_{-n}(S)\beta_{-n}\end{pmatrix} + Y_{*n}. \tag{5}$$

In (5) Y_{*n} contains the interaction term between this mode and other modes only [Eq. (19) of (S.)]. In the approximation which neglects the interaction term Y_{*n}, the eigenvalue equation for determining eigenvalues and eigenfunctions is

$$\begin{aligned}&[\omega_{*n}(S) - \{\omega_p(S) + \omega_q(S)\}]\psi_{p,q}^{*n} = \sum_{p',q'} v_{p,q;p',q'}\psi_{p',q'}^{*n} - \sum_{r',s'} v_{p,q;r',s'}\chi_{r',s'}^{*n} \\ &[\omega_{*n}(S) - \{\omega_r(S) + \omega_s(S)\}]\chi_{r,s}^{*n} = \sum_{p',q'} v_{r,s;p',q'}\psi_{p',q'}^{*n} - \sum_{r',s'} v_{r,s;r',s'}\chi_{r',s'}^{*n},\end{aligned} \tag{6}$$

with

$$\omega_i(S) = \epsilon_i + 2 \times \left\{\sum_r v_{i,r;i,r} - \sum_{r,n} \frac{\bar{R}_{i,r}^n \bar{R}_{i,r}^n}{\omega_n(S) - \{\omega_i(S) + \omega_r(S)\}} - \sum_{p,-n} \frac{\bar{R}_{i,p}^{-n}\bar{R}_{i,p}^{-n}}{\omega_{-n}(S) - \{\omega_i(S) + \omega_p(S)\}}\right\},$$
$$\bar{R}_{i,j}^{*n} = \sum_{p,q} v_{i,j;p,q}\psi_{p,q}^{*n} - \sum_{r,s} v_{i,j;r,s}\chi_{r,s}^{*n},$$
$$v_{i,j;l,m} = \tfrac{1}{4}(V_{i,j;l,m} - V_{i,j;m,l} - V_{j,i;l,m} + V_{j,i;m,l}),$$

and ξ is determined by ψ and χ.

We can show that the quantity $\omega_i(S)$, defined by (6), is the single-particle energy in this approximation, from the following consideration. Using the operators α^* and β in (3) and shifting them to the left and right, respectively, we can rewrite the Hamiltonian in the following form;

$$\begin{aligned}H = \sum_p \Big\{&\epsilon_p + 2\sum_s v_{p,s;p,s} - 2\sum_{q,-n} \frac{\bar{R}_{p,q}^{-n}\bar{R}_{p,q}^{-n}}{\omega_{-n}(S) - \{\omega_p(S) + \omega_q(S)\}} \\ &- 2\sum_{s,n} \frac{\bar{R}_{p,s}^{n}\bar{R}_{p,s}^{n}}{\omega_n(S) - \{\omega_p(S) + \omega_s(S)\}}\Big\} a_p^* a_p \\ + \sum_r \Big\{&\epsilon_r + 2\sum_s v_{r,s;r,s} - 2\sum_{q,-n} \frac{\bar{R}_{r,q}^{-n}\bar{R}_{r,q}^{-n}}{\omega_{-n}(S) - \{\omega_r(S) + \omega_q(S)\}} \\ &- 2\sum_{s,n} \frac{\bar{R}_{r,s}^{n}\bar{R}_{r,s}^{n}}{\omega_n(S) - \{\omega_r(S) + \omega_s(S)\}}\Big\} b_r b_r^* \\ &+ C + H_1 + H_2,\end{aligned} \tag{7}$$

where

$$C = -\sum_{r,s} v_{r,s;r,s} + \sum_{p,q,-n} \frac{\bar{R}_{p,q}^{-n}\bar{R}_{p,q}^{-n}}{\omega_{-n}(S) - \{\omega_p(S) + \omega_q(S)\}} + \sum_{r,s,n} \frac{\bar{R}_{r,s}^{n}\bar{R}_{r,s}^{n}}{\omega_n(S) - \{\omega_r(S) + \omega_s(S)\}} + 2\sum_{p,r,-n} \frac{\bar{R}_{p,r}^{-n}\bar{R}_{p,r}^{-n}}{\omega_{-n}(S) - \{\omega_p(S) + \omega_r(S)\}},$$
$$H_1 = \tfrac{1}{2}\sum_{r,s,n} \bar{R}_{s,r}^{n}\alpha_n^* b_r^* b_s^* - \tfrac{1}{2}\sum_{r,s,-n} \bar{R}_{s,r}^{-n} b_r^* b_s^* \beta_{-n} + \sum_{r,s,p'',r''} \bar{R}_{s,r}^{p'',r''} b_r^* b_s^* a_{p''}^* b_{r''},$$

and

$$H_2 = \tfrac{1}{2}\sum_{p,q,n} \bar{R}_{q,p}^{n}\alpha_n^* a_p a_q - \tfrac{1}{2}\sum_{p,q,-n} \bar{R}_{q,p}^{-n} a_p a_q \beta_{-n} + \sum_{p,q,p'',r''} \bar{R}_{q,p}^{p'',r''} a_{p''}^* b_{r''} a_p a_q - \sum_{p,s,n} \bar{R}_{s,p}^{n}\alpha_n^* b_s^* a_p + \sum_{p,s,-n} \bar{R}_{s,p}^{-n} b_s^* a_p \beta_{-n} - 2\sum_{s,p,p'',r''} \bar{R}_{s,p}^{p'',r''} b_s^* a_{p''}^* b_{r''} a_p.$$

The definition of $\bar{R}$ is given by (18) of (S.). When we take the modified Hamiltonian $H^{(\mathrm{mod})}$ defined below, we have the equation of motion for the one-particle mode,

$$[a_p^*, H^{(\mathrm{mod})}]_- = -\omega_p(S) a_p^*,$$

with

$$H^{(\mathrm{mod})} = \sum_p \omega_p(S) a_p^* a_p + \sum_r \omega_r(S) b_r b_r^* + C + H_1 \tag{8}$$

(noting the definition of $\omega_i(S)$, and the relation $[a_p^*, H_1] = 0$). From (8) we get ($|N\rangle$ is the ground state),

$$H^{(\mathrm{mod})} a_p^* \mid N\rangle = \{\omega_p(S) + E_N\} a_p^* \mid N\rangle. \tag{8'}$$

Equation (8′) shows that $\omega_i(S)$ is the single-particle energy in this approximation. But since $H^{(\mathrm{mod})}$ cannot be solved easily, we must content ourselves with omitting H_1 in $H^{(\mathrm{mod})}$. Thus we can write the modified Hamiltonian in the following compact form, using the definition of the C_i operator

$$H^{(\mathrm{mod})} = \sum_i \omega_i(S) C_i^* C_i + C. \tag{9}$$

In this approximation the ground-state energy could be written in terms of $\omega_i(S)$ or the reaction matrix $\bar{R}$ [(24) of (S.)].

Now we consider the excitation state which contains one additional particle above and one additional hole below the Fermi surface. To investigate the state, the following pair scattering modes γ_m^* and δ_{-m} must be constructed;

$$\left.\begin{matrix}\gamma_m^* \\ \delta_{-m}\end{matrix}\right\} = \sum_{p,r} \Phi_{p,r}^{*m} a_p^* b_r^* + \sum_{p,q} \mathrm{X}_{p,q}^{*m} a_p^* a_q + \sum_{r,s} \Xi_{r,s}^{*m} b_s^* b_r + \sum_{r,p} \Theta_{r,p}^{*m} b_r a_p. \tag{10}$$

The reason is as follows. If we can find the operator γ_m^* which satisfies

$$[\gamma_m^*, H]_- = -\omega_m \gamma_m^*, \qquad \omega_m > 0, \tag{11}$$

we get,

$$H\gamma_m^* \mid N\rangle = (\omega_m + E_N)\gamma_m^* \mid N\rangle,$$

where particle number of the state is still conserved. Then $\gamma_m^* \mid N\rangle$ represents an excited state of the N-particle system and from its definition it corresponds to the state with one particle above and one hole below the Fermi surface, and ω_m is the excitation energy of the state.

For construction and evaluation of the pair scattering mode (10), we use the same technique, as we did in the case of the scattering mode. Using (3) we have,

$$\begin{aligned}
&[\sum_{p,r} \Phi_{p,r}^{*m} a_p^* b_r^* + \sum_{p,q} \mathrm{X}_{p,q}^{*m} a_p^* a_q + \sum_{r,s} \Xi_{r,s}^{*m} b_s^* b_r \\
&\quad + \sum_{r,p} \Theta_{r,p}^{*m} b_r a_p, H]_- = \sum_{p,r} a_p^* b_r^* \{-(\omega_p - \omega_r)\Phi_{p,r}^{*m} \\
&\quad - \sum_{p',r'} \tilde{V}_{p,r';r,p'} \Phi_{p',r'}^{*m} + \sum_{p',q'} B_{p,q';r,p'}^{-} \mathrm{X}_{p',q'}^{*m} \\
&\quad - \sum_{r',s'} B_{p,s';r,r'}^{+} \Xi_{r',s'}^{*m} + \sum_{r',p'} \tilde{U}_{p,p';r,r'} \Theta_{r',p'}^{*m}\} \\
&\quad + \sum_{p,q} a_p^* a_q \{-(\omega_p - \omega_q)\mathrm{X}_{p,q}^{*m} \\
&\quad - \sum_{p',r'} \tilde{V}_{p,r';q,p'} \Phi_{p',r'}^{*m} + \sum_{p',q'} B_{p,q';q,p'}^{-} \mathrm{X}_{p',q'}^{*m} \\
&\quad - \sum_{r',s'} B_{p,s';q,r'}^{+} \Xi_{r',s'}^{*m} + \sum_{r',p'} \tilde{U}_{p,p';q,r'} \Theta_{r',p'}^{*m}\} \\
&\quad + \sum_{s,r} b_s^* b_r \{-(\omega_r - \omega_s)\Xi_{r,s}^{*m} \\
&\quad + \sum_{p',r'} \tilde{V}_{r,r';s,p'} \Phi_{p',r'}^{*m} - \sum_{p',q'} B_{r,q';s,p'}^{-} \mathrm{X}_{p',q'}^{*m} \\
&\quad + \sum_{r',s'} B_{r,s';s,r'}^{+} \Xi_{r',s'}^{*m} - \sum_{r',s'} \tilde{U}_{r,p';s,r'} \Theta_{r',p'}^{*m}\} \\
&\quad + \sum_{r,p} b_r a_p \{-(\omega_r - \omega_p)\Theta_{r,p}^{*m} \\
&\quad - \sum_{p',r'} \tilde{V}_{r,r';p,p'} \Phi_{p',r'}^{*m} + \sum_{p',q'} B_{r,q';p,p'}^{-} \mathrm{X}_{p',q'}^{*m} \\
&\quad - \sum_{r',s'} B_{r,s';p,r'}^{+} \Xi_{r',s'}^{*m} + \sum_{r',p'} \tilde{U}_{r,p';p,r'} \Theta_{r',p'}^{*m}\} \\
&\quad + [\sum_{p,r} a_p^* b_r^* \{\omega_p - \omega_p(S) - \omega_r + \omega_r(S)\}\Phi_{p,r}^{*m} \\
&\quad + \sum_{p,q} a_p^* a_q \{\omega_p - \omega_p(S) - \omega_q + \omega_q(S)\}\mathrm{X}_{p,q}^{*m} \\
&\quad + \sum_{r,s} b_s^* b_r \{\omega_r - \omega_r(S) - \omega_s + \omega_s(S)\}\Xi_{r,s}^{*m} \\
&\quad + \sum_{r,p} b_r a_p \{\omega_r - \omega_r(S) - \omega_p + \omega_p(S)\}\Theta_{r,p}^{*m} \\
&\quad + \sum_{p,r} \Phi_{p,r}^{*m}(M_{r,p} + N_{r,p}) \\
&\quad + \sum_{p,q} \mathrm{X}_{p,q}^{*m}(M_{q,p} - M_{p,q}^{\dagger}) \\
&\quad + \sum_{r,s} \Xi_{r,s}^{*m}(N_{r,s}^{\dagger} - N_{s,r}) \\
&\quad + \sum_{r,p} \Theta_{r,p}^{*m}(-M_{r,p}^{\dagger} - N_{r,p}^{\dagger})],
\end{aligned} \tag{12}$$

where

$$\tilde{V}_{a,b;c,d} = 2\Big[v_{a,b;c,d} - \sum_n \frac{\bar{R}_{a,b}^n \bar{R}_{c,d}^n}{\omega_n(S) - \{\omega_a(S) + \omega_b(S)\}} + \sum_{-n} \frac{\bar{R}_{a,b}^{-n} \bar{R}_{c,d}^{-n}}{\omega_{-n}(S) - \{\omega_c(S) + \omega_d(S)\}}\Big],$$

$$\tilde{U}_{a,b;c,d} = 2\Big[v_{a,b;c,d} - \sum_n \frac{\bar{R}_{a,b}^n \bar{R}_{c,d}^n}{\omega_n(S) - \{\omega_c(S) + \omega_d(S)\}} + \sum_{-n} \frac{\bar{R}_{a,b}^{-n} \bar{R}_{c,d}^{-n}}{\omega_{-n}(S) - \{\omega_a(S) + \omega_b(S)\}}\Big],$$

$$B_{a,b;c,d}^{*} = 2\Big[\sum_{*n} \frac{\bar{R}_{a,b}^{*n} \bar{R}_{c,d}^{*n}}{\omega_{*n}(S) - \{\omega_a(S) + \omega_b(S)\}} - \sum_{*n} \frac{\bar{R}_{a,b}^{*n} \bar{R}_{c,d}^{*n}}{\omega_{*n}(S) - \{\omega_c(S) + \omega_d(S)\}}\Big],$$

and the definitions of $M_{a,b}$ and $N_{a,b}$ are given by Eq. (29) of (S.). By setting (12) equal to the following quantity (representing the quantity in the square bracket by Z_{*m}),

$$(12) = -\omega_{*m}(\sum_{p,r} \Phi_{p,r}^{*m} a_p^* b_r^* + \sum_{p,q} \mathrm{X}_{p,q}^{*m} a_p^* a_q + \sum_{r,s} \Xi_{r,s}^{*m} b_s^* b_r + \sum_{r,p} \Theta_{r,p}^{*m} b_r a_p) + Z_{*m},$$

and constructing equations for Φ, X, Ξ, and Θ, we can get the approximate normal mode γ_m^* and δ_{-m}.

$$
\begin{aligned}
&[\omega_{\pm m} - (\omega_p - \omega_r)]\Phi^{\pm m}_{p,r} \\
&= \sum_{p',r'} \tilde{V}_{p,r';r,p'}\Phi^{\pm m}_{p',r'} - \sum_{p',q'} B^{-}_{p,q';r,p'}X^{\pm m}_{p',q'} \\
&\quad + \sum_{r',s'} B^{+}_{p,s';r,r'}\Xi^{\pm m}_{r',s'} - \sum_{r',p'} \tilde{U}_{p,p';r,r'}\Theta^{\pm m}_{r',p'}, \\
&[\omega_{\pm m} - (\omega_p - \omega_q)]X^{\pm m}_{p,q} \\
&= \sum_{p',r'} \tilde{V}_{p,r';q,p'}\Phi^{\pm m}_{p',r'} - \sum_{p',q'} B^{-}_{p,q';q,p'}X^{\pm m}_{p',q'} \\
&\quad + \sum_{r',s'} B^{+}_{p,s';q,r'}\Xi^{\pm m}_{r',s'} - \sum_{r',p'} \tilde{U}_{p,p';q,r'}\Theta^{\pm m}_{r',p'}, \\
&[\omega_{\pm m} - (\omega_r - \omega_s)]\Xi^{\pm m}_{r,s} \\
&= -\sum_{p',r'} \tilde{V}_{r,r';s,p'}\Phi^{\pm m}_{p',r'} + \sum_{p',q'} B^{-}_{r,q';s,p'}X^{\pm m}_{p',q'} \\
&\quad - \sum_{r',s'} B^{+}_{r,s';s,r'}\Xi^{\pm m}_{r',s'} + \sum_{r',p'} \tilde{U}_{r,p';s,r'}\Theta^{\pm m}_{r',p'}, \\
&[\omega_{\pm m} - (\omega_r - \omega_p)]\Theta^{\pm m}_{r,p} \\
&= \sum_{p',r'} \tilde{V}_{r,r';p,p'}\Phi^{\pm m}_{p',r'} - \sum_{p',q'} B^{-}_{r,q';p,p'}X^{\pm m}_{p',q'} \\
&\quad + \sum_{r',s'} B^{+}_{r,s';p,r'}\Xi^{\pm m}_{r',s'} - \sum_{r',p'} \tilde{U}_{r,p';p,r'}\Theta^{\pm m}_{r',p'}.
\end{aligned}
\tag{13}
$$

$B^{\pm}$ represents the rather weak interaction induced by the scattering and may be regarded as small. The leading term in each term of $B^{\pm}$ begins with a term of the order of λ^3 in the expansion of the coupling constant λ, and $B^{\pm}$ contains the difference of such terms. In this approximation ($B^{\pm} = 0$), the eigenvalue equation (13) reduces to the simple form in which essential coupling exists only for Φ and Θ, and X and Ξ can be regarded as so called attached field. Thus the equation for Φ and Θ in (13) can be written as

$$
\begin{aligned}
&[\omega_{\pm m} - (\omega_p - \omega_r)]\Phi^{\pm m}_{p,r} \\
&= \sum_{p',r'} \tilde{V}_{p,r';r,p'}\Phi^{\pm m}_{p',r'} - \sum_{r',p'} \tilde{V}_{p,p';r,r'}\Theta^{\pm m}_{r',p'}, \\
&[\omega_{\pm m} - (\omega_r - \omega_p)]\Theta^{\pm m}_{r,p} \\
&= \sum_{p',r'} \tilde{V}_{r,r';p,p'}\Phi^{\pm m}_{p',r'} - \sum_{r',p'} \tilde{V}_{r,p';p,r'}\Theta^{\pm m}_{r',p'}.
\end{aligned}
\tag{14}
$$

In this reduction, the following relation has been used,

$$\tilde{V}_{a,b;c,d} = \tilde{V}_{c,d;a,b} = \tilde{U}_{a,b;c,d}.$$

The solutions of (14) have both types of solution: $\omega \gtrless 0$. We denote these as $\omega_{\pm m}$, corresponding to the case $\omega_m > 0$ and $\omega_{-m} < 0$, respectively.

The wave functions Φ and Θ have the orthonormality relations;

$$
\begin{aligned}
&\sum_{p,r} \Phi^{m}_{p,r}\Phi^{m'*}_{p,r} - \sum_{r,p} \Theta^{m}_{r,p}\Theta^{m'*}_{r,p} = \delta_{m,m'}, \\
&\sum_{\substack{\omega_m>0 \\ \omega_m<0}} \Phi^{m}_{p,r}\Phi^{m*}_{p',r'} - \sum_{\substack{\omega_m>0 \\ \omega_m<0}} \Theta^{m}_{r,p}\Theta^{m*}_{r',p'} = \delta_{p,p'}\,\delta_{r,r'}.
\end{aligned}
\tag{15}
$$

The following relations can be easily found from (14), and these relations have been used in obtaining (15),

$$\Theta^{m}_{r,p} = -\Phi^{-m}_{p,r}, \qquad \Phi^{m}_{p,r} = -\Theta^{-m}_{r,p},$$

and

$$\omega_m = -\omega_{-m}. \tag{16}$$

X and Ξ are determined by Φ and Θ. We can see [from (14)] that even when the interaction v contains a hard-core repulsion, it can be replaced by the reaction matrix $\tilde{V}$.

Now we introduce a matrix T defined by

$$
\begin{aligned}
T^{\pm m}_{a,b} &= \sum_{p',r'} \tilde{V}_{a,r';b,p'}\Phi^{\pm m}_{p',r'} \\
&\quad - \sum_{r',p'} \tilde{V}_{a,p';b,r'}\Theta^{\pm m}_{r',p'} = T^{\mp m}_{b,a}.
\end{aligned}
\tag{17}
$$

By substituting T into (13) (but $B^{\pm} = 0$), the attached field X and Ξ are expressed in terms of T;

$$
\begin{aligned}
X^{\pm m}_{p,q} &= \frac{T^{\pm m}_{p,q}}{\omega_{\pm m} - (\omega_p - \omega_q)} = -X^{\mp m}_{q,p}, \\
\Xi^{\pm m}_{r,s} &= -\frac{T^{\pm m}_{r,s}}{\omega_{\pm m} - (\omega_r - \omega_s)} = -\Xi^{\mp m}_{s,r}.
\end{aligned}
\tag{18}
$$

Thus the pair-scattering mode γ^* and δ can be expressed by Φ, Θ, and T; and conversely we obtain the expression of $a^*_p b^*_r$ and $b_r a_p$ in terms of the pair scattering mode γ^* and δ using the orthonormality relations (15).

$$
\begin{aligned}
a^*_p b^*_r &= \sum_m \Phi^{m}_{p,r}\gamma^*_m - \sum_m \Theta^{m}_{r,p}\gamma_m \\
&\quad + \sum_{p',q'} a^*_{p'}a_{q'}\left\{\sum_m \frac{\Theta^{m}_{r,p}T^{m}_{q',p'}}{\omega_m - (\omega_{q'} - \omega_{p'})}\right. \\
&\quad \left. - \sum_m \frac{\Phi^{m}_{p,r}T^{m}_{p',q'}}{\omega_m - (\omega_{p'} - \omega_{q'})}\right\} \\
&\quad + \sum_{r',s'} b^*_{s'}b_{r'}\left\{-\sum_m \frac{\Theta^{m}_{r,p}T^{m}_{s',r'}}{\omega_m - (\omega_{s'} - \omega_{r'})}\right. \\
&\quad \left. + \sum_m \frac{\Phi^{m}_{p,r}T^{m}_{r',s'}}{\omega_m - (\omega_{r'} - \omega_{s'})}\right\},
\end{aligned}
$$

$$b_r a_p = (a^*_p b^*_r)^*. \tag{19}$$

Here we used the relation;

$$\gamma_m = -\delta_{-m}, \qquad \gamma^*_m = -\delta^*_{-m}. \tag{20}$$

We substitute the value of $a^*_p b^*_r$ and $b_r a_p$ in $Z_{\pm m}$ in (12) and express them as functions of γ^* and γ. Now since $Z_{\pm m}$ contains γ^* and γ, we shift γ^* to the extreme left, and γ to the extreme right in $Z_{\pm m}$. Noting that this procedure of shift for the scattering mode α^* and β has been done already, we can rewrite $Z_{\pm m}$ in the form;

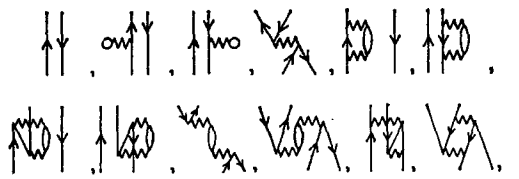

FIG. 1. Some excited states of a system with one additional particle above and one hole below the Fermi surface.

$$Z_{\pm m} = \sum_{p,r} a_p^* b_r^* (\omega_p - \Delta_p - \omega_r + \Delta_r)\Phi_{p,r}^{\pm m} + \sum_{p,q} a_p^* a_q (\omega_p - \Delta_p - \omega_q + \Delta_q)X_{p,q}^{\pm m} + \sum_{r,s} b_s^* b_r (\omega_r - \Delta_r - \omega_s + \Delta_s)\Xi_{r,s}^{\pm m} + \sum_{r,p} b_r a_p (\omega_r - \Delta_r - \omega_p + \Delta_p)\Theta_{r,p}^{\pm m} + Z'_{\pm m}, \quad (21)$$

where

$$\Delta_a = \omega_a(S) + 2\sum_{p,q,s,m} \frac{T_{s,q}^m T_{a,p}^m \tilde{R}_{a,q}^{p,s}}{[\omega_m - (\omega_s - \omega_q)][\omega_m - (\omega_a - \omega_q)]} + 2\sum_{r,s,p,m} \frac{T_{s,a}^m T_{r,p}^m \tilde{R}_{a,r}^{p,s}}{[\omega_m - (\omega_s - \omega_a)][\omega_m - (\omega_r - \omega_p)]}.$$

The term $Z'_{\pm m}$ contains only the interaction term between α^*, β, γ^*, γ and other modes. We do not give the explicit form here for economy of writing. Then in the approximation which neglects $Z'_{\pm m}$, the unknown parameter ω_a should be determined by

$$\omega_a = \Delta_a. \quad (22)$$

Φ, Θ, and $\omega_{\pm m}$ should be evaluated by Eq. (14) with (22).

This substitution of γ^* and γ and shifting process to the extreme left and right should also be done in $Y_{\pm n}$ in (5). Then $Y_{\pm n}$ separates into two parts. One part is given by $Y'_{\pm n}$ which only contain the interaction term between α^*, β, γ^*, γ and other modes, just as in $Z'_{\pm m}$. The other part gives the effect of changing $\omega_a(S)$ in (6) to ω_a defined in (22). Accordingly from now on, we must replace $\omega_a(S)$ in every

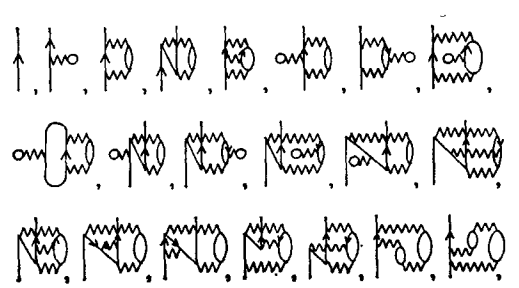

FIG. 2. Some excited states of a system with one additional particle above the Fermi surface.

equation given so far, by ω_a. Thus we obtain modified eigenvalue equations for determining the scattering mode, the pair-scattering mode and eigenvalues $\omega_{\pm n}$, $\omega_{\pm m}$ simultaneously, by changing $\omega_a(S)$ in (6) and (14) to ω_a. The modified Hamiltonian given by (8) must be changed too, by the effect of introducing the pair scattering mode; we have,

$$[a_p^*, H^{(\mathrm{mod})}]_- = -\omega_p a_p^*,$$
$$H^{(\mathrm{mod})} = \sum_i \omega_i C_i^* C_i + C',$$
$$C' = C - 2 \times \sum_{r,r',p,s,m} \frac{T_{s,r}^m T_{r',p}^m \tilde{R}_{r,r'}^{p,s}}{[\omega_m - (\omega_s - \omega_r)][\omega_m - (\omega_{r'} - \omega_p)]}. \quad (23)$$

In this approximation the energy of the ground state taking into account the pair-scattering mode is given by [see (24) of (S.)]

$$+2\sum_{p,q,r,s,m} \frac{T_{s,q}^m T_{r,p}^m \tilde{R}_{s,p}^{q,r}}{[\omega_m - (\omega_s - \omega_q)][\omega_m - (\omega_r - \omega_p)]}, \quad (24)$$

with the replacement of $\omega_a(S)$ in (24) of (S.) by ω_a given by (22).

DISCUSSION

As stated before, $\gamma_e^* \mid N\rangle$, $(\omega_e > 0)$ is an excited state with one additional particle above and one additional hole below the Fermi surface: that is, one-particle excitation. The excitation energy is in this approximation ω_e, which is a positive eigenvalue of the equation for the pair-scattering mode γ_e^*. Similarly, if we construct the double pair-scattering mode, we can get the state of two-particle excitation, and so on.

The state of the system with one additional particle above the Fermi surface is expressed by $a_e^* \mid N\rangle$, $(\omega_e > \mu)$. The energy of the additional particle in this approximation which neglects the interaction between α^*, β, γ^*, γ and other modes, is ω_e, which is an eigenvalue of (23). This gives the difference of binding energy between the ground state of the N-particle system and a some state of the $N+1$ particle system. Similarly the difference of binding energy between the ground state of the N particle system and a some state of the $N+2$ system, is given by an eigenvalue in (6) $(\omega_e > 2\mu)$.

We show the order of our approximation by giving diagrams in Figs. 1–3. (We omit the diagrams obtained by exchanging the lines of particles and holes.) For the case (1) and (3) we give diagrams up to second order in the expansion of the coupling constant λ, for simplicity, but to third order for the second case in conjunction with the Fig. 4 for the ground state. We draw these diagrams by ex-

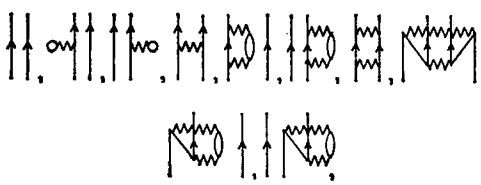

FIG. 3. Some excited states of a system with two additional particles above the Fermi surface.

panding each term in the eigenvalue equations in a power series in λ. As is easily seen from the diagrams, our results contain the contribution from the ladder type diagrams which are important to the evaluation of the approximate excitation energy and ground state energy in the low density Fermion system (nuclear matter). Our results also hold for the Fermion system in the high-density region, even when it has a hard-core repulsion or a Coulomb type interaction between the constituent particles. For the latter case it is known that the pair scattering mode should be taken into account. This corresponds to adding the ring diagrams (or cluster diagrams) in the evaluation of the energy (Fig. 4). These two cases combine in some low-density systems in which the major contribution to the ground-state energy may come from the ladder-type diagrams but some excited states are highly collective and require a knowledge of the ring diagrams in the presence of hard repulsive cores. Such cases have been discussed in connection with the nuclear giant dipole absorption for example.

Now, consider the grand partition function defined by

$$Z = \mathrm{Tr}\ \{e^{-\beta(H^{(\mathrm{mod})}-\mu N)}\}. \tag{25}$$

In (25), $\beta = 1/kT$ and $H^{(\mathrm{mod})}$ is the modified Hamiltonian given in (23). If we write Z in the form

$$Z = e^{-\beta\Omega}, \tag{26}$$

all the thermodynamic properties of the system in this approximation may be derived very simply from Ω. From the definition of $H^{(\mathrm{mod})}$ (omitting C' term), Ω is given by

$$\Omega = -(1/\beta)\sum_i \ln\,(1 + e^{-\beta(\omega_i-\mu)}), \tag{27}$$

for the case of noninteracting system, as is well known. The occupation-probability function is just the same type as the Fermi distribution function, except the replacement of ϵ_i by ω_i. The occupation probability of the individual-particle energy levels at zero temperature is one for levels below the true Fermi energy and zero for energies above the Fermi level.

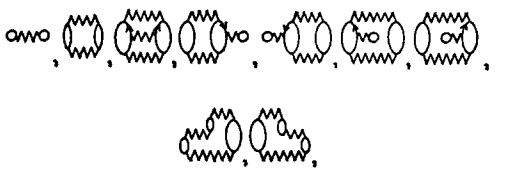

FIG. 4. The ground state of a system.

Finally we mention the diagrams which are contained in the evaluation of the occupation probability n_i, which is defined by;

$$\begin{aligned} n_i &= \mathrm{Tr}\ \{e^{-\beta(H_0+H_I^{(\mathrm{mod})}-\mu N)}C_i^*C_i\}/Z, \\ H_I^{(\mathrm{mod})} &= H^{(\mathrm{mod})} - H_0. \end{aligned} \tag{28}$$

As is familiar from field theory, (28) may be written in terms of the Dyson ordering operator

$$\begin{aligned} n_i &= e^{\beta(\mu-\epsilon_i)}\frac{Z_0}{Z} \\ &\times\left\langle C_iC_i^* + \sum_{n=1}^{\infty}\frac{(-)^n}{n!}\int_0^\beta\int_0^\beta\cdots\int_0^\beta du_1\cdots du_n \right. \\ &\left.\times\, C_iP[H_I^{(\mathrm{mod})}(u_1)\cdots H_I^{(\mathrm{mod})}(u_n)]C_i^*\right\rangle_{\mathrm{all\ d}}. \end{aligned} \tag{29}$$

In (29)

$$\begin{aligned} H_I^{(\mathrm{mod})}(u) &= e^{uH_0}H_I^{(\mathrm{mod})}e^{-uH_0}, \\ \langle A\rangle &= \mathrm{Tr}\ \{e^{-\beta(H_0-\mu N)}A\}/\mathrm{Tr}\ \{e^{-\beta(H_0-\mu N)}\}, \\ Z_0 &= \mathrm{Tr}\ \{e^{-\beta(H_0-\mu N)}\}. \end{aligned}$$

The subscript all d. on the average means that in evaluating this trace we are to take all diagrams. When we take only "connected" diagrams, (29) becomes

$$\begin{aligned} n_i &= e^{\beta(\mu-\epsilon_i)} \\ &\times\left\langle C_iC_i^* + \sum_{n=1}^{\infty}\frac{(-)^n}{n!}\int_0^\beta\int_0^\beta\cdots\int_0^\beta du_1\cdots du_n \right. \\ &\left.\times\, C_iP[H_I^{(\mathrm{mod})}(u_1)\cdots H_I^{(\mathrm{mod})}(u_n)]C_i^*\right\rangle_{\mathrm{c}}, \end{aligned} \tag{30}$$

where the subscript c means that we are to take only connected diagrams. Thus we can give the diagrams which are contained within the frame work of our approach in the evaluation of the average in (30) by the method of Bloch and DeDominicis[4]

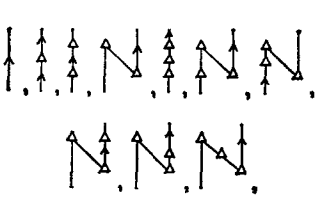

FIG. 5. Diagrams contained in the evaluation of n_i.

[4] C. Bloch and C. DeDominicis, Nuclear Phys. 1, 459 (1958).

(Fig. 5). In Fig. 5, the symbol Δ represents the contribution of all single-particle diagrams shown in Fig. 2, and the diagrams which contain hole lines correspond to the abnormal diagrams defined by Luttinger.[5,6] This is the graphical representation of the evaluation of the function

$$n_i = \frac{1}{e^{\beta(\omega_i-\mu)}+1}.$$

ACKNOWLEDGMENTS

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APPENDIX

ENERGY SPECTRUM OF A FINITE NUCLEUS

In this Appendix the procedure for getting the energy spectrum by looking at the normal modes is extended to a case of finite nuclei consisting of a core nucleus plus one additional nucleon and two additional nucleons, say, such as Ca^{41} and Ca^{42}. The core nucleus means a nucleus consisting of closed neutron and proton shells such as Ca^{40}. The eigenvalue equations for determining the energy spectrum are obtained for each quantum number J (the total angular momentum of the nucleus), when a spherical two-body interaction is assumed.

Although the mechanism producing the analogous states in the finite and infinite systems is essentially the same, the way in which the mechanism works in the finite system differs from that in the infinite system because of its shell structure. We shall describe here how modifications of the scattering modes are to be made so as to be appropriate in the case of real nuclei. The prescription will be made so as to bring out analogies in the methods used to those employed in describing the infinite system.

We consider a system of nucleons (protons and neutrons) which are moving in a certain spherically symmetric self-consistent well. We choose, as basic functions of the second quantization representation, the wave functions of a nucleon in each well, and states are designated by $\psi^{(r)}(n,(l)\,j,m)$; (r designates proton or neutron), as is usually used when formulating the problem in the j-j coupling scheme. Let us introduce the Fermi operators $C^{*(r)}_{n,j,m}$ and $C^{(r)}_{n,j,m}$ which create and destroy one nucleon of the r kind in the state $\psi^{(r)}(n,j,m)$. The Hamiltonian for the system of interacting nucleons is then

$$H = \sum_{r=p,n} H^{(r)} + H^{(r,r')}, \tag{A1}$$

with

$$H^{(r)} = \sum_{n,j,m} \epsilon^{(r)}_{n,j} C^{*(r)}_{n,j,m} C^{(r)}_{n,j,m} + \sum_{n,j,m} C^{*(r)}_{n_1,j_1,m_1} C^{*(r)}_{n_2,j_2,m_2} \times \tfrac{1}{2} V^{(r)}(n_1,j_1,m_1;n_2,j_2,m_2 \mid n_4,j_4,m_4;n_3,j_3,m_3) \times C^{(r)}_{n_3,j_3,m_3} C^{(r)}_{n_4,j_4,m_4},$$

and,

$$H^{(r,r')} = \sum_{n,j,m} C^{*(r)}_{n_1,j_1,m_1} C^{*(r')}_{n_2,j_2,m_2} \times V^{(r,r')}(n_1,j_1,m_1;n_2,j_2,m_2 \mid n_4,j_4,m_4;n_3,j_3,m_3) \times C^{(r')}_{n_3,j_3,m_3} C^{(r)}_{n_4,j_4,m_4}.$$

Here $\epsilon^{(r)}_{n,j}$ is the single nucleon energy of the r kind in the $\psi^{(r)}(n,j,m)$ state, and

$$V^{(r)}(n_1,j_1,m_1;n_2,j_2,m_2 \mid n_4,j_4,m_4,n_3,j_3,m_3) = \iint \psi^{*(r)}_{n_1,j_1,m_1}(1)\cdot\psi^{*(r)}_{n_2,j_2,m_2}(2)\cdot V^{(r)}(1,2) \times \psi^{(r)}_{n_4,j_4,m_4}(1)\cdot\psi^{(r)}_{n_3,j_3,m_3}(2)\cdot d\tau_1^{(r)}\, d\tau_2^{(r)},$$

$$V^{(r,r')}(n_1,j_1,m_1;n_2,j_2,m_2 \mid n_4,j_4,m_4;n_3,j_3,m_3) = \iint \psi^{*(r)}_{n_1,j_1,m_1}(1)\cdot\psi^{*(r')}_{n_2,j_2,m_2}(2)\cdot V^{(r,r')}(1,2) \times \psi^{(r)}_{n_4,j_4,m_4}(1)\cdot\psi^{(r')}_{n_3,j_3,m_3}(2)\cdot d\tau_1^{(r)}\, d\tau_2^{(r')}.$$

We consider for simplicity a core nucleus consisting of closed proton and neutron shells. We denote the ground state of the core nucleus by $|0\rangle$ and its energy by E_c, and treat it as the physical vacuum referring to absent nucleons and holes. Following the analogy with the infinite case, we shall define the separation of the operator $C^{*(r)}_{n,j,m}$ into a creation operator of a r-nucleon and a destruction operator of a r-hole as follows[7];

$$\begin{aligned} C^{*(r)}_{n,j,m} &= a^{*(r)}_{n,j,m}, \qquad \omega^{(r)}_{n,j} \geq \mu^{(r)}_1, \\ C^{*(r)}_{n,j,m} &= b^{(r)}_{n,j,m}, \qquad \omega^{(r)}_{n,j} < \mu^{(r)}_1. \end{aligned} \tag{A2}$$

Here $\omega^{(r)}_{n,j}$ is the "true" one r-nucleon energy of the state $\psi^{(r)}(n,j,m)$ which is defined to be compatible self-consistently with the equation of the eigenvalue problem which we shall establish later and $\mu^{(r)}_1$ is the binding energy of the one additional r-nucleon to the core nucleus. By this definition the Hamiltonian $H^{(r)}$, for example, in (1) can be split into the following parts;

$$H^{(r)} = H^{(r)}_0 + H^{(r)}_I,$$

[5] W. Kohn and J. M. Luttinger, Phys. Rev. **118**, 41 (1960).
[6] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
[7] We use the letters without prime in the case $\omega_{n,j}{}^{(r)} \geq \mu_1{}^{(r)}$, and the letters with a prime in the case $\omega_{n',j'}{}^{(r)} < \mu_1{}^{(r)}$.

$$H_0^{(r)} = \sum_{n,j,m} \omega_{n,j}^{(r)} a_{n,j,m}^{*(r)} a_{n,j,m}^{(r)} - \sum_{n',j',m'} \omega_{n',j'}^{(r)} b_{n',j',m}^{*(r)} b_{n',j',m'}^{(r)} + \sum_{n',j',m'} \epsilon_{n',j'},$$

$$H_I^{(r)} = \sum_{i,j,k} (a_{i_1,j_1,k_1}^{*(r)} + b_{i_1,j_1,k_1}^{(r)})(a_{i_2,j_2,k_2}^{*(r)} + b_{i_2,j_2,k_2}^{(r)}) \times \tfrac{1}{2} V^{(r)}(i_1, j_1, k_1; i_2, j_2, k_2 \mid i_4, j_4, k_4; i_3, j_3, k_3) \times (a_{i_3,j_3,k_3}^{(r)} + b_{i_3,j_3,k_3}^{*(r)})(a_{i_4,j_4,k_4}^{(r)} + b_{i_4,j_4,k_4}^{*(r)}) + \sum_{n,j,m} (\epsilon_{n,j} - \omega_{n,j}) a_{n,j,m}^{*(r)} a_{n,j,m}^{(r)} - \sum_{n',j',m'} (\epsilon_{n',j'} - \omega_{n',j'}) b_{n',j',m}^{*(r)} b_{n',j',m'}^{(r)}; \quad \text{(A3)}$$

where the suffices (i, j, k) stand for (n, j, m) or (n', j', m'). Now the scattering eigenmode operators α^* and β in the finite system are to be defined in the following way,

$$\left.\begin{matrix} \alpha_{J,s}^{*(r)} \\ \beta_{J,-s}^{(r)} \end{matrix}\right\} = \sum_{\lambda_1,\rho_1,\lambda_2,\rho_2,M} \psi_{\lambda_1,\rho_1,\lambda_2,\rho_2:J}^{(r),*s} [a_{\lambda_1,\rho_1}^{*(r)}, a_{\lambda_2,\rho_2}^{*(r)}]_{J,M} + \sum_{\lambda_1',\rho_1',\lambda_2',\rho_2',M} \chi_{\lambda_1',\rho_1',\lambda_2',\rho_2':J}^{(r),*s} [b_{\lambda_1',\rho_1'}^{(r)}, b_{\lambda_2',\rho_2'}^{(r)}]_{J,M} + 2 \sum_{\lambda_1,\rho_1,\lambda_2',\rho_2',M} \xi_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r),*s} [a_{\lambda_1,\rho_1}^{*(r)}, b_{\lambda_2',\rho_2'}^{(r)}]_{J,M} \quad \text{(A4)}$$

and

$$\left.\begin{matrix} \alpha_{J,s}^{*(r,r')} \\ \beta_{J,-s}^{(r,r')} \end{matrix}\right\} = \sum_{\lambda_1,\rho_1,\lambda_2,\rho_2,M} \psi_{\lambda_1,\rho_1,\lambda_2,\rho_2:J}^{(r,r'),*s} [a_{\lambda_1,\rho_1}^{*(r)}, a_{\lambda_2,\rho_2}^{*(r')}]_{J,M} + \sum_{\lambda_1',\rho_1',\lambda_2',\rho_2',M} \chi_{\lambda_1',\rho_1',\lambda_2',\rho_2':J}^{(r,r'),*s} [b_{\lambda_1',\rho_1'}^{(r)}, b_{\lambda_2',\rho_2'}^{(r')}]_{J,M} + \sum_{\lambda_1,\rho_1,\lambda_2',\rho_2';M} \xi_{\lambda_1,\rho_1,\lambda_2',\rho_2':M}^{(r,r'),*s} [a_{\lambda_1,\rho_1}^{*(r)}, b_{\lambda_2',\rho_2'}^{(r')}]_{J,M} + \sum_{\lambda_1',\rho_1',\lambda_2,\rho_2,M} \psi_{\lambda_1',\rho_1',\lambda_2,\rho_2:J}^{(r,r'),*s} [b_{\lambda_1',\rho_1'}^{(r)}, a_{\lambda_2,\rho_2}^{*(r')}]_{J,M}. \quad \text{(A4')}$$

Where a term of the square bracket

$$[a_{\lambda_1,\rho_1}^{*(r)}, a_{\lambda_2,\rho_2}^{*(r)}]_{J,M},$$

for example, equals

$$\sum_{\sigma_1+\sigma_2=M} a_{\lambda_1,\rho_1,\sigma_1}^{*(r)} a_{\lambda_2,\rho_2,\sigma_2}^{*(r)} (\rho_1, \sigma_1, \rho_2, \sigma_2 \mid JM),$$

with the Wigner coefficient $(\rho_1, \sigma_1, \rho_2, \sigma_2 \mid JM)$. The reason is as follows. When we can find the operators $\alpha_{J,s}^{*(r)}$ and $\alpha_{J,s}^{*(r,r')}$ which satisfy

$$[\alpha_{J,s}^{*(r)}, H]_- = -\omega_{J,s}^{(r)} \alpha_{J,s}^{*(r)}, \qquad \omega_{J,s}^{(r)} \geq \mu_2^{(r)}$$

and

$$[\alpha_{J,s}^{*(r,r')}, H]_- = -\omega_{J,s}^{(r,r')} \alpha_{J,s}^{*(r,r')}, \qquad \omega_{J,s}^{(r,r')} \geq \mu_2^{(r,r')}, \quad \text{(A5)}$$

we get

$$H\alpha_{J,s}^{*(r)} \mid 0\rangle = (\omega_{J,s}^{(r)} + E_c)\alpha_{J,s}^{*(r)} \mid 0\rangle,$$

and

$$H\alpha_{J,s}^{*(r,r')} \mid 0\rangle = (\omega_{J,s}^{(r,r')} + E_c)\alpha_{J,s}^{*(r,r')} \mid 0\rangle, \quad \text{(A5')}$$

where $\mu_2^{(r)}$ is the binding energy of the two additional r-kind nucleons added to the core nucleus, and $\mu_2^{(r,r')}$ the same one referred to the additional one neutron and one proton.

Then $\alpha_{J,s}^{*(r)} \mid 0\rangle$ and $\alpha_{J,s}^{*(r,r')} \mid 0\rangle$ represent the ground state or some excited states labeled by the quantum number J, respectively, and from the eigenvalues $\omega_{J,s}^{(r)}$ and $\omega_{J,s}^{(r,r')}$, we can find out the energy separations of the spectrum of each nucleus in terms of the J value.

For construction and evaluation of the scattering modes, we use the same technique, as done in the infinite case. But because of the complicatedness and tediousness, we omit here full calculations. For our purpose the following outline will be sufficient.

We evaluate the anticommutator of the modes defined above with the Hamiltonian using (A3), (A4), and (A4') and put the quantity equal to the right-hand side of the next equation,

$$\left[\begin{pmatrix} \alpha_{J,s}^{*(r)} \\ \beta_{J,-s}^{(r)} \end{pmatrix}, H\right]_- = -\begin{pmatrix} \omega_{J,s}^{(r)} & \alpha_{J,s}^{*(r)} \\ \omega_{J,-s}^{(r)} & \beta_{J,-s}^{(r)} \end{pmatrix} + Y_{*s}^{(r)} \quad \text{(A6)}$$

and

$$\left[\begin{pmatrix} \alpha_{J,s}^{*(r,r')} \\ \beta_{J,-s}^{(r,r')} \end{pmatrix}, H\right]_- = -\begin{pmatrix} \omega_{J,s}^{(r,r')} & \alpha_{J,s}^{*(r,r')} \\ \omega_{J,-s}^{(r,r')} & \beta_{J,-s}^{(r,r')} \end{pmatrix} + Y_{*s}^{(r,r')}. \quad \text{(A6')}$$

In (A6) and (A6') Y_{*s} contains the interaction term between α^*, β and other modes, respectively. We do not give the explicit form here for economy of writing. Then in the approximation which neglects the interaction term Y_{*s}, the eigenvalue equations for determining eigenvalues and eigenfunctions are:

$$[\omega_{J,s}^{(r)} - (\omega_{\lambda_1,\rho_1}^{(r)} + \omega_{\lambda_2,\rho_2}^{(r)})] \times \psi_{\lambda_1,\rho_1,\lambda_2,\rho_2:J}^{(r),*s} = \sum_{n_1,j_1,n_2,j_2} \times \tilde{V}^{(r)}(\lambda_1, \rho_1, \lambda_2, \rho_2: JM \mid n_1, j_1, n_2, j_2: JM) \times \psi_{n_1,j_1,n_2,j_2:J}^{(r),*s} - \sum_{n_1',j_1',n_2',j_2'} \times \tilde{V}^{(r)}(\lambda_1, \rho_1, \lambda_2, \rho_2: JM \mid n_1', j_1', n_2', j_2': JM) \times \chi_{n_1',j_1',n_2',j_2':J}^{(r),*s},$$

$$[\omega_{J,s}^{(r)} - (\omega_{\lambda_1',\rho_1'}^{(r)} + \omega_{\lambda_2',\rho_2'}^{(r)})] \times \chi_{\lambda_1',\rho_1',\lambda_2',\rho_2':J}^{(r),*s} = \sum_{n_1,j_1,n_2,j_2} \times \tilde{V}^{(r)}(\lambda_1', \rho_1', \lambda_2', \rho_2': JM \mid n_1, j_1, n_2, j_2: JM) \times \psi_{n_1,j_1,n_2,j_2:J}^{(r),*s} - \sum_{n_1',j_1',n_2',j_2'} \times \tilde{V}^{(r)}(\lambda_1', \rho_1', \lambda_2', \rho_2': JM \mid n_1', j_1', n_2', j_2': JM) \times \chi_{n_1',j_1',n_2',j_2':J}^{(r),*s}, \quad \text{(A7)}$$

and

$$
\begin{aligned}
&[\omega_{J,\pm s}^{(r,r')} - (\omega_{\lambda_1,\rho_1}^{(r)} + \omega_{\lambda_2,\rho_2}^{(r')})] \\
&\times \psi_{\lambda_1,\rho_1,\lambda_2,\rho_2:J}^{(r,r'),\pm s} = \sum_{n_1,j_1,n_2,j_2} \\
&\times V^{(r,r')}(\lambda_1, \rho_1, \lambda_2, \rho_2: JM \mid n_1, j_1, n_2, j_2: JM) \\
&\times \psi_{n_1,j_1,n_2,j_2:J}^{(r,r'),\pm s} - \sum_{n_1',j_1',n_2',j_2'} \\
&\times V^{(r,r')}(\lambda_1, \rho_1, \lambda_2, \rho_2: JM \mid n_1', j_1', n_2', j_2': JM) \\
&\times \chi_{n_1',j_1',n_2',j_2':J}^{(r,r'),\pm s}, \\
&[\omega_{J,\pm s}^{(r,r')} - (\omega_{\lambda_1',\rho_1'}^{(r)} + \omega_{\lambda_2',\rho_2'}^{(r')})] \\
&\times \chi_{\lambda_1',\rho_1',\lambda_2',\rho_2':J}^{(r,r'),\pm s} = \sum_{n_1,j_1,n_2,j_2} \\
&\times V^{(r,r')}(\lambda_1', \rho_1', \lambda_2', \rho_2': JM \mid n_1, j_1, n_2, j_2: JM) \\
&\times \psi_{n_1,j_1,n_2,j_2:J}^{(r,r'),\pm s} - \sum_{n_1',j_1',n_2',j_2'} \\
&\times V^{(r,r')}(\lambda_1', \rho_1', \lambda_2', \rho_2': JM \mid n_1', j_1', n_2', j_2': JM) \\
&\times \chi_{n_1',j_1',n_2',j_2':J}^{(r,r'),\pm s} \qquad \text{(A7')}
\end{aligned}
$$

with

$$
\begin{aligned}
\omega_{a,b}^{(r)} = \epsilon_{a,b}^{(r)} &+ 2 \sum_{n',j',J} \frac{2J+1}{2b+1} \\
&\times \tilde{V}^{(r)}(a, b, n', j': JM \mid a, b, n', j': JM) \\
&+ \sum_{n',j',J} \frac{2J+1}{2b+1} \\
&\times V^{(r,r')}(a, b, n', j': JM \mid a, b, n', j': JM) \\
&- 2 \sum_{n,j,J,-s} \frac{2J+1}{2b+1} \frac{\bar{R}_{a,b,n,j:J}^{(r),-s} \bar{R}_{a,b,n,j:J}^{(r),-s}}{\omega_{J,-s}^{(r)} - (\omega_{a,b}^{(r)} + \omega_{n,j}^{(r)})} \\
&- \sum_{n,j,J,-s} \frac{2J+1}{2b+1} \frac{\bar{R}_{a,b,n,j:J}^{(r,r'),-s} \bar{R}_{a,b,n,j:J}^{(r,r'),-s}}{\omega_{J,-s}^{(r,r')} - (\omega_{a,b}^{(r)} + \omega_{n,j}^{(r')})} \\
&- 2 \sum_{n',j',J,s} \frac{2J+1}{2b+1} \frac{\bar{R}_{a,b,n',j':J}^{(r),s} \bar{R}_{a,b,n',j':J}^{(r),s}}{\omega_{J,s}^{(r)} - (\omega_{a,b}^{(r)} + \omega_{n',j'}^{(r)})} \\
&- \sum_{n',j',J,s} \frac{2J+1}{2b+1} \frac{\bar{R}_{a,b,n',j':J}^{(r,r'),s} \bar{R}_{a,b,n',j':J}^{(r,r'),s}}{\omega_{J,s}^{(r,r')} - (\omega_{a,b}^{(r)} + \omega_{n',j'}^{(r')})}, \qquad \text{(A7'')}
\end{aligned}
$$

where

$$
\begin{aligned}
\bar{R}_{a,b,c,d:J}^{(r),\pm s} &= \sum_{n_1,j_1,n_2,j_2} \\
&\times \tilde{V}^{(r)}(a, b, c, d: JM \mid n_1, j_1, n_2, j_2: JM) \\
&\times \psi_{n_1,j_1,n_2,j_2:J}^{(r),\pm s} - \sum_{n_1',j_1',n_2',j_2'} \\
&\times \tilde{V}^{(r)}(a, b, c, d: JM \mid n_1', j_1', n_2', j_2': JM) \\
&\times \chi_{n_1',j_1',n_2',j_2':J}^{(r),\pm s}, \\
\bar{R}_{a,b,c,d:J}^{(r,r'),\pm s} &= \sum_{n_1,j_1,n_2,j_2} \\
&\times V^{(r,r')}(a, b, c, d: JM \mid n_1, j_1, n_2, j_2: JM) \\
&\times \psi_{n_1,j_1,n_2,j_2:J}^{(r,r'),\pm s} - \sum_{n_1',j_1',n_2',j_2'} \\
&\times V^{(r,r')}(a, b, c, d: JM \mid n_1', j_1', n_2', j_2': JM) \\
&\times \chi_{n_1',j_1',n_2',j_2':J}^{(r,r'),\pm s},
\end{aligned}
$$

$$
\begin{aligned}
\tilde{V}^{(r)}&(a, b, c, d: JM \mid a', b', c', a': JM) \\
&= \frac{1}{2} \iint [\psi_{a,b}^{(r)}(1), \psi_{c,d}^{(r)}(2)]_{JM}^{*} \\
&\times V^{(r)}(1, 2)[\psi_{a',b'}^{(r)}(1), \psi_{c',d'}^{(r)}(2)]_{JM}\, d\tau_1^{(r)}\, d\tau_2^{(r)} \\
&- \text{exchange term}, \\
V^{(r,r')}&(a, b, c, d: JM \mid a', b', c', d': JM) \\
&= \iint [\psi_{a,b}^{(r)}(1), \psi_{c,d}^{(r')}(2)]_{JM}^{*} \\
&\times V^{(r,r')}(1, 2)[\psi_{a',b'}^{(r)}(1), \psi_{c',d'}^{(r')}(2)]_{JM}\, d\tau_1^{(r)}\, d\tau_2^{(r')}.
\end{aligned}
$$

In this approximation, $\omega_{a,b}^{(r)}$ defined above is the "true" nucleon energy in the state $\psi_{a,b,m}^{(r)}$. (A7) and (A7') are not independent of each other. They are dependent on each other through the single nucleon energy $\omega^{(r)}$ and $\omega^{(r')}$. (A7), (A7'), and (A7''), should be solved so as to be simultaneously self-consistent. The solutions of (A7) and (A7'), have both types of solutions $\omega_J^{(r)} \geq \mu_2^{(r)}$, $\omega_J^{(r)} < \mu_2^{(r)}$, and $\omega_J^{(r,r')} \geq \mu_2^{(r,r')}$, $\omega_J^{(r,r')} < \mu_2^{(r,r')}$. We denote these as $\omega_{J,\pm s}^{(r)}$ and $\omega_{J,\pm s}^{(r,r')}$, corresponding to the cases $\omega_{J,s} \geq \mu_2$ and $\omega_{J,-s} < \mu_2$, respectively.

The attached fields

$$
\xi_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r),\pm s}, \qquad \xi_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r,r'),\pm s}
$$

and

$$
\eta_{\lambda_1',\rho_1',\lambda_2,\rho_2:J}^{(r,r'),\pm s}
$$

are determined by the following equations;

$$
\begin{aligned}
\xi_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r),\pm s} &= \bar{R}_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r),\pm s} / [\omega_{J,\pm s}^{(r)} - (\omega_{\lambda_1,\rho_1}^{(r)} + \omega_{\lambda_2',\rho_2'}^{(r)})], \\
\xi_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r,r'),\pm s} &= \bar{R}_{\lambda_1,\rho_1,\lambda_2',\rho_2':J}^{(r,r'),\pm s} / [\omega_{J,\pm s}^{(r,r')} - (\omega_{\lambda_1,\rho_1}^{(r)} + \omega_{\lambda_2',\rho_2'}^{(r')})],
\end{aligned}
$$

and

$$
\eta_{\lambda_1',\rho_1',\lambda_2,\rho_2:J}^{(r,r'),\pm s} = \bar{R}_{\lambda_1',\rho_1',\lambda_2,\rho_2:J}^{(r,r'),\pm s} / [\omega_{J,\pm s}^{(r,r')} - (\omega_{\lambda_1',\rho_1'}^{(r)} + \omega_{\lambda_2,\rho_2}^{(r')})].
$$

The expression for the energy spectrum for the nucleus consisting of a core nucleus and two nucleons is given by the set of the eigenvalue equations (A7), (A7'), and (A7'') which are to be self-consistently solved. They give the expression for the energy splitting of the nucleus in terms of the quantum number J. In the case in which some knowledge of the ring diagrams is required, one must add the pair-scattering modes γ^* and δ (particle-hole interaction) as shown in the infinite case.

Locally Maxwellian Solutions for a "Positronium" Plasma

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Exact locally Maxwellian solutions of a neutral "positronium" plasma are explicitly presented. They correspond to a flow which is a superposition of a parallel flow, a radial expansion, and a rigid-body rotation.

CONSIDER a neutral plasma consisting of two species + and − whose particles possess equal magnitudes of charge and equal mass (i.e., $e_+ = e$, $e_- = -e, m_+ = m_- = m$). In the absence of external forces there exist exact, nonequilibrium, locally Maxwellian solutions for the distribution functions $f_\pm(\mathbf{x}, \boldsymbol{\xi}, t)$ of these species. These distribution functions satisfy the transport equations

$$\frac{\partial f_\pm}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f_\pm}{\partial \mathbf{x}} \pm \frac{e}{m}\left[\mathbf{E} + \frac{1}{c}\,\boldsymbol{\xi}\times\mathbf{B}\right] \times \frac{\partial f_\pm}{\partial \boldsymbol{\xi}} = J^\pm(f_+, f_-), \tag{1}$$

where the electromagnetic fields **E**, **B** satisfy Maxwell's equations with electric charge and current densities given by

$$n(\mathbf{x}, t) = e\int [f_+ - f_-]\, d\boldsymbol{\xi}$$
$$\mathbf{J}(\mathbf{x}, t) = e\int \boldsymbol{\xi}(f_+ - f_-]\, d\boldsymbol{\xi}, \tag{2}$$

respectively. The $J^\pm$ for the case of the Boltzmann transport equation are

$$J^+ = C^{++} + C^{+-}$$
$$J^- = C^{--} + C^{-+} \tag{3}$$

with the usual collision terms[1,2]

$$C^{+-} = -\int d\boldsymbol{\xi}'\,|\boldsymbol{\xi} - \boldsymbol{\xi}'| \int d\Omega\sigma^{(+,-)} \times [f^+(\mathbf{x}, \boldsymbol{\xi}, t)f^-(\mathbf{x}, \boldsymbol{\xi}', t) - f^+(\mathbf{x}, \boldsymbol{\xi}_1, t)f^-(\mathbf{x}, \boldsymbol{\xi}_1', t)], \quad \text{etc.} \tag{4}$$

where $\sigma^{(+,-)}$ is the appropriate collision cross section. More generally, $J^\pm$ must (1) be invariant under Galilean transformations in phase space, (2) identically vanish for the equilibrium Maxwellian distributions, and (3) conserve the usual three additive collisional invariants,[2] as for example the $J^\pm$ of the Fokker-Planck equation, etc.

When $f^\pm$ is set equal to the locally Maxwellian distribution functions $f_\pm^0(\mathbf{x}, \boldsymbol{\xi}, t)$,

$$f_\pm^0(\mathbf{x}, \boldsymbol{\xi}, t) = \frac{\rho(\mathbf{x}, t)}{[2\pi RT(\mathbf{x}, t)]^{\frac{3}{2}}} \exp\left\{-\frac{[\boldsymbol{\xi} - \mathbf{u}(\mathbf{x}, t)]^2}{2RT(\mathbf{x}, t)}\right\} = f^0(\mathbf{x}, \boldsymbol{\xi}, t), \qquad R = k/m; \tag{5}$$

then, by virtue of the previously listed properties of $J^\pm$,

$$J^\pm(f_+^0, f_-^0) = 0. \tag{6}$$

On substituting (5) into (2), we find that n and **J** vanish identically and Maxwell's equations reduce to the form which they possess for a vacuum. A perfectly acceptable solution of these equations is obtained then by setting

$$\mathbf{E} = 0 \quad \text{and} \quad \mathbf{B} = 0. \tag{7}$$

Introducing (6) and (7) into the transport equations (1) we see that these equations simplify to a single partial differential equation,

$$\frac{\partial f^0}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f^0}{\partial \mathbf{x}} = 0, \tag{8}$$

from which, together with (5), we obtain the density ρ, mean velocity u, and temperature T previously obtained by Grad[2] in the case of a single-component uncharged Boltzmann gas. After a translation in space and time, Grad's solution can be written [Eq. (A2.21) of reference 2 for $\alpha \neq 0$, see (A2.14) for the more general case]

$$RT(t) = -1/2(a_4 + \alpha t^2),$$
$$u(\mathbf{x}, t) = -\frac{\mathbf{a} - 2\alpha t\mathbf{x} + \boldsymbol{\Omega}\times\mathbf{x}}{2(a_4 + \alpha t^2)},$$
$$\ln\left\{\frac{\rho(\mathbf{x}, t)}{[2\pi RT(\mathbf{x}, t)]^{\frac{3}{2}}}\right\} = a_0 - \frac{4\alpha a_4 x^2 + 4\alpha t\mathbf{a}\cdot\mathbf{x} - (\mathbf{a} + \boldsymbol{\Omega}\times\mathbf{x})^2}{4(a_4 + \alpha t^2)}, \tag{9}$$

with a_0, α, a_4, **a**, and $\boldsymbol{\Omega}$ constants. Thus this locally Maxwellian plasma can undergo a flow which is a superposition of a parallel flow, a radial expansion, and a rigid body rotation.

In regard to the H theorem[2] for such a plasma, these solutions play the analogous role[2] to that played by the locally Maxwellian solutions for a Boltzmann gas. We are investigating the question of whether such solutions exist in the presence of external fields (particularly gravitational fields).

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Studies in Nonequilibrium Rate Processes. V. The Relaxation of Moments Derived from a Master Equation

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A study has been made of the relaxation of the moments of probability distributions whose time evolution are governed by a master equation. The necessary and sufficient condition for the first moment, $M_1(t)$, to undergo a simple exponential relaxation is found to be

$$\sum_{n=0}^{\infty} nA_{nm} = \beta m + \gamma,$$

where A_{nm} is the transition probability per unit time for transitions from state m to n, and where β and γ are constants. The necessary and sufficient condition under which the first k moments, $M_1(t)$, $M_2(t)$, $\cdots$, $M_k(t)$, satisfy a closed system of linear equations is found to be

$$\sum_{n=0}^{\infty} n^r A_{nm} = \sum_{i=0}^{k} \beta_{ri} m^i.$$

Near equilibrium, i.e., as $t \to \infty$, all the moments $M_r(t)$ obey, *to a good approximation*, a simple exponential relaxation law irrespective of the form of the A_{nm}.

For systems described by the Fokker-Planck equation

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial}{\partial x}[b_1(x)P(x, t)] + \tfrac{1}{2}\frac{\partial^2}{\partial x^2}[b_2(x)P(x, t)],$$

the necessary and sufficient condition that the first moment $M_1(t)$ undergo a simple exponential relaxation is found to be $b_1(x) = \beta x + \gamma$ and the necessary and sufficient condition for the 2nd moment, $M_2(t)$ to have a simple exponential relaxation is $2xb_1(x) + b_2 = \beta_{22}x^2 + \gamma_2$. It is shown that these conditions are equivalent to the conditions on the A_{nm} stated above.

I. INTRODUCTION

In an earlier paper of this series, one of us (K.E.S.), in collaboration with Montroll, has presented the theory for the relaxation of a system of harmonic oscillators in contact with a heat bath.[1] Starting with the master equation

$$\frac{dx_n(t)}{dt} = \sum_{m=0}^{\infty} \{W_{nm}x_m(t) - W_{mn}x_n(t)\} = \sum_{m=0}^{\infty} A_{nm}x_m(t), \tag{1}$$

where $x_n(t)$ is the fraction of oscillators with energy $nh\nu$ at time t and where the W_{nm} are the transition probabilities per unit time for transitions from state m to n, we showed that the first moment of the distribution,

$$M_1(t) = \sum_{n=0}^{\infty} nx_n(t),$$

obeyed a simple exponential relaxation law of the form, where α is a constant,

$$dM_1(t)/dt = -\alpha[M_1(t) - M_1(\infty)] \tag{2}$$

independent of the initial distribution $\{x_n(0)\}$. This result, which had been obtained previously by Bethe and Teller,[2] is somewhat surprising in its simplicity since the relaxation of the distribution $\{x_n(t)\}$, as a function of the initial distribution $\{x_n(0)\}$, follows a quite complicated behavior. In general, the solution of the transport equation (1) is given by a linear combination of eigenfunctions $\mu_i(n)$ as

$$x_n(t) = \sum_i c_i\mu_i(n)e^{\lambda_i t}, \tag{3}$$

where the λ_i are the eigenvalues of the matrix $\mathbf{A} = (A_{nm})$ and the c_i are related to the initial distribution $\{x_n(0)\}$. While $\lambda_0 = 0$ in order that $x_n(t) \to x_n^{equil}$ as $t \to \infty$, the λ_i ($j \neq 0$) are different from zero so that the solution (3) will in general not reduce to the simple exponential form (2) for the moment $M_1(t)$.

As has been pointed out previously[3] the simple exponential relaxation of the moment M_1 exhibited in Eq. (2) depends entirely on the form of the transition probabilities W_{nm} (or A_{nm}) which enter into the kinetic equation (1). It is the purpose of this paper to derive the necessary and sufficient conditions on the form of the transition probabilities A_{nm} under which the moment equation (2) is obtained from the master equation (1). This result will then

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be generalized to obtain the necessary and sufficient conditions on the form of the A_{nm} in order that the first k moments, $M_1(t)$, $M_2(t)$, $\cdots$, $M_k(t)$, satisfy a closed system of linear equations. We shall also derive the necessary and sufficient conditions for the exponential relaxation of the first and second moments, $M_1(t)$ and $M_2(t)$, for systems described by the Fokker-Planck equation derived from the master equation (1).

II. RELAXATION OF THE MOMENT $M_1(t)$

Our consideration in this section is restricted to systems whose time evolution is described by the master equation [see Eq. (1)]. In general, this equation, for systems with discrete states, can be written as

$$\frac{dP(n, t)}{dt} = \sum_{m=0}^{\infty} A_{nm}P(m, t) \quad n = 0, 1, \cdots \infty, \tag{4}$$

where $P(n, t)$ is the probability that the system will be found in state n at time t, and where the A_{nm} are the elements of the transition probability matrix. The $P(n, t)$ have the obvious normalization

$$\sum_{n=0}^{\infty} P(n, t) = 1. \tag{5}$$

For systems with continuous variables, Eq. (4) reads

$$\frac{\partial P(x, t)}{\partial t} = \int_0^{\infty} A(x, y)P(y, t)\, dy, \tag{6}$$

where $P(x, t)\, dx$ is the probability that the variable $x(t)$ is in the range from x to $x + dx$ at time t and where $A(x, y)$, one of the elements of the transition probability matrix, is the probability per unit time for a transition from y to x. We shall limit our discussion here to systems with discrete variables; all of our results, however, carry over readily to systems with continuous variables. The only change, essentially, is the replacement of summation by integration.

We begin by inquiring under what conditions the time evolution of the first moment, defined by

$$M_1(t) \equiv \sum_{n=0}^{\infty} nP(n, t), \tag{7}$$

can be written as

$$dM_1(t)/dt = \beta M_1(t) + \gamma, \tag{8}$$

where β and γ are constants. From Eq. (4) and the definition (7) it follows that

$$\frac{dM_1(t)}{dt} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} nA_{nm}P(m, t). \tag{9}$$

A comparison of Eqs. (7) and (8) and use of the normalization (5) shows that the relation

$$\sum_{n=0}^{\infty} nA_{nm} = \beta m + \gamma \tag{10}$$

is a sufficient condition for the simple exponential relaxation (8) to hold. Since we consider here only stationary processes, i.e., A_{nm} is not a function of the time, and since all the other quantities appearing in Eq. (10) are independent of the time t, it is evident that condition (10) will hold for all time t. In addition, in order for Eq. (10) to be a sufficient condition for the validity of the moment relaxation equation (8) we require that the relation (10) hold for all values of m.

It can readily be shown that Eq. (10) is also a necessary condition. The initial condition for $P(n, t)$ can be chosen arbitrarily subject only to the conditions [see also Eq. (5)]

$$P(n, 0) \geq 0, \sum_{n=0}^{\infty} P(n, 0) = 1. \tag{11}$$

Let us then choose the special initial condition

$$P(s, 0) = 1; \quad P(j, 0) = 0 \quad \text{for all} \quad j \neq s. \tag{12}$$

Then from Eq. (9) it follows that

$$\left.\frac{dM_1(t)}{dt}\right|_{t=0} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} nA_{nm}P(m, 0) = \sum_{n=0}^{\infty} nA_{ns}. \tag{13}$$

Equation (8) becomes

$$\left.\frac{dM_1(t)}{dt}\right|_{t=0} = \beta M_1(0) + \gamma = \beta \sum_{n=0}^{\infty} nP(n, 0) + \gamma$$
$$= \beta s P(s, 0) + \gamma = \beta s + \gamma. \tag{14}$$

A comparison of the r.h.s. of Eqs. (13) and (14) shows that Eq. (10) is also a necessary condition.

As an example of the above relations we now discuss briefly the relaxation of $M_1(t)$ for a system of harmonic oscillators in weak interaction with a heat bath at temperature T. It has been shown in reference 1 that for such a system the transition probabilities A_{nm}, for transitions from m to n, are given by

$$(1/\kappa)A_{nm} = (n + 1)\, \delta_{n+1,m} - [n + (n + 1)e^{-\theta}]\, \delta_{nm} + ne^{-\theta}\, \delta_{n-1,m}, \tag{15}$$

where κ is a rate constant, the δ's are Kronecker deltas, and where $\theta = h\nu/kT$ with ν equal to the frequency of the oscillator. Substitution of (15) into the l.h.s. of Eq. (10) yields

$$\sum_{n=0}^{\infty} nA_{nm} = \kappa[(e^{-\theta} - 1)m + e^{-\theta}] = \beta m + \gamma, \tag{16}$$

which is of the correct form to give the exponential moment relaxation (8) with a "relaxation time" equal to $(-\beta)^{-1} = [\kappa(1 - e^{-\theta})]^{-1}$ as obtained in reference 1. Note that

$$\frac{\gamma}{\beta} = \frac{e^{-\theta}}{e^{-\theta} - 1} = -\left(\frac{1}{e^{\theta} - 1}\right) = -\frac{E_v(\infty)}{h\nu}, \qquad (17)$$

as required for the first moment

$$M_1(t) = h\nu \sum_{n=0}^{\infty} nP(n, t) = E_v(t),$$

where $E_v(t)$ is the vibrational energy of the oscillators at time t, to relax to its equilibrium value as $t \to \infty$.

III. RELAXATION OF THE MOMENTS $M_r(t)$

The development presented above can readily be extended to study the relaxation of the moments

$$M_r(t) \equiv \sum_{n=0}^{\infty} n^r P(n, t).$$

Specifically, we ask under what conditions on the A_{nm} the first k moments $M_1(t)$, $M_2(t)$, $\cdots$, $M_k(t)$ satisfy the *closed* system of linear equations

$$\begin{aligned}
\frac{dM_1(t)}{dt} &= \beta_{11}M_1(t) + \beta_{12}M_2(t) + \cdots + \beta_{1k}M_k(t) + \gamma_1 \\
\frac{dM_2(t)}{dt} &= \beta_{21}M_1(t) + \beta_{22}M_2(t) + \cdots + \beta_{2k}M_k(t) + \gamma_2 \\
&\vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\quad \vdots \\
\frac{dM_k(t)}{dt} &= \beta_{k1}M_1(t) + \beta_{k2}M_2(t) + \cdots + \beta_{kk}M_k(t) + \gamma_k.
\end{aligned} \qquad (18)$$

In vector notation Eqs. (18) become

$$d\mathbf{M}(t)/dt = \mathbf{BM} + \mathbf{G}. \qquad (19)$$

The time evolution of the rth moment is given, in analogy with Eq. (9), by

$$\frac{dM_r(t)}{dt} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} n^r A_{nm} P(m, t). \qquad (20)$$

If now the transition probabilities A_{nm}, in analogy to Eq. (10), obey the relation[4]

$$\sum_{n=0}^{\infty} n^r A_{nm} = \gamma_r + \beta_{r1}m + \beta_{r2}m^2 + \cdots + \beta_{rk}m^k \qquad (21)$$

for all $r = 1, 2, \cdots k$, then the moment relaxation equation (20) becomes

$$dM_r(t)/dt = \gamma_r + \beta_{r1}M_1(t) + \beta_{r2}M_2(t) + \cdots + \beta_{rk}M_k(t). \qquad (22)$$

This is of the form of Eqs. (18) so that the relation (21) on the A_{nm} is a sufficient condition for Eqs. (18) to hold. That relation (21) is also a necessary condition can easily be verified by repeating the development in Eqs. (11) through (14).

As a specific example, we shall again discuss the relaxation of a system of harmonic oscillators with A_{nm} given by Eq. (15). Substitution of A_{nm} into the l.h.s. of Eq. (21) yields

$$\begin{aligned}
\frac{1}{\kappa}\sum_{n=0}^{\infty} n^r A_{nm} &= m(m-1)^r \\
&- \{m^r[m + (m+1)e^{-\theta}] + (m+1)^{r+1}e^{-\theta}\},
\end{aligned} \qquad (23)$$

Performing the indicated expansions then yields a polynomial of rth degree in m

$$\begin{aligned}
\frac{1}{\kappa}\sum_{n=0}^{\infty} n^r A_{nm} &= r(e^{-\theta} - 1)m^r \\
&+ \tfrac{1}{2}[r^2(e^{-\theta} + 1) + r(e^{-\theta} - 1)]m^{r-1} + \cdots + e^{-\theta},
\end{aligned} \qquad (24)$$

which is of the form (21). That the higher moments for a system of relaxing harmonic oscillators form a closed system of equations where the factorial moments, f_m, depend only upon the mth and lower moments has been shown by Montroll and Shuler[1] who obtained the equation

$$df_m/dt + m(1 - e^{-\theta})f_m = m^2 e^{-\theta} f_{m-1} \qquad (25)$$

for the factorial moments

$$f_m(t) \equiv \sum_{n=0}^{\infty} n(n-1)\cdots(n-m+1)P(n, t) \qquad m = 1, 2, \cdots k \qquad (26)$$

The formal general solution of the moment equation (19) is

$$\begin{aligned}
\mathbf{M}(t) &= e^{\mathbf{B}t}\mathbf{M}(0) + e^{\mathbf{B}t}\int_0^t e^{-\mathbf{B}\tau}\, d\tau\mathbf{G} \\
&= e^{\mathbf{B}t}\mathbf{M}(0) + e^{\mathbf{B}t}\mathbf{B}^{-1}(\mathbf{I} - e^{-\mathbf{B}t})\mathbf{G}
\end{aligned} \qquad (27)$$

To evaluate $\mathbf{M}(t)$ explicitly it will be necessary to find the eigenvalues of the matrix $\mathbf{B}$. A particularly simple case arises when $\beta_{rj} = 0$ for $r < j$ where then the rth moment, $M_r(t)$ depends only on the lower moments $M_{r-i}(t)$, with $i = 0, 1, \cdots r - 1$. Under this condition, $\mathbf{B}$ assumes the triangular form

[4] Note that for $r = 0$,

$$\sum_{n=0}^{\infty} n^r A_{nm} = \sum_{n=0}^{\infty} A_{nm} = 0$$

as can readily be seen from Eqs. (4) and (5). This is a consequence of the conservation of particles (mass) during the relaxation.

$$\mathbf{B} = \begin{bmatrix} \beta_{11} & 0 & \cdots & 0 \\ \beta_{21} & \beta_{22} & 0 & \cdots & 0 \\ \vdots & & & & \\ \beta_{k1} & \beta_{k2} & \cdots & \beta_{kk} \end{bmatrix}. \tag{28}$$

For $\beta_{11} \neq \beta_{22} \neq \cdots \beta_{kk}$, the eigenvalues of $\mathbf{B}$ are distinct and are, explicitly,

$$\lambda_1 = \beta_{11}, \qquad \lambda_2 = \beta_{22}, \cdots, \lambda_k = \beta_{kk}, \tag{29}$$

and by the Lagrange-Sylvester interpolation formula one then finds

$$\mathbf{M}(t) = \sum_{j=1}^{k}{}' \frac{(\mathbf{B} - \beta_{11}\mathbf{I}) \cdots (\mathbf{B} - \beta_{kk}\mathbf{I})}{(\beta_{jj} - \beta_{11}) \cdots (\beta_{jj} - \beta_{kk})} \cdot \left[e^{\beta_{jj}t}\mathbf{M}_k(0) + \frac{(e^{\beta_{jj}t} - 1)}{\beta_{jj}} \mathbf{G} \right], \tag{30}$$

where the prime indicates that the term $\mathbf{B} - \beta_{jj}\mathbf{I}$ is missing from the numerator and the zero term is missing from the denominator. Simple analytical forms for $\mathbf{M}(t)$ can also be obtained for other special cases of the matrix $\mathbf{B}$ for which the eigenvalues λ_i can be evaluated.

IV. RELAXATION OF THE MOMENTS NEAR EQUILIBRIUM

In an attempt to reduce the relaxation of physical systems to a mathematically amenable basis, the assumption is made frequently that the relaxation of some of the macroscopic variables related to the moments of the distribution such as temperature, momentum, number density, etc., follows the simple exponential course given by Eq. (2). The classic example of this is, of course, Newton's law of cooling

$$dT(t)/dt = -\alpha[T(t) - T(\infty)] \tag{31}$$

but more sophisticated and recent examples can be found in the literature. As discussed above, such a simple exponential relaxation will be found only under special conditions and certainly not in general.

Near equilibrium, however, such a simple exponential relaxation will be found to hold, to a good approximation, for all moments $M_r(t)$ for systems whose time evolution is described by the master equations (1) *or* (6), *irrespective of the forms of the A_{nm}.* As $t \to \infty$, one can neglect, to a good approximation, all but the lowest (nonzero) eigenvalue λ_1 of the expansion (3) and write[5]

$$P(n, t) \mid_{t\to\infty} \cong c_0\mu_0(n) + c_1\mu_1(n)e^{-\lambda_1 t}. \tag{32}$$

[5] As has been shown in reference (3), all the eigenvalues are real.

From the definition of the moments

$$M_r(t) \equiv \sum_{n=0}^{\infty} n^r P(n, t)$$

one then finds that

$$\left.\frac{dM_r(t)}{dt}\right|_{t\to\infty} = -\lambda_1 c_1 e^{-\lambda_1 t} \sum_{n=0}^{\infty} n^r \mu_1(n). \tag{33}$$

From (32) one obtains

$$M_r(t) \mid_{t\to\infty} = M_r(\infty) = c_0 \sum_{n=0}^{\infty} n^r \mu_0(n), \tag{34}$$

so that

$$M_r(t) \mid_{t\to\infty} = M_r(\infty) + c_1 e^{-\lambda_1 t} \sum_{n=0}^{\infty} n^r \mu_1(n). \tag{35}$$

The use of (35) in Eq. (33) then yields

$$\left.\frac{dM_r(t)}{dt}\right|_{t\to\infty} = -\lambda_1[M_r(t) - M_r(\infty)], \tag{36}$$

which is of the same form as Eq. (2). In this development, we assume that all the moments $M_r(t)$ exist. Since macroscopic state variables can be expressed in terms of the moments of the probability distribution,[6] simple exponential relaxation laws for these state variables will be found to hold near equilibrium.

V. RELAXATION OF THE MOMENTS $M_1(t)$ AND $M_2(t)$ OF THE FOKKER-PLANCK EQUATION

We shall now consider the relaxation of the moments

$$\begin{aligned} M_1(t) &\equiv \int_0^\infty xP(x, t)\, dx \\ M_2(t) &\equiv \int_0^\infty x^2 P(x, t)\, dx \end{aligned} \tag{37}$$

of the Fokker-Planck (F-P) equation

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial}{\partial x}[b_1(x)P(x, t)] + \tfrac{1}{2}\frac{\partial^2}{\partial x^2}[b_2(x)P(x, t)], \tag{38}$$

with[7]

$$b_1 = \int_0^\infty (y - x)A(y, x)\, dy \tag{39}$$

$$b_2 = \int_0^\infty (y - x)^2 A(y, x)\, dy. \tag{40}$$

[6] In the case of translational relaxation, for instance, the zeroth moment is proportional to the density, the first moment to the momentum, and the second moment to the temperature since $kT \sim \langle mv^2 \rangle \equiv m \sum_v v^2 P(v, t)$.

[7] We shall assume here, to be consistent with the previous discussion on the discrete master equation, that the range of the continuous variable y extends from 0 to ∞.

As is well known[8] the F-P Eq. (38) can readily be derived from the master equation (6) under certain restrictive assumptions on the form of the moments $b_n(x)$ and the probability distribution $P(x, t)$.

A. Relaxation of the Moment $M_1(t)$

To obtain the relaxation equation for the first moment $M_1(t)$ defined in Eq. (37) we multiply the F-P Eq. (38) by x and integrate over all x:

$$\int_0^\infty \frac{\partial[xP(x, t)]}{\partial t}\,dx = \frac{dM_1(t)}{dt} = -\int_0^\infty x\,\frac{\partial}{\partial x}\,[b_1(x)P(x, t)]\,dx + \tfrac{1}{2}\int_0^\infty x\,\frac{\partial^2}{\partial x^2}\,[b_2(x)P(x, t)]\,dx. \quad (41)$$

Partial integration on the r.h.s. of Eq. (41) leads to

$$\frac{dM_1(t)}{dt} = -[xb_1(x)P(x, t)]\Big|_0^\infty + \int_0^\infty b_1(x)P(x, t)\,dx + \frac{1}{2}\left[xP(x, t)\,\frac{\partial b_2(x)}{\partial x} + xb_2(x)\,\frac{\partial P(x, t)}{\partial x}\right]\Big|_0^\infty - \tfrac{1}{2}[b_2(x)P(x, t)]\Big|_0^\infty. \quad (42)$$

In order to arrive at the moment relaxation equation (8) we must impose some general conditions on the distribution function $P(x, t)$ and the coefficient $b_2(x)$:

(i) $b_2(x)$ can be represented as a polynomial in x without a constant term.[9]

(ii) $P(x, t)$ goes to zero sufficiently rapidly as $x \to \infty$ that all the bracketed terms in (42) go to zero at the upper limit $x = \infty$.

Under these conditions, all the bracketed terms in Eq. (42) go to zero at both limits and Eq. (42) reduces to

$$\frac{dM_1(t)}{dt} = \int_0^\infty b_1(x)P(x, t)\,dx. \quad (43)$$

If we make use of the continuum analog of the normalization (5), i.e.,

$$\int_0^\infty P(x, t)\,dx = 1, \quad (44)$$

it follows that the necessary and sufficient condition for the exponential relaxation of $M_1(t)$ is

$$b_1(x) = \beta_1 x + \gamma_1. \quad (45)$$

As an example of this relation we shall again consider our previous example of the relaxation of a system of harmonic oscillators in a heat bath. The F-P equation for the relaxation of a system of classical oscillators in a heat bath has been found to be,[10] using our present notation,

$$\frac{1}{k_{10}}\,\frac{\partial P(x, t)}{\partial t} = -\frac{\partial}{\partial x}\,[(1 - \theta x)P(x, t)] + \frac{1}{2}\,\frac{\partial^2}{\partial x^2}\,[2xP(x, t)], \quad (46)$$

where k_{10} is a rate constant and where $P(x, t)\,dx$ is the probability that the oscillators will have an energy between $h\nu x$ and $h\nu\ (x + dx)$ at time t. Rubin and Shuler have shown[10] that the relaxation of the first moment, the mean vibrational energy $\langle E_v\rangle = h\nu \int_0^\infty xP(x, t)\,dx$, is indeed exponential with β of Eq. (8) given by $(-k_{10}\theta)$. A comparison of the condition (45) with the $b_1(x)$ of Eq. (46) shows that $b_1(x)$ is of the proper form and that $\beta_1 = -k_{10}\theta$ as required. In addition, it will be noted that $b_2(x) = 2x$ is of the proper form in being a polynomial in x without a constant term.

B. Relaxation of the Moment $M_2(t)$

The relaxation equation for the second moment $M_2(t)$ defined in Eq. (37) is obtained in a manner completely analogous to that used for $M_1(t)$. We multiply the F-P Eq. (38) by x^2 and integrate over all x to obtain

$$\int_0^\infty \frac{\partial[x^2P(x, t)]}{\partial t}\,dx = \frac{dM_2(t)}{dt} = -\int_0^\infty x^2\,\frac{\partial}{\partial x}\,[b_1(x)P(x, t)]\,dx + \frac{1}{2}\int_0^\infty x^2\,\frac{\partial^2}{\partial x^2}\,[b_2(x)P(x, t)]\,dx. \quad (47)$$

Partial integration of the r.h.s. of Eq. (47) leads to

$$\frac{dM_2(t)}{dt} = \int_0^\infty P(x, t)[2xb_1(x) + b_2(x)]\,dx - [x^2b_1(x)P(x, t)]\Big|_0^\infty + \frac{1}{2}\left[x^2b_2(x)\,\frac{\partial P(x, t)}{\partial x} + x^2P(x, t)\,\frac{\partial b_2(x)}{\partial x}\right]\Big|_0^\infty - [xb_2(x)P(x, t)]\Big|_0^\infty. \quad (48)$$

[8] See, e.g., N. G. van Kampen, Ned. Tijdschr. Natuurk. **26**, 225 (1960); Can. J. Phys. **30**, 551 (1961).

[9] The absence of a constant term is necessary for the last bracketed term in (42) to go to zero at the limit $x = 0$. If the range of the variable x is from $-\infty$ to ∞, no assumption has to be made about the form of $b_2(x)$ provided that $P(x, t)$ also goes to zero sufficiently rapidly as $x \to -\infty$.

[10] R. J. Rubin and K. E. Shuler, J. Chem. Phys. **25**, 59 (1956).

Making use again of our assumption (ii) on the form of the $P(x, t)$ we find that the bracketed terms in Eq. (48) vanish since they go to zero at both the upper and lower limit.[11] Equation (48) then reduces to

$$\frac{dM_2(t)}{dt} = \int_0^\infty P(x, t)[2xb_1(x) + b_2(x)]\, dx. \tag{49}$$

For $M_2(t)$ to follow a simple exponential relaxation, i.e.,

$$dM_2(t)/dt = \beta_{22}M_2(t) + \gamma_2, \tag{50}$$

the necessary and sufficient conditions on the $b_1(x)$ and $b_2(x)$ are found to be

$$2xb_1(x) + b_2(x) = \beta_{22}x^2 + \gamma_2. \tag{51}$$

For $M_2(t)$ to follow the relaxation law given in Eqs. (18), i.e.,

$$dM_2(t)/dt = \beta_{22}M_2(t) + \beta_{21}M_1(t) + \gamma_2, \tag{52}$$

the necessary and sufficient conditions on the $b_1(x)$ and $b_2(x)$ are found to be

$$2xb_1(x) + b_2(x) = \beta_{22}x^2 + \beta_{21}x + \gamma_2. \tag{53}$$

If $b_1(x)$ is given by Eq. (45), i.e., $M_1(t)$ undergoes a simple exponential relaxation, then $b_2(x)$ in Eq. (53) will be a quadratic polynomial in x.

As an example of the relaxation of the second moment $M_2(t)$ for a system described by a F-P equation of the form of Eq. (38), we consider the relaxation of the mean translational energy $\langle E_t \rangle$ of a dilute electron gas dispersed in a heat bath of molecules. For this example of a Rayleigh gas the Fokker-Planck equation for the electron distribution function $f(v, t)$ can be written, using certain assumptions about the electron-molecule collision cross sections, as[12]

$$\frac{\partial f(v, t)}{\partial t} = \frac{A}{v^2}\frac{\partial}{\partial v}\left\{\frac{kT}{M}v^2\frac{\partial f(v, t)}{\partial v} + \frac{m}{M}v^3 f(v, t)\right\}, \tag{54}$$

where A is a constant, m is the mass of the electron, and M is the mass of the heavy molecule. Using the transformation $v^2 f(v, t) = P(v, t)$, Eq. (54) can be rewritten as

$$\frac{\partial P(v, t)}{\partial t} = -\frac{A}{M} \times \left\{\frac{\partial}{\partial v}\left[\left(\frac{2kT}{v} - mv\right)P(v, t)\right] + kT\frac{\partial^2 P(v, t)}{\partial v^2}\right\}, \tag{55}$$

where $P(v, t)\, dv$ is the probability that an electron has a velocity between v and $v + dv$ at time t and where $P(v, t)$ is normalized as shown in Eq. (44). From Eq. (55) we find

$$\begin{aligned} b_1(v) &= (A/M)(2kT/v - mv) \\ b_2(v) &= 2(A/M)kT. \end{aligned} \tag{56}$$

Combining these quantities as shown in the condition (51) we obtain

$$2vb_1(v) + b_2(v) = (2A/M)(3kT - mv^2), \tag{57}$$

which is clearly of the required form with

$$\begin{aligned} \beta_{22} &= -2Am/M \\ \text{and} \qquad \gamma_2 &= 6AkT/M. \end{aligned} \tag{58}$$

We should therefore predict an exponential relaxation for the second moment

$$M_2(t) = \int_0^\infty v^2 P(v, t)\, dv = \frac{2}{3m}\langle E_t(t)\rangle$$

of the electron gas with a relaxation time $-\beta_{22}^{-1}$ given by

$$-\beta_{22}^{-1} = \tfrac{1}{2}M/Am. \tag{59}$$

This is indeed the result obtained by Osipov[12] by another method.[13] Note that

$$\gamma_2/\beta_{22} = -3kT/m = -\langle E_t(\infty)\rangle 2/m, \tag{60}$$

as required [see also Eq. (17)] for the mean translational energy to relax to its equilibrium value as $t \to \infty$.[14]

The development presented in this section provides a convenient and easy test of the relaxation of the moments of distribution functions whose temporal development is described by the F-P equation (38). If the relations (45), (51), or (53) hold for the coefficients $b_1(x)$ and $b_2(x)$, then the moments relax according to Eqs. (8), (50), or (52). The relaxation times $-\beta_1^{-1}$ and $-\beta_{22}^{-1}$ are, respectively, the reciprocals of the coefficients of x and x^2 in Eqs. (45) and (51), and the equilibrium values of the moments, $M_1(\infty)$ and $M_2(\infty)$, are, respectively, $(-\gamma_1/\beta_1)$ and $(-\gamma_2/\beta_{22})$. It is thus possible to write down the explicit expressions for the relaxation of the moments

[11] Note that we can dispense here with the requirement that the constant term in the polynomial $b_2(x)$ be equal to zero. The last term in Eq. (48) will go to zero at the lower limit even with a nonzero constant term in the polynomial $b_2(x)$ since $b_2(x)P(x, t)$ is now multiplied by x.

[12] S. L. Kahalas and H. C. Kashian, Phys. Fluids **2**, 100 (1959); D. I. Osipov, Bull. of the Moscow Univ., Series III **1**, 13 (1961) (in Russian).

[13] Our β_{22} is Osipov's α and our A is his V/λ. Osipov was concerned with the relaxation of the translational temperature of a relaxing Maxwellian velocity distribution of electrons which is, of course, proportional to the mean energy (see footnote 6).

[14] The results of Keilson and Storer, Quart. Appl. Math **10**, 243 (1952) on the relaxation of $M_1(t)$ and $M_2(t)$ for the velocity distribution of the Brownian Motion F-P equation are also in complete agreement with the results presented above.

without a knowledge of the distribution function $P(x, t)$ from the solution of the Fokker-Planck equation. If none of the relations (45), (51), or (53) are found to hold, then one at least knows that the moments $M_1(t)$ and $M_2(t)$ do not obey the simple relaxation equations (8), (50), or (52).

C. Equivalence of the Conditions on the A_{nm} the $A(y, x)$

We now wish to demonstrate that the conditions (45), (51), and (53) are completely equivalent to the previously derived conditions (10) and (21) on the A_{nm}. If we perform the indicated integrations in Eqs. (39) and (40) for the moments $b_1(x)$ and $b_2(x)$ we obtain

$$b_1(x) = \int_0^\infty yA(y, x)\, dy \tag{61}$$

and

$$b_2(x) = \int_0^\infty y^2 A(y, x)\, dy - 2x \int_0^\infty yA(y, x)\, dy, \tag{62}$$

where we have made use of the result[4] that $\int_0^\infty A(y, x)\, dy = 0$. The integrals in Eqs. (61) and (62) are the continuums analogs of the summation

$$\sum_{n=0}^{\infty} nA_{nm} \quad \text{and} \quad \sum_{n=0}^{\infty} n^2 A_{nm}$$

in the expressions (10) and (21). If we now assume that the necessary and sufficient conditions on the A_{nm} of Eqs. (10) and (21) also apply to the $A(y, x)$, i.e.,

$$\int_0^\infty yA(y, x)\, dy = \beta_1 x + \gamma_1 \tag{63}$$

$$\int_0^\infty y^2 A(y, x)\, dy = \beta_{22}x^2 + \beta_{21}x + \gamma_2, \tag{64}$$

we obtain, from (61) and (62),

$$b_1(x) = \beta_1 x + \gamma_1 \tag{65}$$

$$b_2(x) = x^2(\beta_{22} - 2\beta_1) + x(\beta_{21} - 2\gamma_1) + \gamma_2. \tag{66}$$

Note that Eq. (65) is identical with Eq. (45). Multiplication of Eq. (65) by $2x$ and addition to Eq. (66) leads to

$$2xb_1(x) + b_2(x) = \beta_{22}x^2 + \beta_{21}x + \gamma_2, \tag{67}$$

which is identical with Eq. (53). For the simple exponential relaxation of $M_2(t)$ as given by Eq. (50), it is necessary that $\beta_{21} = 0$. Under this condition Eq. (67) becomes identical with Eq. (51). The conditions (63) and (64) on the $A(y, x)$ are thus equivalent to the conditions (45), (51), and (53) on the coefficients $b_1(x)$ and $b_2(x)$ of the F-P equation.

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Double-Tensor Operators for Configurations of Equivalent Electrons*

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To every irreducible representation W of the rotation group in $2l + 1$ dimensions that is used to classify states of the electronic configurations l^n, there correspond two couples (v, S), where v and S stand for the seniority number and total spin, respectively. Determinantal product states are introduced to examine this correspondence in detail. It is shown that for two double tensors $\mathbf{W}^{(\kappa k)}$ and $\mathbf{W}^{(\kappa' k)}$, the set of reduced matrix elements

$$(l^n v_1 W \xi S_1 L \,||W^{(\kappa k)}||\, l^n v_1' W' \xi' S_1' L'),$$

for fixed n, v_1, v_1', W, and W', is proportional to the set

$$(l^n v_2 W \xi S_2 L \,||W^{(\kappa' k)}||\, l^n v_2' W' \xi' S_2' L'),$$

where ξ and ξ' are additional labels that may be required to define the states uniquely, provided (a) the two couples (v_1, S_1) and (v_2, S_2) are distinct, (b) the two couples (v_1', S_1') and (v_2', S_2') are distinct, and (c) the sum $\kappa + \kappa' + k$ is odd. The amplitudes of the double tensors are chosen so that the constant of proportionality is equal to the ratio of two 3-j symbols, multiplied by a phase factor. An explicit expression for this factor is given for f electrons, and a number of applications are discussed.

I. SYMMETRY

CONJUGATE electronic configurations of the type l^n and l^{4l+2-n} share many properties. Perhaps the most familiar is the occurrence of identical term schemes; as a consequence of this, a table of the terms occurring in the configurations l^0, l^1, l^2, $\cdots$, l^{4l+2} exhibits a symmetry about the half filled shell, l^{2l+1}. A glance at Table I[7] of Condon and Shortley,[1] which lists the terms of all configurations of the type p^n, d^n, and f^n, makes it obvious that other kinds of symmetry exist. The most striking is the symmetry with respect to L (the quantum number of the total orbital angular momentum) of the terms of maximum multiplicity about the quarter- and three-quarter-filled shells. For example, the terms of f^5 with S (the quantum number of the total spin angular momentum) equal to 5/2 are ^6P, ^6F, and ^6H; while those of f^2 with S equal to 1 are ^3P, ^3F, and ^3H. At first sight, it appears difficult to find similar types of symmetry for terms possessing less than the maximum value of S. However, this is because the quantum number that should be associated with a sequence of L values is not S, but M_S. With this clue, we can uncover a large number of symmetries of a rather spectacular kind in Condon and Shortley's table; for example, the L values of the terms of f^5 that can produce components with $M_S = \pm 3/2$, namely,

$$SP^3D^3F^5G^4H^4I^3K^2LM, \tag{1}$$

are precisely the same as the L values of the terms of f^4 that can produce components with $M_S = \pm 1$. [The superscript to a letter of the sequence (1) indicates the number of times the corresponding L value occurs.]

We can gain some understanding of the recurrence of a sequence of L values by listing the irreducible representations W of R_{2l+1}, the rotation group in $2l + 1$ dimensions, to which the representation $\mathfrak{D}_L$ of R_3 belong. From Table 2 of Elliott *et al.*,[2] we find, for example, that sequence (1) corresponds to the irreducible representations (110), (211), and (111) of R_7, both for f^4 and f^5. The problem of explaining why certain sequences of L values recur in different configurations can thus be made equivalent to the problem of explaining why certain sequences of W values recur. In the latter form, the problem is seen to be closely connected to an observation of Racah,[3] namely, that to every representation W of the type used in classifying states of l^n, there correspond two values of the couple (v, S), where v stands for the seniority. If we denote two such couples by (v_1, S_1) and (v_2, S_2), then, according to Eq. (54) of Racah,[3]

$$v_1 + 2S_2 = v_2 + 2S_1 = 2l + 1. \tag{2}$$

For the representations (110), (211), and (111) of our example, we find, from Table 2 of Elliott

* Work done under the auspices of the U. S. Atomic Energy Commission.

[1] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, New York, 1935).

[2] J. P. Elliott, B. R. Judd, and W. A. Runciman, Proc. Roy. Soc. (London) **A240**, 509 (1957).

[3] G. Racah, Phys. Rev. **76**, 1352 (1949).

et al.,[2] that the couples (v, S) are (5, 5/2), (5, 3/2), and (3, 3/2) for f^5 and (2, 1), (4, 1), and (4, 2) for f^4.

In themselves, the symmetries with respect to L possess little more than a curiosity value. Our reason for introducing them lies in the hope that they will lead to symmetries with respect to matrix elements. It is well known that the matrix elements of most operators exhibit simple symmetry properties about the half-filled shell, and for states of maximum multiplicity it is usually not difficult to derive relations between matrix elements in symmetrical positions on either side of the quarter- or three-quarter-filled shell [see, for example, Eq. (15) of Judd[4]]. It therefore seems reasonable to anticipate analogous relations for other types of symmetry. This expectation is strengthened by Eq. (73) of Racah,[3] which relates matrix elements of the part e_2 of the Coulomb interaction between states defined by one couple (v_1, S_1) to those between states defined by the corresponding couple (v_2, S_2). Furthermore, Wybourne[5] has shown that many matrix elements of the spin-orbit interaction between states belonging to the two representations W and W' of R_7 are proportional to similar matrix elements in other configurations. Some of his results are examples of Eqs. (67) and (69b) of Racah,[6] and are of no interest here; of the others, in each case the pair of couples (v_1, S_1) and (v_2, S_2) corresponding to W, and also the pair (v_1', S_1') and (v_2', S_2') corresponding to W', separately satisfy Eqs. (2).

The first aim of this paper is to explore the symmetries within configurations of the type l^n. Most single-particle interactions of atomic spectroscopy can be concisely expressed as the components of double tensors, and the second objective is to derive relations between the matrix elements of such operators. Since the spin-orbit interaction is the scalar part of a double tensor of rank one with respect to spin, and of similar rank with respect to orbit, the second part of the program can be regarded as a generalization of Wybourne's[5] work to arbitrary double tensors.

II. DOUBLE TENSORS

In order to define the operators with which we shall be concerned, we first introduce the tensors $\mathbf{t}^{(\kappa)}$ and $\mathbf{v}^{(k)}$ that act in the spin and orbital spaces, respectively, of a single electron, and for which

$$(s\,||t^{(\kappa)}||\,s) = (2\kappa + 1)^{\frac{1}{2}}$$

and

$$(l\,||v^{(k)}||\,l) = (2k + 1)^{\frac{1}{2}}.$$

The $(2\kappa + 1)(2k + 1)$ products

$$w_{\pi q}^{(\kappa k)} = t_{\pi}^{(\kappa)} v_q^{(k)} \qquad (-\kappa \leq \pi \leq \kappa;\ -k \leq q \leq k)$$

form the components of the double tensor $\mathbf{w}^{(\kappa k)}$, for which

$$(sl\,||w^{(\kappa k)}||\,sl) = (2\kappa + 1)^{\frac{1}{2}}(2k + 1)^{\frac{1}{2}}. \tag{3}$$

Many-electron tensor operators for the configuration l^n can be easily constructed by summing the operators for the n individual electrons; thus

$$\mathbf{W}^{(\kappa k)} = \sum_i (\mathbf{w}^{(\kappa k)})_i$$

and

$$\mathbf{V}^{(k)} = \sum_i (\mathbf{v}^{(k)})_i.$$

We note

$$\mathbf{V}^{(k)} = \mathbf{W}^{(0k)}\sqrt{2}.$$

The set of quantum numbers $WSLM_SM_L$ is not always sufficient to specify a state of l^n completely. We therefore include the additional symbol ξ; for f electrons this can often be replaced by an irreducible representation U of the group G_2.[3] All reduced matrix elements of $\mathbf{W}^{(\kappa k)}$ can be calculated by means of the formula

$$\begin{aligned}(l^n W\xi SL\,||W^{(\kappa k)}||\,l^n W'\xi' S'L') &= n[(2S + 1)(2\kappa + 1)(2S' + 1)(2L + 1)\\ &\quad\times (2k + 1)(2L' + 1)]^{\frac{1}{2}}\\ &\quad\times \sum_{\bar{\psi}} (\psi\{|\,\bar{\psi})(\psi'\{|\,\bar{\psi})(-1)^{\tau}\\ &\quad\times \begin{Bmatrix} S & \kappa & S' \\ s & \bar{S} & s \end{Bmatrix}\begin{Bmatrix} L & k & L' \\ l & \bar{L} & l \end{Bmatrix},\end{aligned} \tag{4}$$

where

$$\tau = \bar{S} + s + S + \kappa + \bar{L} + l + L + k,$$

and where ψ, ψ', and $\bar{\psi}$ are abbreviations for $W\xi SL$, $W'\xi'S'L'$, and $\bar{W}\bar{\xi}\bar{S}\bar{L}$, respectively. However the construction of the fractional parentage coefficients $(\psi\{|\,\bar{\psi})$ and $(\psi'\{|\,\bar{\psi})$, and the summation over the parent terms $\bar{\psi}$, are often extremely tedious to perform. In seeking to establish relations between different reduced matrix elements, we aim to circumvent this procedure as much as possible.

III. DETERMINANTAL PRODUCT STATES

In Sec. I we mentioned the correspondence between the states f^5 with $M_S = \pm 3/2$, and those

[4] B. R. Judd, Phys. Rev. **125**, 613 (1962).
[5] B. G. Wybourne, J. Chem. Phys. **35**, 334 (1961).
[6] G. Racah, Phys. Rev. **63**, 367 (1943).

of f^4 with $M_S = \pm 1$. For both configurations, the state for which $M_L = L = 9$ can be expressed as a single determinantal product state. However, without examining the phases of our states in detail, we cannot be sure whether, for example, we should identify

$$|f^5, {}^4M, M_S = -3/2, M_L = 9)$$

with

$$\{3^+, 3^-, 2^-, 1^-, 0^-\}$$

or with

$$-\{3^+, 3^-, 2^-, 1^-, 0^-\}.$$

We shall return to questions of phase later. For the moment, we avoid the difficulty by introducing the new states

$$|l^n W\xi SLM_S M_L\rangle$$

characterized by angular brackets, whose phases are at our disposal. We can therefore write

$$|f^5, {}^4M, M_S = -3/2, M_L = 9\rangle \equiv \{3^+, 0^-, 1^-, 2^-, 3^-\} \quad (5)$$

and

$$|f^4, {}^3M, M_S = -1, M_L = 9\rangle \equiv \{3^+, 1^-, 2^-, 3^-\}. \quad (6)$$

Operating on Eq. (5) with $W^{(12)}_{0-2}$, and using Eq. (3), we find

$$\begin{aligned} W^{(12)}_{0-2}\,|f^5, {}^4M, M_S = -3/2, M_L = 9\rangle &\equiv (5/84)^{\frac{1}{2}}\{1^+, 0^-, 1^-, 2^-, 3^-\} \\ &+ (5/42)^{\frac{1}{2}}\{3^+, -2^-, 1^-, 2^-, 3^-\} \\ &+ (1/7)^{\frac{1}{2}}\{3^+, -1^-, 0^-, 2^-, 3^-\}. \end{aligned} \quad (7)$$

Similarly, from Eq. (6), we get

$$\begin{aligned} W^{(02)}_{0-2}\,|f^4, {}^3M, M_S = -1, M_L = 9\rangle &\equiv (5/84)^{\frac{1}{2}}\{1^+, 1^-, 2^-, 3^-\} \\ &+ (5/42)^{\frac{1}{2}}\{3^+, 1^-, 0^-, 3^-\} \\ &+ (1/7)^{\frac{1}{2}}\{3^+, -1^-, 2^-, 3^-\}. \end{aligned} \quad (8)$$

The striking similarity between Eqs. (7) and (8) prompts us to ask the following questions:

(i) Can the determinantal product states of f^5 for which $M_S = -3/2$ be put into a one-to-one correspondence with the determinatal product states of f^4 for which $M_S = -1$?

(ii) If (i) is true, what is its generalization?

(iii) If it can be established that the determinantal product state $\{a_\gamma\}$ of l^{n_a} corresponds to the unique determinantal product state $\{b_\gamma\}$ of l^{n_b}, and vice versa, what are the conditions on κ, k, q, κ', k', and q' if $c_{\gamma\rho}$ and $d_{\gamma\rho}$ in the expansions

$$W^{(\kappa k)}_{0q}\{a_\gamma\} = \sum_\rho c_{\gamma\rho}\{a_\rho\} \quad (9)$$

and

$$W^{(\kappa' k')}_{0q'}\{b_\gamma\} = \sum_\rho d_{\gamma\rho}\{b_\rho\} \quad (10)$$

are to satisfy

$$c_{\gamma\rho} = d_{\gamma\rho} \quad (11)$$

for all γ and ρ?

Questions (i) and (ii) can be taken together. Suppose that the g integers m_i ($i = 1, 2, \cdots, g$), constituting the set P_α, satisfy the inequalities

$$l \geq m_1 > m_2 > \cdots > m_i > \cdots > m_g \geq -l \quad (12)$$

and that the h integers m'_j ($j = 1, 2, \cdots, h$), constituting the set P'_β, satisfy the inequalities

$$l \geq m'_1 > m'_2 > \cdots > m'_i > \cdots > m'_h \geq -l. \quad (13)$$

We denote the combined set of $g + h$ integers by Q_γ. We can construct two determinantal product states, corresponding to any such set Q_γ, according to the following rules:

(a) Delete from

$$\{l^+, (l-1)^+, \cdots, (-l)^+, l^-, (l-1)^-, \cdots, (-l)^-\},$$

the state corresponding to a completely filled shell, those entries $(m_l)^+$ for which m_l coincides with a member of P_α, and also those entries $(m_l)^-$ for which m_l coincides with a member of P'_β.

(b) Delete from

$$\{l^+, (l-1)^+, \cdots, (-l)^+\},$$

the state corresponding to a half-filled shell with maximum M_S, those entries $(m_l)^+$ for which m_l is a member of P_α, and insert the sequence

$$(-m'_1)^-, (-m'_2)^-, \cdots, (-m'_h)^-$$

between $(-l)^+$ and the final bracket.

The resulting quantities, which we denote by $\{a_\gamma\}$ and $\{b_\gamma\}$, respectively, are

$$\begin{aligned} \{a_\gamma\} \equiv \{&l^+, \cdots, (m_i+1)^+, \\ &(m_i-1)^+, \cdots (-l)^+, l^-, \cdots, (m'_i+1)^-, \\ &(m'_i-1)^-, \cdots, (-l)^-\} \end{aligned} \quad (14)$$

and

$$\begin{aligned} \{b_\gamma\} \equiv \{&l^+, \cdots, (m_i+1)^+, \\ &(m_i-1)^+, \cdots, (-l)^+, (-m'_1)^-, \\ &(-m'_2), \cdots, (-m'_j)^-, \cdots, (-m'_h)^-\}. \end{aligned} \quad (15)$$

The first, $\{a_\gamma\}$, is a determinantal product state of $l^{4l+2-g-h}$; the second, $\{b_\gamma\}$, of $l^{2l+1-g+h}$. The values of M_S for these two states, which we write as M_{Sa} and M_{Sb}, are given by

$$M_{Sa} = \tfrac{1}{2}(h - g)$$

and

$$M_{Sb} = \tfrac{1}{2}(2l + 1 - g - h).$$

Upon writing

$$4l + 2 - g - h = n_a$$

and

$$2l + 1 - g + h = n_b,$$

we see

$$M_{Sa} = -\tfrac{1}{2}(2l + 1 - n_b) \tag{16}$$

and

$$M_{Sb} = -\tfrac{1}{2}(2l + 1 - n_a). \tag{17}$$

If two entries of a determinantal product state are interchanged, the state becomes multiplied by -1. Two determinantal product states, whose entries can be perfectly matched by a process of rearrangement, are equivalent. The inequalities (12) and (13) impose a standard ordering on the entries of the states (14) and (15), and guarantee that no two determinantal product states $\{a_\gamma\}$ and $\{a_\delta\}$, deriving from two distinct sets Q_γ and Q_δ, are equivalent. Similar remarks apply to states of the type $\{b_\gamma\}$. If we suppose l, g, and h to be fixed, it follows that to each state $\{a_\gamma\}$ of l^{n_a} there corresponds a unique state $\{b_\gamma\}$ of l^{n_b}, and vice versa. From inequalities (12) and (13), g and h are nonnegative integers, not exceeding $2l + 1$. Provided we restrict our attention to configurations l^n for which $n \leq 2l + 1$ —and, in view of the familiar symmetry with respect to the half-filled shell, nothing is gained by considering configurations in the second half of the shell—these conditions imply only that $n_a + n_b$ must be an odd integer greater than or equal to $2l + 1$. Given, then, two configurations l^{n_a} and l^{n_b} comprising an odd and an even number of electrons, the total number being at least $2l + 1$, the states of l^{n_a} for which M_S is determined by Eq. (16) can be put into a one-to-one correspondence with those of l^{n_b}, for which M_S is determined by Eq. (17). This statement answers questions (i) and (ii) above.

Having established a method for drawing correspondences between states of the types $\{a_\gamma\}$ and $\{b_\gamma\}$, it is straightforward to construct the right-hand sides of Eqs. (9) and (10) in detail, and to pick out corresponding coefficients $c_{\gamma\rho}$ and $d_{\gamma\rho}$. For Eq. (11) to be valid for arbitrary l, the conditions on κ, k, q, κ', k', and q' turn out to be

$$\begin{aligned} q' &= q, \\ k' &= k, \\ (-1)^{\kappa+\kappa'+k} &= -1. \end{aligned} \tag{18}$$

The last equation holds if $\kappa + \kappa' + k$ is odd. These equations provide the answers to question (iii).

IV. MATRIX ELEMENTS

The infinitesimal operators of the group R_{2l+1} can be taken to be $W_{0q}^{(0k)}$, where k is odd.[3] Any one of these operators, acting on a member $\{a_\gamma\}$ of the collection of determinantal product states of l^{n_a} with $M_S = M_{Sa}$, generates a linear combination of states of the collection. It follows that the collection of states $\{a_\gamma\}$ for all possible Q_γ forms a basis for a representation of R_{2l+1}. Now for every operation with $W_{0q}^{(0k)}$ on a state $\{a_\gamma\}$ of l^{n_a}, we can construct a corresponding operation on the state $\{b_\gamma\}$ of l^{n_b}. According to Eqs. (18), the appropriate operator is again the infinitesimal operator $W_{0q}^{(0k)}$ of R_{2l+1}. Hence the transformation properties of the basis functions $\{a_\gamma\}$ are identical to those of the basis functions $\{b_\gamma\}$. We conclude that the irreducible representations W, into which the two representations with these bases decompose, are also identical. This accounts for the recurrence of sequences of W values, the existence of which was mentioned in Sec. I.

The correspondence between the transformation properties of the two sets of basis functions $\{a_\gamma\}$ and $\{b_\gamma\}$ holds not only for R_{2l+1}, but also for any of its subgroups, since the infinitesimal operators of the latter can be chosen from those operators $W_{0q}^{(0k)}$ for which k is odd. The labels L and M_L can be interpreted as irreducible representations of R_3 and R_2; hence, given a particular expansion

$$|\, l^{n_a} v_1 W \xi S_1 L M_{Sa} M_L\rangle = \sum_\rho \lambda_\rho \{a_\rho\} \tag{19}$$

for l^{n_a}, we can be sure that the linear combination

$$\sum_\rho \lambda_\rho \{b_\rho\} \tag{20}$$

corresponds to the same set of quantum numbers W, L, and M_L. The symbol ξ can also be carried over if its choice influences the properties of the linear combination of determinantal product states with respect to the tensors $W_{0q}^{(0k)}$ for which k is odd. However, since either n_a or n_b is odd and the other even, the couple (v_2, S_2) associated with the expression (20) cannot be the same as (v_1, S_1). We may therefore write

$$|\, l^{n_b} v_2 W\xi S_2 L M_{S_b} M_L\rangle = \sum_\rho \lambda_\rho \{b_\rho\}, \qquad (21)$$

with the understanding the v_1, v_2, S_1, and S_2 satisfy Eqs. (2).

The construction of the matrix elements follows easily. If we operate on the right-hand sides of Eqs. (19) and (20) with $W^{(\kappa k)}_{0q}$ and $W^{(\kappa' k)}_{0q}$, respectively, where $\kappa + \kappa' + k$ is odd, the resultant linear combinations of determinantal product states correspond perfectly. The matrix elements are readily completed in a quite general fashion, and we obtain the result

$$\langle l^{n_a} v_1' W'\xi' S_1' L' M_{S_a} M_{L'} \,|W^{(\kappa k)}_{0q}|\, l^{n_a} v_1 W\xi S_1 L M_{S_a} M_L\rangle$$
$$= \langle l^{n_b} v_2' W'\xi' S_2' L' M_{S_b} M_{L'} \,|W^{(\kappa' k)}_{0q}|\, l^{n_b} v_2 W\xi S_2 L M_{S_b} M_L\rangle.$$

To bring the notation into line with that of Eq. (4), we reverse the labelings of the states, and replace the angular brackets by regular ones. The latter operation introduces a phase factor $(-1)^x$, where x is independent of κ, κ', and k. Passing to reduced matrix elements, we obtain

$$\frac{(l^{n_a} v_1 W\xi S_1 L \,||W^{(\kappa k)}||\, l^{n_a} v_1' W'\xi' S_1' L')}{(l^{n_b} v_2 W\xi S_2 L \,||W^{(\kappa' k)}||\, l^{n_b} v_2' W'\xi' S_2' L')}$$
$$= (-1)^{S_a - S_1 - M_{Sb} + M_{Sa} + x}$$
$$\times \begin{pmatrix} S_2 & \kappa' & S_2' \\ -M_{Sb} & 0 & M_{Sb} \end{pmatrix} \begin{pmatrix} S_1 & \kappa & S_1' \\ -M_{Sa} & 0 & M_{Sa} \end{pmatrix}^{-1}$$
$$= (-1)^{x + (n_b + v_2 - v_1 - n_a)/2}$$
$$\times \begin{pmatrix} \frac{1}{2}(2l + 1 - v_1) & \kappa' & \frac{1}{2}(2l + 1 - v_1') \\ \frac{1}{2}(2l + 1 - n_a) & 0 & -\frac{1}{2}(2l + 1 - n_a) \end{pmatrix}$$
$$\times \begin{pmatrix} \frac{1}{2}(2l + 1 - v_2) & \kappa & \frac{1}{2}(2l + 1 - v_2') \\ \frac{1}{2}(2l + 1 - n_b) & 0 & -\frac{1}{2}(2l + 1 - n_b) \end{pmatrix}^{-1} \qquad (22)$$

The last line of the above equation follows from Eqs. (2), (17), and (18). To complete the program outlined in the last paragraph of Sec. I we have but to determine x.

V. PHASE

Racah[3] has shown that the fractional parentage coefficients can be factorized according to

$$(\psi\{|\, \bar\psi) \equiv (l^n v W\xi S L\{|\, l^{n-1}\bar v \bar W \bar\xi \bar S \bar L)$$
$$= (l^n v S\{|\, l^{n-1}\bar v \bar S + l)(W\xi L \mid \bar W \bar\xi \bar L + l).$$

If the fractional parentage coefficients are always constructed as a product of these two parts, we can be sure that the second factor does not contain any hidden phase factors dependent on n. Under these conditions, we can often use Eq. (4) to gain information about x.

Suppose, for example, that we make the substitutions $\kappa = k = \kappa' = 1, v_1' = v_1 - 2$, and $S_1' = S_1 - 1$ in the reduced matrix elements of Eq. (22). Equations (2) must be satisfied by the primed quantities, and we deduce that $v_2' = v_2 + 2$, $S_2' = S_2 + 1$. The ratio of the reduced matrix elements can be related by Eq. (67) of Racah[6] to a ratio for which n_a and n_b assume the special values v_1 and $v_2 + 2$, respectively. The couple $(\bar v, \bar S)$ for the matrix element of the numerator can now be only $(v_1 - 1, S_1 - \frac{1}{2})$; that for the matrix element of the denominator, only $(v_2 + 1, S_2 + \frac{1}{2})$. Both of these couples correspond to the same $\bar W$; hence, if Eq. (4) is used to compute the ratio, the sum

$$\sum_{\bar L \bar\xi} (W\xi L \mid \bar W \bar\xi \bar L + l)(W'\xi' L' \mid \bar W \bar\xi \bar L + l)$$
$$\times (-1)^\sigma \begin{Bmatrix} L & 1 & L' \\ l & \bar L & l \end{Bmatrix}, \qquad (23)$$

where

$$\sigma = \bar L + l + L + 1,$$

occurs in both numerator and denominator, and therefore cancels. Equations (52) of Racah[3] give the magnitudes of the coefficients of the type

$$(l^n v S\{|\, l^{n-1}\bar v \bar S + l).$$

The phase of such a quantity is independent of n,[3] and following Racah, we denote it by $\epsilon(vS\{|\, \bar v \bar S)$. The result of the calculation is

$$\frac{(l^{n_a} v_1 W\xi S_1 L \,||W^{(11)}||\, l^{n_a} v_1 - 2\ W'\xi' S_1 + 1\ L')}{(l^{n_b} v_2 W\xi S_2 L \,||W^{(11)}||\, l^{n_b} v_2 + 2\ W'\xi' S_2 - 1\ L')}$$
$$= -\frac{\epsilon(v_1 S_1\{|\, v_1 - 1, S_1 - 1/2)\epsilon(v_1 - 2, S_1 + 1\{|\, v_1 - 1, S_1 - 1/2)}{\epsilon(v_2 S_2\{|\, v_2 + 1, S_2 + 1/2)\epsilon(v_2 + 2, S_2 - 1\{|\, v_2 + 1, S_2 + 1/2)}\, \Xi \qquad (24)$$

where

$$\Xi = \left[\frac{(n_a + 2 - v_1)(4l + 4 - n_a - v_1)(2S_1 - 1)2S_1(2S_1 + 1)}{(n_b - v_2)(4l + 2 - n_b - v_2)(2S_2 + 1)(2S_2 + 2)(2S_2 + 3)}\right]^{\frac{1}{2}}.$$

So much for the left-hand side of Eq. (22). The right-hand side, involving the ratio of two 3-j symbols, evaluates to

$$(-1)^{x+1}\Xi. \tag{25}$$

The immediate conclusion, independent of the choice made for the phases $\epsilon(vS\{|\ \bar{v}\bar{S})$, is that x is independent of ξ, ξ', L, and L', and depends solely on the spins and seniorities of the states involved in the matrix elements. Equations (2) permit us to narrow down the dependence simply to the seniorities.

The above analysis can be repeated for other special cases. There are not many to consider, since the seniorities and spins with common subscripts can differ by, at most, 2 and 1, respectively, if the matrix elements are not to vanish. If $S_1' = S_1$, however, $\bar{S}$ can sometimes assume two values, and we cannot be sure that the simple factorization that allowed us to cancel the summations (23) still prevails. This difficulty can be circumvented, if the matrix elements are not completely diagonal with respect to v, W, ξ, and L, by making use of the fact that the corresponding reduced matrix elements of $\mathbf{W}^{(01)}$, being proportional to those of $\mathbf{L}$, must vanish. The sum over $\bar{L}$ and $\bar{\xi}$ for $\bar{S} = S_1 - \frac{1}{2}$ can now be related to the similar sum for $\bar{S} = S_1 + \frac{1}{2}$, and, with a little manipulation, the dependence of the ratio of the reduced matrix elements on ξ, L, ξ', and L' can again be removed. This method, which has been previously used by Elliott *et al.*,[2] breaks down if one of the matrix elements is completely diagonal in all quantum numbers; but in this case it is easy to see that the other matrix element must also be completely diagonal, and hence $(-1)^x = 1$. The result of working through the various special cases is that the conclusions of the preceding paragraph are true in general: x is always independent of ξ, ξ', L, and L', and depends only on the seniorities.

Thus

$$x = x(v_1, v_2, v_1', v_2'). \tag{26}$$

The precise form of x depends on the phases $\epsilon(vS\{|\ \bar{v}\bar{S})$. If these are still at our disposal, then we can go no further in our determination of x. However, for some values of l a particular choice has been made; for example, Eqs. (56) of Racah[3] determine the phases of $\epsilon(vS\{|\ \bar{v}\bar{S})$ for f electrons. We may therefore compare expressions, such as (24) and (25), for all the various types of couples (v, S); the resulting values of x required to lead to agreement as to phase for f electrons can be summarized in the equation

$$x = v_1\ \delta(v_1, v_1') + v_2\ \delta(v_2, v_2') + 1.$$

Upon putting this value of x into Eq. (22) the ratio of the two reduced matrix elements is made unambiguous.

VI. APPLICATIONS

We may specialize Eq. (22) in several ways. A prudent step is to check that it reproduces those special cases that are already known. Wybourne[5] expresses his results for the matrices of the spin-orbit coupling in terms of the matrix elements of a quantity Λ defined by

$$(l^n W\xi SLJM_J\ |\sum_i (\mathbf{s}_i\cdot\mathbf{l}_i)|\ l^n W'\xi'S'L'JM_J)$$
$$= (-1)^{J+y}\begin{Bmatrix} S & L & J \\ L' & S' & 1 \end{Bmatrix}(l^n W\xi SL\ |\Lambda|\ l^n W'\xi'S'L'),$$

where $y = 0$ or $-\frac{1}{2}$ according as n is even or odd. From Eq. (25) of Racah,[6] we may easily prove

$$\frac{(\psi_1\ |\Lambda|\ \psi_1')}{(\psi_2\ |\Lambda|\ \psi_2')} = (-1)^{S_1'-S_2'+y_2-y_1}\frac{(\psi_1\ ||W^{(11)}||\ \psi_1')}{(\psi_2\ ||W^{(11)}||\ \psi_2')}, \tag{27}$$

where

$$\psi_1 \equiv l^{n_a}v_1 W\xi S_1 L,$$
$$\psi_1' \equiv l^{n_a}v_1' W'\xi' S_1' L',$$
$$\psi_2 \equiv l^{n_b}v_2 W\xi S_2 L,$$

and

$$\psi_2' \equiv l^{n_b}v_2' W'\xi' S_2' L'.$$

By combining Eqs. (22) and (27), the ratio of the matrix elements of Λ for any set of states ψ_1, ψ_1', ψ_2, and ψ_2' can readily be found. Of the 31 entries in Table III of Wybourne,[5] 20 are special cases of this kind; the remainder are examples of Eqs. (67) and (69b) of Racah.[6] We obtain complete agreement with Wybourne for 16 of the 20, but the signs of the right-hand sides of the sixth, ninth, tenth, and eleventh equations of his Table IIIb are incorrect, and should be reversed. In a private communication, Wybourne has confirmed these four corrections.[7]

Although we have distinguished between Eq. (22) (for which $v_1 \neq v_2$ and $v_1' \neq v_2'$) and Eqs. (67) and

[7] Table III of Wybourne contains other errors that are more obviously typographical. Of these, three possess a mathematical significance: In the second equation of Table III a, the representation (110) on the extreme right should be (111); in the fifth equation of this table, the seniority number 4 should be replaced by 3; and in the last equation of Table IIIc, the factor $-[2(2)/3]^{1/2}$ should read $-[2(2)^{1/2}/3]$.

(69b) of Racah[6] (for which $v_1 = v_2$ and $v_1' = v_2'$), it should be pointed out that Racah's equations can be derived from Eq. (22). It is only necessary to compare Eq. (22), as it stands, to a similar equation in which n_a possesses its minimum value, namely the larger of v_1 and v_1'. Suppose, for example, we take $v_1 = v_1' = v$ and choose $\kappa + k$ to be even. For Eq. (22) to be valid, we must have $\kappa' = 1$. We set $n_a = v$ in Eq. (22) and then $n_a = n$. The matrix elements

$$(\psi_2' \,||W^{(1k)}||\, \psi_2)$$

can be easily eliminated, and we get

$$\frac{(l^n v W\xi SL \,||W^{(\kappa k)}||\, l^n v W'\xi' S'L')}{(l^v v W\xi SL \,||W^{(\kappa k)}||\, l^v v W'\xi' S'L')}$$

$$= (-1)^{(v-n)/2} \begin{pmatrix} \tfrac{1}{2}(2l+1-v) & 1 & \tfrac{1}{2}(2l+1-v) \\ \tfrac{1}{2}(2l+1-n) & 0 & -\tfrac{1}{2}(2l+1-n) \end{pmatrix}$$

$$\times \begin{pmatrix} \tfrac{1}{2}(2l+1-v) & 1 & \tfrac{1}{2}(2l+1-v) \\ \tfrac{1}{2}(2l+1-v) & 0 & -\tfrac{1}{2}(2l+1-v) \end{pmatrix}^{-1}$$

$$= (2l+1-n)/(2l+1-v),$$

which agrees with Eq. (69b) of Racah.[6]

The applications of Eq. (22) that have been considered so far simply reproduce established results. However, it is only necessary to take k to be even to obtain a large number of new equations. This is because $\kappa + \kappa'$ must be odd, and so κ cannot equal κ'. We may therefore relate the matrix elements of $\mathbf{W}^{(12)}$ in one configuration to those of $\mathbf{W}^{(02)}$ in another; in fact, for any matrix element of $\mathbf{W}^{(12)}$, a matrix element of $\mathbf{W}^{(02)}$ in another configuration can be found to which it is related by Eq. (22). Since tensors of the type $\mathbf{W}^{(12)}$ and $\mathbf{W}^{(02)}$ are used in the study of hyperfine structure and crystalline field effects, respectively, a considerable amount of labor can be saved by taking advantage of this relation. For example, on setting $v_1 = v_1'$, $S_1 = S_1'$, $v_2 = v_2'$, and $S_2 = S_2'$ in Eq. (22), we obtain, for even k,

$$\frac{(l^{n_a} v_1 W\xi S_1 L \,||W^{(1k)}||\, l^{n_a} v_1 W\xi' S_1 L')}{(l^{n_b} v_2 W\xi S_2 L \,||V^{(k)}||\, l^{n_b} v_2 W\xi' S_2 L')}$$

$$= -\left[\frac{(2l+1-v_2)(2l+2-v_2)(2l+3-v_2)}{2(2l+1-n_b)^2}\right]^{\frac{1}{2}}. \tag{28}$$

This result is independent of v_1 and S_2, and relates, for example, the matrix elements of part of the hyperfine interaction for the quartets of f^5 to the matrix elements of $\mathbf{V}^{(2)}$ for the terms of f^4 with a seniority of 4. Matrix elements of the latter kind are the easier to evaluate, since fewer parents are involved. Equation (28) should therefore be useful in calculating, for example, the contribution to the hyperfine structure of PmI $4f^5\ {}^6H_J$ coming from admixtures of quartet states.

Transient Response of a Dipole Antenna

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The transient current in a long dipole antenna excited by a step-function voltage across an infinitesimal center gap has recently been calculated by Wu. A simpler derivation of Wu's result is given using double Fourier transformation.

IN a recent paper,[1] Wu calculates the current in a long dipole antenna driven by a voltage impressed across an infinitesimal center gap. The impressed voltage is a step function of both space and time, and the current is found up until the time that the discontinuity spreading out from the gap first reaches the ends of the dipole. Since Wu's analysis, while ingenious, is somewhat roundabout, the following more direct solution may be of interest.

In a cylindrical coordinate system (ρ, φ, z), the resultant electric field at the surface of the antenna, which is the negative of the applied electric field, may be expressed as[2]

$$E_z(a, z, t) = -\delta(z)U(t)$$
$$= \lim_{s\to 0} \frac{1}{4\pi^2} \int_{C_\gamma} \frac{\sinh \frac{1}{2}\gamma s}{\frac{1}{2}\gamma s} e^{\gamma z}\, d\gamma \int_{C_p} \frac{e^{pct}}{p}\, dp, \qquad (1)$$

where c is the velocity of light, and the contours C_γ and C_p are up the imaginary axes, with C_p indented to the right of $p = 0$.

The electromagnetic field will be transverse magnetic and derivable from a stream function $\Pi(\rho, z, t)$ which satisfies the scalar wave equation.[2] Such a function may be written in the form

$$\Pi(\rho, z, t)$$
$$= \frac{1}{4\pi^2} \int_{C_\gamma} \int_{C_{p'}} A(p, \gamma) \frac{K_0(\lambda\rho)}{K_0(\lambda a)} e^{\gamma z + pct}\, dp\, d\gamma, \qquad (2)$$

where

$$\lambda = (p^2 - \gamma^2)^{\frac{1}{2}}. \qquad (3)$$

In order to represent outgoing or damped waves at infinity, λ must lie in the fourth quadrant or on its boundaries when Im $p < 0$, and in the first quadrant or on its boundaries when Im $p > 0$. To carry out the p integration when $\gamma = i\beta$, where $\beta \neq 0$, take the contour C_p' shown in Fig. 1, indented

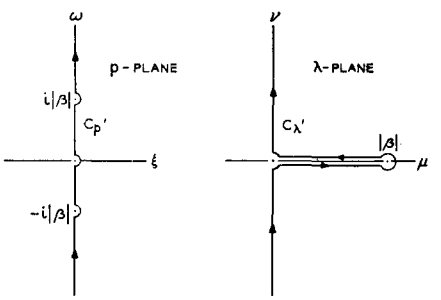

FIG. 1. Contours of integration.

to pass to the right of $p = \pm i\beta$. It is easy to verify that if λ is taken to be negative imaginary when p lies on C_p' below $-i\,|\beta|$, then λ describes the contour C_λ' shown in Fig. 1 as p describes C_p', and so only outgoing or damped waves are included in the integral (2). If $\beta = 0$, then C_p' coincides with C_p and $\lambda = p$. To make the Bessel functions single valued, the λ plane may be cut along the negative real axis.

The electric field corresponding to (2) at the surface of the antenna is

$$E_z(a, z, t)$$
$$= -\frac{1}{4\pi^2} \int_{C_\gamma} \int_{C_{p'}} A(p, \gamma) \frac{\eta_0 \lambda^2}{p} e^{\gamma z + pct}\, dp\, d\gamma, \qquad (4)$$

where η_0 is the characteristic impedance of free space, so that the function $A(p, \gamma)$ may be determined by comparison with (1). The antenna current, which is proportional to the surface magnetic field, is given by

$$I(z, t) = -2\pi a \left.\frac{\partial \Pi}{\partial \rho}\right|_{\rho=a}$$
$$= -\frac{a}{2\pi\eta_0} \int_{C_\gamma} \int_{C_{p'}} \frac{K_1(\lambda a)}{\lambda K_0(\lambda a)} e^{\gamma z + pct}\, dp\, d\gamma, \qquad (5)$$

where the convergence factor $(\sinh \frac{1}{2}\gamma s)/\frac{1}{2}\gamma s$ has been dropped on the assumption that z and t are not simultaneously zero.

To simplify the expression for $I(z, t)$, we observe

[1] T. T. Wu, J. Math. Phys. **2**, 892 (1961).
[2] S. A. Schelkunoff, *Electromagnetic Waves* (D. van Nostrand Company, Inc., New York, 1943), pp. 34–35 and 375–377.

that the integrand of (5) does not have a pole at $p = 0$, so the center part of C_p' may be deformed into an infinite semicircle in the left half-plane, over which the integrand vanishes when $t > 0$. The final stage of deformation is shown as C_p'' in Fig. 2, where nothing is left but the integrals around the branch cuts from $p = \pm i\,|\beta|$ to $\pm i\infty$. The corresponding contour in the λ plane is C_λ''. It is easy to show that during the deformation C_λ does not leave the right half-plane, in which the function $K_0(\lambda a)$ has no zeros; furthermore, the ratio $K_1(\lambda a)/K_0(\lambda a)$ approaches 1 as $|\lambda|$ approaches ∞. The contributions from the circles around $p = \pm i\,|\beta|$ can be shown to be of the order of $1/|\log \delta|$, where δ is the radius of these circles in the p plane, so the contributions vanish as $\delta \to 0$.

If we now set

$$\gamma = i\beta, \qquad p = i\omega, \qquad \nu = (\omega^2 - \beta^2)^{\frac{1}{2}}, \tag{6}$$

where ν is real, we can write down the four integrals along the branch lines. Expressing the modified Bessel functions $K_{0,1}(\pm i\nu a)$ in terms of Hankel functions and combining terms gives

$$\begin{aligned} I(z, t) &= \frac{ai}{\pi\eta_0}\int_{-\infty}^{\infty}\int_{|\beta|}^{\infty}\left[\frac{H_1^{(1)}(\nu a)}{\nu H_0^{(1)}(\nu a)} - \frac{H_1^{(2)}(\nu a)}{\nu H_0^{(2)}(\nu a)}\right]\sin(\omega ct)e^{i\beta z}\,d\omega\,d\beta \\ &= \frac{4}{\pi^2\eta_0}\int_{-\infty}^{\infty}\int_{|\beta|}^{\infty}\frac{\sin(\omega ct)e^{i\beta z}\,d\omega\,d\beta}{\nu^2[J_0^2(\nu a) + N_0^2(\nu a)]}, \end{aligned} \tag{7}$$

where in the last step we have used the Wronskian relationship between the Hankel functions. Changing the inner variable of integration from ω to ν and then inverting the order of integration and using the result[3]

$$\int_{-\infty}^{\infty}\frac{\sin[ct(\beta^2+\nu^2)^{\frac{1}{2}}]}{(\beta^2+\nu^2)^{\frac{1}{2}}}e^{i\beta z}\,d\beta = \begin{cases} 0 & \text{if } |z| > ct, \\ \pi J_0[\nu(c^2t^2 - z^2)^{\frac{1}{2}}] & \text{if } |z| < ct, \end{cases} \tag{8}$$

we find that the antenna current vanishes for $|z| > ct$. For $|z| < ct$ it is given by

$$I(z, t) = \frac{4}{\pi\eta_0}\int_0^{\infty}\frac{J_0[\nu(c^2t^2 - z^2)^{\frac{1}{2}}]}{J_0^2(\nu a) + N_0^2(\nu a)}\frac{d\nu}{\nu}, \tag{9}$$

a result which is clearly equivalent to Wu's Eq. (17).

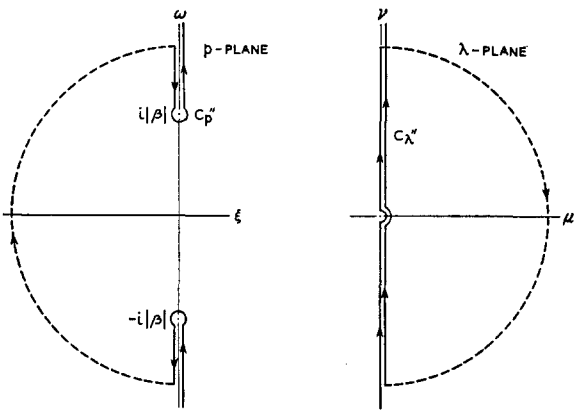

FIG. 2. Contours of integration.

[3] W. Magnus and F. Oberhettinger, *Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1954), p. 118.

An Approach to Gravitational Radiation by a Method of Spin Coefficients*

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A new approach to general relativity by means of a tetrad or spinor formalism is presented. The essential feature of this approach is the consistent use of certain complex linear combinations of Ricci rotation coefficients which give, in effect, the spinor affine connection. It is applied to two problems in radiation theory; a concise proof of a theorem of Goldberg and Sachs and a description of the asymptotic behavior of the Riemann tensor and metric tensor, for outgoing gravitational radiation.

I. INTRODUCTION

IN the study of gravitational radiation, two techniques have recently gained prominence; the tetrad calculus[1-6] and the spinor calculus.[7-9] In the present paper (Secs. II, III,[10] and IV) it is shown how the two techniques can be used to derive a very compact and useful set of equations, which are essentially linear combinations of the equations for the Riemann tensor expressed in terms of either Ricci rotation coefficients or the spinor affine connection. In Sec. V, we give a short proof of a theorem of Goldberg and Sachs[11] to the effect that if in empty space there exists a null geodesic congruence with vanishing shear, then the Riemann tensor of the space must be algebraically specilized (i.e., the Riemann tensor is not Petrov type I nondegenerate).

The last application of our formalism is to the asymptotic behavior of the Riemann tensor and metric tensor in empty space. In Sec. VI a coordinate system and tetrad are built around a hypersurface-orthogonal null-vector field. In Sec. VII, this special coordinate system and tetrad are used to prove essentially the following theorem. If a particular complex (tetrad) component of the Riemann tensor (complex because we are using a complex tetrad system) has an asymptotic behavior $O(r^{-5})$, the other four complex components are, respectively, $O(r^{-4})$, $O(r^{-3})$, $O(r^{-2})$, and $O(r^{-1})$. The last component represents the pure radiation field. Special cases of this theorem have been known for some time.[12,13] Our theorem is also a slight generalization of a similar result recently obtained by Bondi and Sachs.[6]

II. TETRAD CALCULUS

We deal with a four-dimensional Riemannian space with a signature -2. Into this space a tetrad system of vectors l_μ, m_μ, $\bar{m}_\mu$, n_μ is introduced, l_μ and n_μ being real null vectors and m_μ with its complex conjugate $\bar{m}_\mu$ being complex null vectors. The vector m_μ can be defined from a pair of real, orthogonal unit space-like vectors a_μ and b_μ by $m_\mu = (1/\sqrt{2})(a_\mu - ib_\mu)$. The orthogonality properties of the vectors are

$$\begin{gathered} l_\mu l^\mu = m_\mu m^\mu = \bar{m}_\mu \bar{m}^\mu = n_\mu n^\mu = 0, \\ l_\mu n^\mu = -m_\mu \bar{m}^\mu = 1, \\ l_\mu m^\mu = l_\mu \bar{m}^\mu = n_\mu m^\mu = n_\mu \bar{m}^\mu = 0. \end{gathered} \tag{2.1}$$

It is of great convenience to introduce the tetrad notation[14]

$$z_{\mathbf{m}\mu} = (l_\mu, n_\mu, m_\mu, \bar{m}_\mu), \qquad \mathbf{m} = 1, 2, 3, 4.$$

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[4] J. Goldberg and R. Kerr, J. Math. Phys. **2**, 327 (1961).
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[6] H. Bondi and R. Sachs (private communication).
[7] L. Witten, Phys. Rev. **113**, 357 (1959).
[8] R. Penrose, Ann. Phys. (New York) **10**, 171 (1960).
[9] J. Ehlers, Hamburg Lectures.
[10] It is possible, if one has no familiarity with spinors to omit Sec. III, with but a small loss of continuity.
[11] J. Goldberg and R. Sachs (to be published).
[12] R. Sachs (to be published).
[13] I. Robinson and A. Trautman, Phys. Rev. Letters **4**, 431 (1960).
[14] Greek indices (values 1, 2, 3, 4) are tensor indices, bold face **a**, **b** ··· (values 1, 2, 3, 4) are tetrad indices, capital latin A, B ··· (values 0, 1) are spinor indices and small lightface latin a, b ··· (values 0, 1) are spinor "dyad" indices.

The tetrad indices can be raised or lowered by the flat-space metric $\eta_{\mathbf{mn}}$

$$\eta_{\mathbf{mn}} = \eta^{\mathbf{mn}} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix}. \tag{2.2}$$

The following two relations are easily seen to be true;

$$g_{\mu\nu} = z_{\mathbf{m}\mu} z_{\mathbf{n}\nu} \eta^{\mathbf{mn}}$$

$$= l_\mu n_\nu + n_\mu l_\nu - m_\mu \bar{m}_\nu - \bar{m}_\mu m_\nu \tag{2.3a}$$

$$\eta_{\mathbf{mn}} = z_{\mathbf{m}\mu} z_{\mathbf{n}\nu} g^{\mu\nu}. \tag{2.3b}$$

Complex Ricci rotation coefficients are defined by

$$\gamma_{\mathbf{m}}{}^{\mathbf{np}} = z_{\mathbf{m}\mu;\nu} z^{\mathbf{n}\mu} z^{\mathbf{p}\nu}, \tag{2.4}$$

with the symmetry

$$\gamma^{\mathbf{mnp}} = -\gamma^{\mathbf{nmp}}.$$

The tetrad components of the Riemann tensor defined by

$$R_{\mathbf{mnpq}} = R_{\alpha\beta\gamma\delta} z_{\mathbf{m}}^{\alpha} z_{\mathbf{n}}^{\beta} z_{\mathbf{p}}^{\gamma} z_{\mathbf{q}}^{\delta} \tag{2.5}$$

can be expressed in terms of the rotation coefficients by[15]

$$R^{\mathbf{mnpq}} = \gamma^{\mathbf{mnp;q}} - \gamma^{\mathbf{mnq;p}} + \gamma_{\mathbf{l}}{}^{\mathbf{mq}} \gamma^{\mathbf{lnp}} - \gamma_{\mathbf{l}}{}^{\mathbf{mp}} \gamma^{\mathbf{lnq}} + \gamma^{\mathbf{mnl}} (\gamma_{\mathbf{l}}{}^{\mathbf{pq}} - \gamma_{\mathbf{l}}{}^{\mathbf{qp}}), \tag{2.6}$$

with

$$\gamma^{\mathbf{mnp;q}} \equiv \gamma^{\mathbf{mnp}}_{;\mu} z^{\mathbf{q}\mu}.$$

This can easily be derived from the Ricci identity

$$z_{\mathbf{m}\mu;[\alpha\beta]} = \tfrac{1}{2} z_{\mathbf{m}\nu} R^{\nu}_{\mu\alpha\beta} \tag{2.7}$$

by repeated application of (2.4).

The relationship between the Riemann tensor, Weyl tensor, and Ricci tensor goes over in tetrad form unchanged[15]

$$R_{\mathbf{mnpq}} = C_{\mathbf{mnpq}} - \tfrac{1}{2}(\eta_{\mathbf{mp}} R_{\mathbf{nq}} - \eta_{\mathbf{mq}} R_{\mathbf{np}} + \eta_{\mathbf{nq}} R_{\mathbf{mp}} - \eta_{\mathbf{np}} R_{\mathbf{mq}}) - (R/6)(\eta_{\mathbf{mq}} \eta_{\mathbf{np}} - \eta_{\mathbf{mp}} \eta_{\mathbf{nq}}). \tag{2.8}$$

In the tetrad notation the Bianchi identities, $R_{\alpha\beta[\gamma\delta;\mu]} = 0$, take the form

$$R_{\mathbf{mn}[\mathbf{pq};\mathbf{r}]} = \gamma_{\mathbf{m}}{}^{\mathbf{l}}{}_{[\mathbf{r}} R_{\mathbf{pq}]\mathbf{ln}} - \gamma_{\mathbf{n}}{}^{\mathbf{l}}{}_{[\mathbf{r}} R_{\mathbf{pq}]\mathbf{lm}} + 2 R_{\mathbf{mnl}[\mathbf{p}} \gamma_{\mathbf{r}}{}^{\mathbf{l}}{}_{\mathbf{q}]}. \tag{2.9}$$

Though they appear to be considerably more complicated, it will be seen in Sec. IV that with a new notation they take a simple and useful form in empty space.

In Eq. (2.6) we used the intrinsic derivative defined by $\varphi^{;\mathbf{m}} = \varphi_{;\mu} z^{\mathbf{m}\mu}$. It will be of great value to obtain the commutator of two intrinsic derivatives, $\varphi^{;\mathbf{m};\mathbf{n}} - \varphi^{;\mathbf{n};\mathbf{m}}$. We have

$$\varphi^{;\mathbf{m};\mathbf{n}} = (\varphi_{;\mu} z^{\mathbf{m}\mu})_{;\nu} z^{\mathbf{n}\nu} = \varphi_{;\mu\nu} z^{\mathbf{m}\mu} z^{\mathbf{n}\nu} + \varphi_{,\mu} z^{\mathbf{m}\mu}_{;\nu} z^{\mathbf{n}\nu}. \tag{2.10}$$

By interchanging $\mathbf{m}$ and $\mathbf{n}$ in (2.10) and using $z^{\mathbf{m}\mu}{}_{;\nu} z^{\mathbf{n}\nu} = \gamma^{\mathbf{mpn}} z^{\mu}_{\mathbf{p}}$ obtained from (2.4), we see

$$\varphi^{;\mathbf{m};\mathbf{n}} - \varphi^{;\mathbf{n};\mathbf{m}} = \varphi^{;\mathbf{l}} [\gamma^{\mathbf{m}}{}_{\mathbf{l}}{}^{\mathbf{n}} - \gamma^{\mathbf{n}}{}_{\mathbf{l}}{}^{\mathbf{m}}]. \tag{2.11}$$

In Sec. IV it will be advantageous to dispense with the semicolon notation for intrinsic derivatives and use the following;

$$D\varphi \equiv \varphi_{;\mu} l^{\mu}, \qquad \Delta\varphi \equiv \varphi_{;\mu} n^{\mu}$$
$$\delta\varphi \equiv \varphi_{;\mu} m^{\mu}, \qquad \bar{\delta}\varphi \equiv \varphi_{;\mu} \bar{m}^{\mu}. \tag{2.12}$$

III. TWO-COMPONENT SPINOR CALCULUS

The connection between tensors and spinors[16] is achieved by means of a quantity $\sigma^{\mu}{}_{AB'}$, satisfying

$$g_{\mu\nu} \sigma^{\mu}{}_{AB'} \sigma^{\nu}{}_{CD'} = \epsilon_{AC} \epsilon_{B'D'}. \tag{3.1}$$

For each value of μ, $\sigma_{\mu}{}^{AB'}$ is a (2×2) Hermitian matrix. The ϵ's are Levi-Civita symbols, that is, skew-symmetric expressions with $\epsilon_{01} = \epsilon_{0'1'} = \epsilon^{01} = \epsilon^{0'1'} = 1$, and they are used for lowering or raising spinor indices:

$$\xi^A = \epsilon^{AB} \xi_B, \qquad \xi_B = \xi^A \epsilon_{AB},$$
$$\eta^{A'} = \epsilon^{A'B'} \eta_{B'}, \qquad \eta_{B'} = \eta^{A'} \epsilon_{A'B'}. \tag{3.2}$$

(Note the ordering of the indices.) The spinor equivalent of any tensor is a quantity having each tensor index replaced by a pair of spinor indices, one unprimed and one primed[17];

$$X^{\lambda\mu}{}_{\nu} \leftrightarrow X^{AB'CD'}{}_{EF'} = \sigma_{\lambda}{}^{AB'} \sigma_{\mu}{}^{CD'} X^{\lambda\mu}{}_{\nu} \sigma^{\nu}{}_{EF'}.$$

Inversely:

$$X^{\lambda\mu}{}_{\nu} = \sigma^{\lambda}{}_{AB'} \sigma^{\mu}{}_{CD'} X^{AB'CD'}{}_{EF'} \sigma_{\nu}{}^{EF'}.$$

Equation (3.1) tells us that $\epsilon_{AC}\epsilon_{B'D'}$ is the spinor equivalent of $g_{\mu\nu}$.

When taking the complex conjugate of a spinor, unprimed indices become primed, and primed indices become unprimed. For example, the complex conjugate[18] of $X^{AB'CD'}{}_{EF'}$ is $\bar{X}^{A'BC'D}{}_{E'F}$, whence

[15] L. P. Eisenhart, *Riemannian Geometry* (Princeton University Press, Princeton, New Jersey, 1960).

[16] See, for example, W. L. Bade and H. Jehle, Revs. Modern Phys. **25**, 714 (1953).

[17] We use primed rather than dotted indices for typographical reasons.

[18] Many authors omit the bar over the complex conjugate.

the condition for $X^{\lambda\mu}{}_{\nu}$ to be real is the Hermitian property

$$X^{AB'CD'}{}_{EF'} = \bar{X}^{B'AD'C}{}_{F'E}.$$

The covariant derivative $\xi_{A;\mu}$ of the spinor ξ_A is

$$\xi_{A;\mu} = \xi_{A,\mu} - \xi_B \Gamma^B{}_{A\mu}, \tag{3.3}$$

where $\Gamma^B{}_{A\mu}$ is the spinor affine connection. The corresponding quantity $\bar{\Gamma}^{B'}{}_{A'\mu}$ deals with the primed indices. The rules of covariant differentiation for spinor indices are exactly analogous to those for tensor indices. The choice of $\Gamma^B{}_{A\mu}$ is fixed by the requirement that the covariant derivatives of $\sigma^{\mu}{}_{AB'}, \epsilon_{AB}, \epsilon_{A'B'}$ shall all vanish.[16]

Observe that, by (3.1), the four expressions

$$\sigma^{\mu}{}_{00'}, \quad \sigma^{\mu}{}_{11'}, \quad \sigma^{\mu}{}_{01'}, \quad \sigma^{\mu}{}_{10'} \tag{3.4}$$

satisfy the same orthogonality relations (2.1) as the four vectors l^{μ}, n^{μ}, m^{μ}, $\bar{m}^{\mu}$. We would like, therefore, to identify the expressions (3.4) as a convenient tetrad. However, this would not be strictly accurate and is a little misleading. The expressions (3.4) do not really denote vectors as they stand, as is exemplified by the fact that while covariant derivative of $\sigma^{\mu}{}_{AB'}$ is zero, this is not so for l^{μ}, m^{μ}, $\bar{m}^{\mu}$, n^{μ} [see Eq. (2.4)].

To get around this difficulty we introduce two basis spinors o^A, ι^A (a "dyad") normalized thus:

$$o_A \iota^A = \epsilon_{AB} o^A \iota^B = -\iota_A o^A = 1. \tag{3.5}$$

A dyad (in spin space) is analogous to a tetrad in vector space. We may put

$$l^{\mu} = \sigma^{\mu}{}_{AB'} o^A \bar{o}^{B'}, \quad n^{\mu} = \sigma^{\mu}{}_{AB'} \iota^A \bar{\iota}^{B'}, \quad m^{\mu} = \sigma^{\mu}{}_{AB'} o^A \bar{\iota}^{B'} \tag{3.6}$$

The covariant derivatives of these expressions will now involve the covariant derivatives of o^A and ι^B.

As with the tetrads, it is convenient to have a generic symbol for both o^A and ι^A. Define $\zeta_a{}^A$, $\bar{\zeta}_a{}^{A'}$ by

$$\zeta_0{}^A = o^A, \quad \zeta_1{}^A = \iota^A, \quad \bar{\zeta}_{0'}{}^{A'} = \bar{o}^{A'}, \quad \bar{\zeta}_{1'}{}^{A'} = \bar{\iota}^{A'}. \tag{3.7}$$

Then, for example, given a spinor $Y_{AB'C}$, we can define its *dyad components*

$$Y_{ab'c} = Y_{AB'C} \zeta_a{}^A \bar{\zeta}_{b'}{}^{B'} \zeta_c{}^C.$$

The lower-case indices behave the same way algebraically as ordinary (capital) spinor indices, but when covariant differentiation is applied, no term involving an affine connection appears for the lower case indices. Thus, the important formal difference between the lower-case and capital indices is simply the difference with respect to covariant differentiation.

Bearing this in mind, it is permissible to choose the components of $\zeta_a{}^A$ to be the Kronecker delta. The dyad components of any spinor will then, in fact, be identical with its spinor components. It is by no means essential to make this specialization but it will be convenient to do so here. The expression

$$\sigma^{\mu}{}_{ab'} = \sigma^{\mu}{}_{AB'} \zeta_a{}^A \bar{\zeta}_{b'}{}^{B'} \tag{3.8}$$

now gives us l^{μ}, n^{μ}, m^{μ}, $\bar{m}^{\mu}$ as ab' take, respectively, the values $00'$, $11'$, $01'$, $10'$, by (3.6). With this interpretation, the expressions (3.4) may indeed be though of as giving the required tetrad. However, it is essential to maintain the distinction between the dyad and spinor indices when covariant differentiation is involved.

The components of ζ_{aB} are now the same as those of ϵ_{AB}. Hence, $\zeta_{aA;\mu} = -\zeta_{aC}\Gamma^C{}_{A\mu} = \zeta_a^C \Gamma_{CA\mu} = \Gamma_{aA\mu}$ by (3.3). For the analog of the rotation coefficients[19] (2.4), we therefore have

$$\Gamma_{abcd'} = \zeta_{aA;\mu} \zeta_b{}^A \sigma^{\mu}{}_{cd'} \tag{3.9}$$

with the symmetry

$$\Gamma_{abcd'} = \Gamma_{bacd'}. \tag{3.10}$$

Writing

$$\varphi_{\cdots\cdots;\mu} \sigma^{\mu}{}_{ab'} \equiv \partial_{ab'} \varphi_{\cdots\cdots}, \tag{3.11}$$

the intrinsic derivatives (2.12) become

$$D \equiv \partial_{00'}, \quad \Delta \equiv \partial_{11'}, \quad \delta \equiv \partial_{01'}, \quad \bar{\delta} \equiv \partial_{10'}. \tag{3.12}$$

The commutation relations for these derivatives acting on scalars

$$\begin{aligned}\{\partial_{ab'}\partial_{cd'} - \partial_{cd'}\partial_{ab'}\}\varphi \equiv \{&\epsilon^{pq}(\Gamma_{pacd'}\partial_{qb'} - \Gamma_{pcab'}\partial_{qd'}) \\ &+ \epsilon^{r's'}(\bar{\Gamma}_{r'b'd'c}\partial_{as'} - \bar{\Gamma}_{r'd'b'a}\partial_{cs'})\}\varphi\end{aligned} \tag{3.13}$$

can be obtained by direct calculation from (3.13) using (3.8) and (3.9). By a slight extension of this calculation, when the derivatives act on ζ_{aA} we obtain

$$\begin{aligned}\partial_{fe'}\Gamma_{acdb'} - \partial_{db'}\Gamma_{acfe'} &= \epsilon^{pq}\{\Gamma_{apdb'}\Gamma_{acfe'} \\ &+ \Gamma_{acpb'}\Gamma_{qdfe'} - \Gamma_{apfe'}\Gamma_{qcdb'} - \Gamma_{acpe'}\Gamma_{qfdb'}\} \\ &+ \epsilon^{r's'}\{\Gamma_{acdr'}\bar{\Gamma}_{s'b'e'f} - \Gamma_{acfr'}\Gamma_{s'e'b'd}\} \\ &+ \Psi_{acdf}\epsilon_{e'b'} + \Lambda\epsilon_{e'b'}(\epsilon_{cd}\epsilon_{af} + \epsilon_{ab}\epsilon_{cf}) \\ &+ \Phi_{acb'e'}\epsilon_{fd},\end{aligned} \tag{3.14}$$

[19] The quantities (3.9) can be defined directly in terms of derivatives of the $\sigma_{\mu ab'}$, as follows:

$$\Gamma_{abcd'} = \tfrac{1}{2}\epsilon^{p'q'}\{\sigma_{cd'ap'bq'} - \sigma_{cd'bq'ap'} - \sigma_{ap'bq'cd'}\}$$

where

$$\sigma_{ab'cd'ef'} = \sigma^{[\mu}{}_{ab'}\sigma^{\nu]}{}_{cd'}\,\sigma_{\mu ef'},{}_{\nu}$$

or

$$\Gamma_{abcd'} = \tfrac{1}{2}\epsilon^{p'q'}\sigma^{\mu}{}_{aq'}\sigma^{\nu}{}_{cd'}\sigma_{\mu bp'};{}_{\nu}.$$

where the spinors Ψ_{ABCD}, $\Phi_{ABC'D'}$, and Λ correspond, respectively, to the Weyl tensor, trace-free part of the Ricci tensor, and scalar curvature. They have the symmetries:

$$\Psi_{ABCD} = \Psi_{(ABCD)},$$
$$\Phi_{ABC'D'} = \Phi_{(AB)(C'D')} = \bar{\Phi}_{C'D'AB} \tag{3.15}$$

with

$$\Lambda = (1/24)R.$$

The spinor equivalent of the Riemann tensor $R_{\alpha\beta\gamma\delta}$ decomposes as follows[20]:

$$\begin{aligned} -R_{AE'BF'CG'DH'} &= \Psi_{ABCD}\epsilon_{E'F'}\epsilon_{G'H'} \\ &+ \epsilon_{AB}\epsilon_{CD}\bar{\Psi}_{E'F'G'H'} \\ &+ 2\Lambda(\epsilon_{AC}\epsilon_{BD}\epsilon_{E'F'}\epsilon_{G'H'} + \epsilon_{AB}\epsilon_{CD}\epsilon_{E'H'}\epsilon_{F'G'}) \\ &+ \epsilon_{AB}\Phi_{CDE'F'}\epsilon_{G'H'} + \epsilon_{CD}\Phi_{ABG'H'}\epsilon_{E'F'}. \end{aligned} \tag{3.16}$$

The relations[8]

$$\partial_{(A}{}^{P'}\partial_{B)P'}\xi_C = -\Psi_{ABCD}\xi^D + \Lambda\xi_{(A}\epsilon_{B)C}, \tag{3.17}$$
$$\partial_{C(P'}\partial^{C}{}_{Q')}\xi_A = \Phi_{ABP'Q'}\xi^B$$

have been used to obtain (3.14).

The Bianchi identities in spinor form are

$$\begin{aligned} \partial^{D}{}_{G'}\Psi_{ABCD} &= \partial_{(C}{}^{H'}\Phi_{AB)G'H'} \\ \partial^{AG'}\Phi_{ABG'H'} &= -3\,\partial_{BH'}\Lambda \end{aligned} \tag{3.18}$$

from which we obtain

$$\begin{aligned} \partial^{p}{}_{d'}\Psi_{abcp} - \partial_{(c}{}^{t'}\Phi_{ab)d't'} &= \{3\Psi_{pr(ab}\Gamma_{c)}{}^{pr}{}_{d'} \\ &+ \Psi_{abcp}\Gamma^{p}{}_{r}{}^{r}{}_{d'}\} - 2\Gamma^{p}{}_{(ab}{}^{t'}\Phi_{c)pt'd'} \\ &- \{\bar{\Gamma}_{t'd'v'(a}\Phi_{bc)}{}^{t'v'} + \bar{\Gamma}_{t'}{}^{v'}{}_{v'(a}\Phi_{bc)}{}^{t'}{}_{d'}\} \end{aligned} \tag{3.19}$$

and

$$\begin{aligned} 3\,\partial_{ab'}\Lambda &+ \partial^{pt'}\Phi_{apb't'} \\ &= \epsilon^{v'w'}\{\Phi_{ap}{}^{t'}{}_{w'}\bar{\Gamma}_{b't'v'}{}^{p} + \Phi_{apb'}{}^{t'}\bar{\Gamma}_{t'w'v'}{}^{p}\} \\ &- \{\Phi_{prb'}{}^{t'}\Gamma_{a}{}^{pr}{}_{t'} + \Phi_{apb'}{}^{t'}\Gamma^{p}{}_{r}{}^{r}{}_{t'}\}. \end{aligned} \tag{3.20}$$

IV. THE SPIN COEFFICIENTS

In the present section we will show how the formalisms developed in Secs. II and III can be put into a relatively concise form, despite the fact that all summations will be written out explicitly.

Twelve complex functions (called spin coefficients) are defined in terms of either the rotation coefficients (2.4) or spinor affine connection (3.9).

[20] These definitions of Ψ_{ABCD}, $\Phi_{ABC'D'}$ differ by a factor 2 from those given in reference 8. Also, the Riemann tensor used here is the negative of that used in reference 8.

$$\begin{aligned} \kappa &= \gamma_{131} = l_{\mu;\nu}m^{\mu}l^{\nu}, \quad \pi = -\gamma_{241} = -n_{\mu;\nu}\bar{m}^{\mu}l^{\nu}, \\ \epsilon &= \tfrac{1}{2}(\gamma_{121} - \gamma_{341}) = \tfrac{1}{2}(l_{\mu;\nu}n^{\mu}l^{\nu} - m_{\mu;\nu}\bar{m}^{\mu}l^{\nu}), \\ \rho &= \gamma_{134} = l_{\mu;\nu}m^{\mu}\bar{m}^{\nu}, \quad \lambda = -\gamma_{244} = -n_{\mu;\nu}\bar{m}^{\mu}\bar{m}^{\nu}, \\ \alpha &= \tfrac{1}{2}(\gamma_{124} - \gamma_{344}) = \tfrac{1}{2}(l_{\mu;\nu}n^{\mu}\bar{m}^{\nu} - m_{\mu;\nu}\bar{m}^{\mu}\bar{m}^{\nu}), \\ \sigma &= \gamma_{133} = l_{\mu;\nu}m^{\mu}m^{\nu}, \quad \mu = -\gamma_{243} = -n_{\mu;\nu}\bar{m}^{\mu}m^{\nu}, \\ \beta &= \tfrac{1}{2}(\gamma_{123} - \gamma_{343}) = \tfrac{1}{2}(l_{\mu;\nu}n^{\mu}m^{\nu} - m_{\mu;\nu}\bar{m}^{\mu}m^{\nu}), \\ \nu &= -\gamma_{242} = -n_{\mu;\nu}\bar{m}^{\mu}n^{\nu}, \\ \gamma &= \tfrac{1}{2}(\gamma_{122} - \gamma_{342}) = \tfrac{1}{2}(l_{\mu;\nu}n^{\mu}n^{\nu} - m_{\mu;\nu}\bar{m}^{\mu}n^{\nu}), \\ \tau &= \gamma_{132} = l_{\mu;\nu}m^{\mu}n^{\nu}, \end{aligned} \tag{4.1a}$$

or

$\Gamma_{abcd'} =$

cd' \ ab	00	01 or 10	11
00′	κ	ϵ	π
10′	ρ	α	λ
01′	σ	β	μ
11′	τ	γ	ν

. (4.1b)

It is seen that the spin coefficients appear more naturally when dealing with spinors than with tetrad vectors. This fact reappears when Eq. (2.6) is rewritten in terms of these new functions. The equations are rather unattractive until certain linear combinations are taken. These simpler equations are just the ones, (3.14), that arise naturally in the spinor calculus. Equation (3.14) or the appropriate linear combinations of Eq. (2.6) using (2.8), with the notation of (4.1), is

$$\begin{aligned} D\rho - \bar{\delta}\kappa &= (\rho^2 + \sigma\bar{\sigma}) + (\epsilon + \bar{\epsilon})\rho - \bar{\kappa}\tau \\ &- \kappa(3\alpha + \bar{\beta} - \pi) + \Phi_{00} \end{aligned} \tag{4.2a}$$

$$\begin{aligned} D\sigma - \delta\kappa &= (\rho + \bar{\rho})\sigma + (3\epsilon - \bar{\epsilon})\sigma \\ &- (\tau - \bar{\pi} + \bar{\alpha} + 3\beta)\kappa + \Psi_0 \end{aligned} \tag{4.2b}$$

$$\begin{aligned} D\tau - \Delta\kappa &= (\tau + \bar{\pi})\rho + (\bar{\tau} + \pi)\sigma \\ &+ (\epsilon - \bar{\epsilon})\tau - (3\gamma + \bar{\gamma})\kappa + \Psi_1 + \Phi_{01} \end{aligned} \tag{4.2c}$$

$$\begin{aligned} D\alpha - \bar{\delta}\epsilon &= (\rho + \bar{\epsilon} - 2\epsilon)\alpha + \beta\bar{\sigma} - \bar{\beta}\epsilon \\ &- \kappa\lambda - \bar{\kappa}\gamma + (\epsilon + \rho)\pi + \Phi_{10} \end{aligned} \tag{4.2d}$$

$$\begin{aligned} D\beta - \delta\epsilon &= (\alpha + \pi)\sigma + (\bar{\rho} - \bar{\epsilon})\beta \\ &- (\mu + \gamma)\kappa - (\bar{\alpha} - \bar{\pi})\epsilon + \Psi_1 \end{aligned} \tag{4.2e}$$

$$D\gamma - \Delta\epsilon = (\tau + \bar{\pi})\alpha + (\bar{\tau} + \pi)\beta - (\epsilon + \bar{\epsilon})\gamma - (\gamma + \bar{\gamma})\epsilon + \tau\pi - \nu\kappa + \Psi_2 - \Lambda + \Phi_{11} \quad (4.2f)$$

$$D\lambda - \bar{\delta}\pi = (\rho\lambda + \bar{\sigma}\mu) + \pi^2 + (\alpha - \bar{\beta})\pi - \nu\bar{\kappa} - (3\epsilon - \bar{\epsilon})\lambda + \Phi_{20} \quad (4.2g)$$

$$D\mu - \delta\pi = (\bar{\rho}\mu + \sigma\lambda) + \pi\bar{\pi} - (\epsilon + \bar{\epsilon})\mu - \pi(\bar{\alpha} - \beta) - \nu\kappa + \Psi_2 + 2\Lambda \quad (4.2h)$$

$$D\nu - \Delta\pi = (\pi + \bar{\tau})\mu + (\bar{\pi} + \tau)\lambda + (\gamma - \bar{\gamma})\pi - (3\epsilon + \bar{\epsilon})\nu + \Psi_3 + \Phi_{21} \quad (4.2i)$$

$$\Delta\lambda - \bar{\delta}\nu = -(\mu + \bar{\mu})\lambda - (3\gamma - \bar{\gamma})\lambda + (3\alpha + \bar{\beta} + \pi - \bar{\tau})\nu - \Psi_4 \quad (4.2j)$$

$$\delta\rho - \bar{\delta}\sigma = \rho(\bar{\alpha} + \beta) - \sigma(3\alpha - \bar{\beta}) + (\rho - \bar{\rho})\tau + (\mu - \bar{\mu})\kappa - \Psi_1 + \Phi_{01} \quad (4.2k)$$

$$\delta\alpha - \bar{\delta}\beta = (\mu\rho - \lambda\sigma) + \alpha\bar{\alpha} + \beta\bar{\beta} - 2\alpha\beta + \gamma(\rho - \bar{\rho}) + \epsilon(\mu - \bar{\mu}) - \Psi_2 + \Lambda + \Phi_{11} \quad (4.2l)$$

$$\delta\lambda - \bar{\delta}\mu = +(\rho - \bar{\rho})\nu + (\mu - \bar{\mu})\pi + \mu(\alpha + \bar{\beta}) + \lambda(\bar{\alpha} - 3\beta) - \Psi_3 + \Phi_{21} \quad (4.2m)$$

$$\delta\nu - \Delta\mu = (\mu^2 + \lambda\bar{\lambda}) + (\gamma + \bar{\gamma})\mu - \bar{\nu}\pi + [\tau - 3\beta - \bar{\alpha}]\nu + \Phi_{22} \quad (4.2n)$$

$$\delta\gamma - \Delta\beta = (\tau - \bar{\alpha} - \beta)\gamma + \mu\tau - \sigma\nu - \epsilon\bar{\nu} - \beta(\gamma - \bar{\gamma} - \mu) + \alpha\bar{\lambda} + \Phi_{12} \quad (4.2o)$$

$$\delta\tau - \Delta\sigma = (\mu\sigma + \bar{\lambda}\rho) + (\tau + \beta - \bar{\alpha})\tau - (3\gamma - \bar{\gamma})\sigma - \kappa\bar{\nu} + \Phi_{02} \quad (4.2p)$$

$$\Delta\rho - \bar{\delta}\tau = -(\rho\bar{\mu} + \sigma\lambda) + (\bar{\beta} - \alpha - \bar{\tau})\tau + (\gamma + \bar{\gamma})\rho + \nu\kappa - \Psi_2 - 2\Lambda \quad (4.2q)$$

$$\Delta\alpha - \bar{\delta}\gamma = (\rho + \epsilon)\nu - (\tau + \beta)\lambda + (\bar{\gamma} - \bar{\mu})\alpha + (\bar{\beta} - \bar{\tau})\gamma - \Psi_3. \quad (4.2r)$$

The notation for intrinsic derivatives (2.12) has been used. The quantities Ψ_0, Ψ_1, etc., Φ_{00}, etc., and Λ are, respectively, related to components of the Weyl tensor, Ricci tensor, and scalar curvature by the following;

$$\Psi_0 = -C_{1313} = -C_{\alpha\beta\gamma\delta}l^\alpha m^\beta l^\gamma m^\delta = \Psi_{0000} \quad (4.3a)$$

$$\Psi_1 = -C_{1213} = -C_{\alpha\beta\gamma\delta}l^\alpha n^\beta l^\gamma m^\delta = \Psi_{0001}$$

$$\Psi_2 = -\tfrac{1}{2}(C_{1212} + C_{1234}) = -\tfrac{1}{2}C_{\alpha\beta\gamma\delta} \times (l^\alpha n^\beta l^\gamma n^\delta + l^\alpha n^\beta m^\gamma \bar{m}^\delta) = \Psi_{0011}$$

$$\Psi_3 = C_{1224} = C_{\alpha\beta\gamma\delta}l^\alpha n^\beta n^\gamma \bar{m}^\delta = \Psi_{0111}$$

$$\Psi_4 = -C_{2424} = -C_{\alpha\beta\gamma\delta}n^\alpha \bar{m}^\beta n^\gamma \bar{m}^\delta = \Psi_{1111}$$

$$\Phi_{00} = -\tfrac{1}{2}R_{11} = \Phi_{000'0'} = \bar{\Phi}_{00},$$

$$\Phi_{11} = -\tfrac{1}{4}(R_{12} + R_{34}) = \Phi_{010'1'} \quad (4.3b)$$

$$\Phi_{01} = -\tfrac{1}{2}R_{13} = \Phi_{000'1'} = \bar{\Phi}_{10},$$

$$\Phi_{12} = -\tfrac{1}{2}R_{23} = \Phi_{011'1'},$$

$$\Phi_{10} = -\tfrac{1}{2}R_{14} = \Phi_{010'0'} = \bar{\Phi}_{01},$$

$$\Phi_{21} = -\tfrac{1}{2}R_{24} = \Phi_{110'1'},$$

$$\Phi_{02} = -\tfrac{1}{2}R_{33} = \Phi_{001'1'} = \bar{\Phi}_{20},$$

$$\Phi_{22} = -\tfrac{1}{2}R_{22} = \Phi_{111'1'},$$

$$\Phi_{20} = -\tfrac{1}{2}R_{44} = \Phi_{110'0'},$$

$$\Lambda = R/24.$$

With the present notation the commutators (2.11) or (3.13) are

$$(\Delta D - D\Delta)\varphi = [(\gamma + \bar{\gamma})D + (\epsilon + \bar{\epsilon})\Delta - (\tau + \bar{\pi})\bar{\delta} - (\bar{\tau} + \pi)\delta]\varphi \quad (4.4)$$

$$(\delta D - D\delta)\varphi = [(\bar{\alpha} + \beta - \bar{\pi})D + \kappa\Delta - \sigma\bar{\delta} - (\bar{\rho} + \epsilon - \bar{\epsilon})\delta]\varphi$$

$$(\delta\Delta - \Delta\delta)\varphi = [-\bar{\nu}D + (\tau - \bar{\alpha} - \beta)\Delta + \bar{\lambda}\bar{\delta} + (\mu - \gamma + \bar{\gamma})\delta]\varphi$$

$$(\bar{\delta}\delta - \delta\bar{\delta})\varphi = [(\bar{\mu} - \mu)D + (\bar{\rho} - \rho)\Delta - (\bar{\alpha} - \beta)\bar{\delta} - (\bar{\beta} - \alpha)\delta]\varphi.$$

The Bianchi identities (2.9) or (3.18) when written out in general, are very long and unwieldy. However in empty-space, $R_{\alpha\beta} = \Phi_{ABC'D'} = 0$, they do have the simple form[21]

$$D\Psi_1 - \bar{\delta}\Psi_0 = -3\kappa\Psi_2 + [2\epsilon + 4\rho]\Psi_1 - [-\pi + 4\alpha]\Psi_0 \quad (4.5)$$

$$D\Psi_2 - \bar{\delta}\Psi_1 = -2\kappa\Psi_3 + 3\rho\Psi_2 - [-2\pi + 2\alpha]\Psi_1 - \lambda\Psi_0$$

$$D\Psi_3 - \bar{\delta}\Psi_2 = -\kappa\Psi_4 - [2\epsilon - 2\rho]\Psi_3 + 3\pi\Psi_2 - 2\lambda\Psi_1$$

$$D\Psi_4 - \bar{\delta}\Psi_3 = -[4\epsilon - \rho]\Psi_4 + [4\pi + 2\alpha]\Psi_3 - 3\lambda\Psi_2$$

$$\Delta\Psi_0 - \delta\Psi_1 = [4\gamma - \mu]\Psi_0 - [4\tau + 2\beta]\Psi_1 + 3\sigma\Psi_2$$

[21] For completeness, though it is never used in this paper, we give in the Appendix the formulas for the Bianchi identities in the presence of a Maxwell field as well as the Maxwell equations using the notation of this section.

$$\Delta\Psi_1 - \delta\Psi_2 = \nu\Psi_0 + [2\gamma - 2\mu]\Psi_1 - 3\tau\Psi_2 + 2\sigma\Psi_3$$

$$\Delta\Psi_2 - \delta\Psi_3 = 2\nu\Psi_1 - 3\mu\Psi_2 + [-2\tau + 2\beta]\Psi_3 + \sigma\Psi_4$$

$$\Delta\Psi_3 - \delta\Psi_4 = 3\nu\Psi_2 - [2\gamma + 4\mu]\Psi_3 + [-\tau + 4\beta]\Psi_4.$$

Before proceeding to applications of the formalism developed here, it is useful to examine briefly the geometric meaning of some of quantities (4.1) and (4.3) which will be used frequently in the remainder of the paper.

The spin coefficient κ is related to the first curvature of the congruence of which l_μ is the tangent vector by the equation

$$l_{\mu;\nu}l^\nu = -\kappa\bar{m}_\mu - \bar{\kappa}m_\mu + (\epsilon + \bar{\epsilon})l_\mu. \tag{4.6}$$

It is easily seen that if $\kappa = 0$, l_μ is tangent to a geodesic. By a change in scale $l_\mu \to \varphi l_\mu$, $\epsilon + \bar{\epsilon}$ can be made zero. In the case of a geodesic with the above choice of scaling for l_μ we have

$$\rho = \tfrac{1}{2}[-l^\mu{}_{;\mu} + i \text{ curl } l_\mu],$$

where

$$\text{curl } l_\mu = (l_{[\mu;\nu]}l^{[\mu;\nu]})^{\frac{1}{2}} \tag{4.7}$$

and σ is the complex shear of l_μ satisfying[12,22]

$$\sigma\bar{\sigma} = \tfrac{1}{2}[l_{(\mu;\nu)}l^{\mu;\nu} - \tfrac{1}{2}(l^\mu{}_{;\mu})^2].$$

The quantity τ describes how the direction of l_μ changes as we move in the direction n_μ as follows from the equation

$$l_{\mu;\nu}n^\nu = -\tau\bar{m}_\mu - \bar{\tau}m_\mu + (\gamma + \bar{\gamma})l_\mu. \tag{4.8}$$

Again we can make $\gamma + \bar{\gamma}$ zero by the change $l_\mu \to \varphi l_\mu$.

The spin coefficients ν, μ, λ, π are analogous, respectively, to κ, $-\rho$, $-\sigma$, τ, the difference being that the congruence used is given by n_μ instead of l_μ.

If l_μ is taken tangent to a geodesic congruence and we wish to propogate the remainder of the tetrad system parallelly along this congruence, then

$$\kappa = \epsilon = \pi = 0. \tag{4.9}$$

If in addition to being tangent to geodesics, the l_μ are hypersurface orthogonal, that is, proportional to a gradiant field, we have

$$\rho = \bar{\rho}, \tag{4.10}$$

if *equal* to a gradient field

$$\rho = \bar{\rho}, \qquad \tau = \bar{\alpha} + \beta. \tag{4.11}$$

One can understand the meaning of Ψ_0, Ψ_1, Ψ_2, Ψ_3, and Ψ_4 by the following:

Consider the five cases

(a) $\Psi_0 \neq 0$, others zero
(b) $\Psi_1 \neq 0$, others zero
(c) $\Psi_2 \neq 0$, others zero
(d) $\Psi_3 \neq 0$, others zero
(e) $\Psi_4 \neq 0$, others zero.

The Weyl tensor or the tetrad components of the Weyl tensor will have the following algebraic properties in each of the five cases;

(a) Petrov type N (or [4])[8] with propagation vector n_μ,
(b) Petrov type III (or [31]) with propagation vector n_μ,
(c) Petrov type D (or [22]) with propagation vector n_μ and l_μ,
(d) Petrov type III (or [31]) with propagation vector l_μ,
(e) Petrov type N (or [4]) with propagation vector l_μ.

By a propagation vector, we mean a repeated principal null vector.[8]

If in empty space the vector field l_μ satisfies the equation $l_{[\mu}R_{\alpha]\beta\gamma[\delta}l_{\nu]}l^\beta l^\gamma = 0$, then l_μ corresponds to one of the four principal null directions of the Riemann tensor and

$$\Psi_0 = 0. \tag{4.12}$$

If two or more of the principal null directions coincide and are represented by l_μ, they must satisfy $R_{\alpha\beta\gamma[\delta}l_{\mu]}l^\beta l^\gamma = 0$ or

$$\Psi_0 = \Psi_1 = 0. \tag{4.13}$$

(In this case, one refers to the Riemann tensor as being algebraically specialized.)

In the following section it will be shown that in empty space if the l_μ are tangents to a geodetic congruence whose shear σ vanishes, then (4.13) must be satisfied, and conversely.

V. GOLDBERG-SACHS THEOREM

In this section the conciseness attained by the use of spin coefficients will be illustrated by an example. Here and in the remainder of the paper it will be assumed that we are dealing with empty space, i.e.,

$$R_{\alpha\beta} = 0.$$

[22] I. Robinson, J. Math. Phys. **2**, 290 (1961).

First we will prove that if the Riemann tensor is algebraically specialized, having $\Psi_0 = \Psi_1 = 0$, then $\sigma = \kappa = 0$. With these assumptions the pertinent Bianchi identities become

$$3\sigma\Psi_2 = 0,$$

$$-\delta\Psi_2 = -3\tau\Psi_2 + 2\sigma\Psi_3 \tag{5.1a}$$

$$\Delta\Psi_2 - \delta\Psi_3 = -3\mu\Psi_2 + (-2\tau + 2\beta)\Psi_3 + \sigma\Psi_4$$

$$-3\kappa\Psi_2 = 0$$

$$D\Psi_2 = -2\kappa\Psi_3 + 3\rho\Psi_2 \tag{5.1b}$$

$$D\Psi_3 - \bar{\delta}\Psi_2 = -\kappa\Psi_4 - (2\epsilon - 2\rho)\Psi_3 + 3\pi\Psi_2.$$

It is easily seen from this that unless the space is flat, $\sigma = 0$ by (5.1a) and $\kappa = 0$ by (5.1b).

The converse is more difficult to prove. We assume $\sigma = \kappa = 0$ and wish to prove $\Psi_0 = \Psi_1 = 0$. We can, by a transformation of the form $m_\mu \to e^{i\theta}m_\mu$ and by using a suitable scaling of l_μ, set $\epsilon = 0$.

The pertinent Eqs. (4.2) are then

$$D\rho = \rho^2 \tag{4.2a'}$$

$$0 = \Psi_0 \tag{4.2b'}$$

$$D\tau = (\tau + \bar{\pi})\rho + \Psi_1 \tag{4.2c'}$$

$$D\beta = \beta\bar{\rho} + \Psi_1 \tag{4.2e'}$$

$$\delta\rho = \rho(\bar{\alpha} + \beta) + (\rho - \bar{\rho})\tau - \Psi_1. \tag{4.2k'}$$

With the fact that $\Psi_0 = 0$, [Eq. (4.2b')] the needed Bianchi identities and commutator are

$$\delta\Psi_1 = (4\tau + 2\beta)\Psi_1 \tag{5.2}$$

$$D\Psi_1 = 4\rho\Psi_1 \tag{5.3}$$

$$(D\delta - \delta D)\varphi = (\bar{\pi} - \bar{\alpha} - \beta)\, D\varphi + \bar{\rho}\,\delta\varphi. \tag{5.4}$$

There is yet a freedom in the choice of the vector n_μ, the freedom being that of the so-called "null rotations,"

$$\begin{aligned} l_\mu &\to l_\mu \\ m_\mu &\to m_\mu + a l_\mu \\ n_\mu &\to n_\mu + a\bar{m}_\mu + \bar{a}m_\mu + a\bar{a}l_\mu. \end{aligned} \tag{5.5}$$

This rotation of the tetrad does not change l_μ or disturb the relation $\epsilon = 0$. The complex function a can be chosen so that $\tau = 0$. [It is possible to do this only if $\rho \neq 0$. However from (4.2 k') it is easily seen that if $\rho = 0$, then $\Psi_1 = 0$, and our theorem is proved.]

Equations (5.2) and (5.3) are rewritten

$$\begin{aligned} \delta \ln \Psi_1 &= 2\beta \\ D \ln \Psi_1 &= 4\rho. \end{aligned} \tag{5.6}$$

Taking mixed derivatives and subtracting the two expressions, we have

$$(D\delta - \delta D) \ln \Psi_1 = 2\, D\beta - 4\,\delta\rho$$

$$= 2\beta\bar{\rho} - 4\rho(\bar{\alpha} + \beta) + 6\Psi_1 \tag{5.7}$$

after using (4.2 e') and (4.2 b'). The commutator (5.4) with $\varphi = \ln \Psi_1$, and using (5.6) is

$$(D\delta - \delta D) \ln \Psi_1 = 2\beta\bar{\rho} - 4\rho(\bar{\alpha} + \beta) + 4\rho\bar{\pi}. \tag{5.8}$$

Subtracting (5.8) from (5.7) we have

$$\Psi_1 = \tfrac{2}{3}\bar{\pi}\rho.$$

If this is compared with (4.2 c'), $\Psi_1 = -\bar{\pi}\rho$ we have, since ρ is assumed different from zero, $\Psi_1 = \bar{\pi} = 0$. This completes the proof.[23]

VI. SPECIAL COORDINATES

It is always possible, in a hyperbolic Riemannian manifold, to introduce a family of null hypersurfaces $u = \text{const}$, that is,

$$g^{\mu\nu}u_{,\mu}u_{,\nu} = 0. \tag{6.1}$$

The vectors $l^\mu = g^{\mu\nu}u_{,\nu}$ are tangent to the family of null geodesics lying in the hypersurfaces $u = \text{const}$, and satisfy

$$l^\mu{}_{;\nu}l^\nu = 0. \tag{6.2}$$

Robinson and Trautman[13] show that if one chooses as coordinates $u = x^1$ and an affine parameter[24] along the geodesics $r = x^2$, and two coordinates x^3, x^4 that label the geodesics on each surface $u = \text{constant}$, the metric takes the form ($i, j = 3, 4$)

$$g^{\mu\nu} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & g^{22} & g^{23} & g^{24} \\ 0 & g^{23} & & \\ 0 & g^{24} & & g^{ij} \end{bmatrix}. \tag{6.3}$$

(It is not always most convenient to use an affine parameter as x^2. Sachs uses a "luminosity" parameter, $\tilde{r} = 2/l^\mu{}_{;\mu}$ which makes the g^{12} different from unity. However, for our purposes an affine parameter seems simplest.)

With these coordinates the vector l_μ becomes

$$l_\mu = \delta^1_\mu, \qquad l^\mu = \delta^\mu_2. \tag{6.4}$$

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[23] Though we have not seen all the details of the Goldberg-Sachs proof, we believe our proof to be essentially equivalent, but, due to the conciseness of our notation, much shorter.

[24] An affine parameter is a parameter along the geodesic, such that the equation for the geodesic takes the standard form. See, for example, E. M. Schrödinger, *Expanding Universes* (Cambridge University Press, New York, 1956).

To preserve $l_\mu n^\mu = 1$, and $l_\mu m^\mu = 0$, we have ($i = 3, 4$)

$$\begin{aligned} m^\mu &= \omega\ \delta_2^\mu + \xi^i\ \delta_i^\mu \\ n^\mu &= \delta_1^\mu + U\ \delta_2^\mu + X^i\ \delta_i^\mu. \end{aligned} \tag{6.5}$$

The relation between the tetrad components (6.4) and (6.5) and the metric components (6.3) is

$$\begin{aligned} g^{22} &= 2(U - \omega\bar{\omega}), \\ g^{2i} &= X^i - (\xi^i\bar{\omega} + \bar{\xi}^i\omega), \\ g^{ij} &= -(\xi^i\bar{\xi}^j + \bar{\xi}^i\xi^j), \end{aligned} \tag{6.6}$$

($i, j = 3, 4$). This follows from (2.3a).

There is still complete freedom for the rotation of the tetrad vectors m^μ and n^μ leaving l^μ fixed. This freedom is eliminated by demanding m^μ and n^μ be parallelly propagated along l^μ. This requirement, in addition to the knowledge that l_μ is a gradient field, is stated in terms of the spin coefficients by (see Sec. IV)

$$\kappa = \pi = \epsilon = 0, \quad \rho = \bar{\rho}, \quad \tau = \bar{\alpha} + \beta. \tag{6.7}$$

With these simplifications the commutators (4.4) are

$$\begin{aligned} (\Delta D - D\Delta)\varphi &= (\gamma + \bar{\gamma})\ D\varphi \\ &\quad - \tau\ \bar{\delta}\varphi - \bar{\tau}\ \delta\varphi \\ (\delta D - D\delta)\varphi &= [\bar{\alpha} + \beta]\ D\varphi \\ &\quad - \sigma\ \bar{\delta}\varphi - \rho\ \delta\varphi \\ (\delta\Delta - \Delta\delta)\varphi &= -\bar{\nu}\ D\varphi \\ &\quad + \bar{\lambda}\ \bar{\delta}\varphi + [\mu + \bar{\gamma} - \gamma]\ \delta\varphi \\ (\bar{\delta}\delta - \delta\bar{\delta})\varphi &= (\mu - \bar{\mu})\ D\varphi \\ &\quad - [\bar{\alpha} - \beta]\ \bar{\delta}\varphi - [\bar{\beta} - \alpha]\ \delta\varphi \end{aligned} \tag{6.8}$$

with [using (6.5) and (2.12)]

$$\begin{aligned} D &= \partial/\partial r, \qquad \delta = \omega\ \partial/\partial r + \xi^i\ \partial/\partial x^i \\ \Delta &= U\ \partial/\partial r + \partial/\partial u + X^i\ \partial/\partial x^i. \end{aligned} \tag{6.9}$$

In order to relate the tetrad components (or metric components) and the spin coefficients we replace φ by u, r, and x^i, respectively, in the four commutators. The result of this operation is ($i = 3, 4$)

$$D\xi^i = \rho\xi^i + \sigma\bar{\xi}^i \tag{6.10a}$$

$$D\omega = \rho\omega + \sigma\bar{\omega} - (\bar{\alpha} + \beta) \tag{6.10b}$$

$$DX^i = \tau\bar{\xi}^i + \bar{\tau}\xi^i \tag{6.10c}$$

$$DU = \tau\bar{\omega} + \bar{\tau}\omega - (\gamma + \bar{\gamma}) \tag{6.10d}$$

$$\delta X^i - \Delta\xi^i = (\mu + \bar{\gamma} - \gamma)\xi^i + \bar{\lambda}\bar{\xi}^i \tag{6.10e}$$

$$\delta\bar{\xi}^i - \bar{\delta}\xi^i = (\bar{\beta} - \alpha)\xi^i + (\bar{\alpha} - \beta)\bar{\xi}^i \tag{6.10f}$$

$$\delta\bar{\omega} - \bar{\delta}\omega = (\bar{\beta} - \alpha)\omega + (\bar{\alpha} - \beta)\bar{\omega} + (\mu - \bar{\mu}) \tag{6.10g}$$

$$\delta U - \Delta\omega = (\mu + \bar{\gamma} - \gamma)\omega + \bar{\lambda}\bar{\omega} - \bar{\nu}. \tag{6.10h}$$

We will refer to these as the metric equations.

To conclude this section we will write the Eqs. (4.2) and the Bianchi identities using the conditions (6.7).

$$D\rho = \rho^2 + \sigma\bar{\sigma} \tag{6.11a}$$

$$D\sigma = 2\rho\sigma + \Psi_0 \tag{6.11b}$$

$$D\tau = \tau\rho + \bar{\tau}\sigma + \Psi_1 \tag{6.11c}$$

$$D\alpha = \alpha\rho + \beta\bar{\sigma} \tag{6.11d}$$

$$D\beta = \beta\rho + \alpha\sigma + \Psi_1 \tag{6.11e}$$

$$D\gamma = \tau\alpha + \bar{\tau}\beta + \Psi_2 \tag{6.11f}$$

$$D\lambda = \lambda\rho + \mu\bar{\sigma} \tag{6.11g}$$

$$D\mu = \mu\rho + \lambda\sigma + \Psi_2 \tag{6.11h}$$

$$D\nu = \tau\lambda + \bar{\tau}\mu + \Psi_3 \tag{6.11i}$$

$$\Delta\lambda - \bar{\delta}\nu = 2\alpha\nu + (\bar{\gamma} - 3\gamma - \mu - \bar{\mu})\lambda - \Psi_4 \tag{6.11j}$$

$$\delta\rho - \bar{\delta}\sigma = (\beta + \bar{\alpha})\rho + (\bar{\beta} - 3\alpha)\sigma - \Psi_1 \tag{6.11k}$$

$$\delta\alpha - \bar{\delta}\beta = \mu\rho - \lambda\sigma - 2\alpha\beta + \alpha\bar{\alpha} + \beta\bar{\beta} - \Psi_2 \tag{6.11l}$$

$$\delta\lambda - \bar{\delta}\mu = (\alpha + \bar{\beta})\mu + (\bar{\alpha} - 3\beta)\lambda - \Psi_3 \tag{6.11m}$$

$$\delta\nu - \Delta\mu = \gamma\mu - 2\nu\beta + \bar{\gamma}\mu + \mu^2 + \lambda\bar{\lambda} \tag{6.11n}$$

$$\delta\gamma - \Delta\beta = \tau\mu - \sigma\nu + (\mu - \gamma + \bar{\gamma})\beta + \bar{\lambda}\alpha \tag{6.11o}$$

$$\delta\tau - \Delta\sigma = 2\tau\beta + (\bar{\gamma} + \mu - 3\gamma)\sigma + \bar{\lambda}\rho \tag{6.11p}$$

$$\Delta\rho - \bar{\delta}\tau = (\gamma + \bar{\gamma} - \bar{\mu})\rho - 2\alpha\tau - \lambda\sigma - \Psi_2 \tag{6.11q}$$

$$\begin{aligned} \Delta\alpha - \bar{\delta}\gamma &= \rho\nu - \tau\lambda - \lambda\beta \\ &\quad + (\bar{\gamma} - \gamma - \bar{\mu})\alpha - \Psi_3 \end{aligned} \tag{6.11r}$$

$$D\Psi_1 - \bar{\delta}\Psi_0 = 4\rho\Psi_1 - 4\alpha\Psi_0 \tag{6.12a}$$

$$D\Psi_2 - \bar{\delta}\Psi_1 = 3\rho\Psi_2 - 2\alpha\Psi_1 - \lambda\Psi_0 \tag{6.12b}$$

$$D\Psi_3 - \bar{\delta}\Psi_2 = 2\rho\Psi_3 - 2\lambda\Psi_1 \tag{6.12c}$$

$$D\Psi_4 - \bar{\delta}\Psi_3 = \rho\Psi_4 + 2\alpha\Psi_3 - 3\lambda\Psi_2 \tag{6.12d}$$

$$\begin{aligned} \Delta\Psi_0 - \delta\Psi_1 &= [4\gamma - \mu]\Psi_0 \\ &\quad - [4\tau + 2\beta]\Psi_1 + 3\sigma\Psi_2 \end{aligned} \tag{6.12e}$$

$$\begin{aligned} \Delta\Psi_1 - \delta\Psi_2 &= \nu\Psi_0 + [2\gamma - 2\mu]\Psi_1 \\ &\quad - 3\tau\Psi_2 + 2\sigma\Psi_3 \end{aligned} \tag{6.12f}$$

$$\begin{aligned} \Delta\Psi_2 - \delta\Psi_3 &= 2\nu\Psi_1 - 3\mu\Psi_2 \\ &\quad + [-2\tau + 2\beta]\Psi_3 + \sigma\Psi_4 \end{aligned} \tag{6.12g}$$

$$\Delta\Psi_3 - \delta\Psi_4 = 3\nu\Psi_2 - [2\gamma + 4\mu]\Psi_3 + [-\tau + 4\beta]\Psi_4. \quad (6.12h)$$

VII. ASYMPTOTIC BEHAVIOR

We shall now investigate the asymptotic behavior of the Riemann tensor, spin coefficients and metric, for a general type of radiative empty space time. In order to do this, it is necessary to impose some condition of approach to flatness at infinity on the space time. This is usually done in terms of the metric tensor, but it is a little more satisfactory to impose restrictions on the Riemann tensor instead, as we shall do here.

The main condition that will be adopted here is[25]

$$\Psi_0 = O(r^{-5}) \quad (7.1)$$

but a condition

$$D\Psi_0 = O(r^{-6}) \quad (7.2)$$

on the r derivative of Ψ_0 will also be used. Furthermore, an assumption of "uniform smoothness" will be imposed, that as many as four or three derivatives with respect to x^3, x^4 do not spoil the above dependence:

$$d_i\Psi_0 = O(r^{-5}), \cdots, d_i\, d_j\, d_k\, d_l\Psi_0 = O(r^{-5}) \quad (i, j, k, l = 3, 4)$$
$$d_i\, D\Psi_0 = O(r^{-6}), \cdots, d_i\, d_j\, d_k\, D\Psi_0 = O(r^{-6}) \quad (7.3)$$

where

$$d_i \equiv \partial/\partial x^i \qquad (i = 3, 4).$$

It will also be assumed that the hypersurfaces u = const are not so chosen that they are "asymptotically cylindrical" or "asymptotically plane." The exact meaning of this condition will be explained later. It means, in effect, merely that certain very special choices of coordinate system are to be ruled out. From these assumptions[26] we shall prove:

$$\Psi_1 = O(r^{-4}), \qquad \Psi_2 = O(r^{-3})$$
$$\Psi_3 = O(r^{-2}), \qquad \Psi_4 = O(r^{-1}). \quad (7.4)$$

If, in addition, we were to assume that the Riemann tensor (in tetrad form) could be expanded[27] in negative powers of r, for large r, then (7.4) would tell us that the coefficient of $r^{-n}(n = 1, \cdots, 5)$ has the algebraic form of an empty-space Riemann tensor having the direction l^μ as a $(5\text{-}n)$-fold principal null direction. Bondi and Sachs[6] have obtained a similar result under somewhat different (and more restrictive) assumptions.

The choice of Ψ_0 as the quantity whose properties are specified in order to characterize the space-time is in accordance with a certain form of characteristic initial value problem. Given a suitable null hypersurface u = const, the function Ψ_0 on this hypersurface constitutes the main part (and sometimes all) of the initial data[28] for gravitation that is required for continuation. This matter will be discussed elsewhere,[29] but it is worth pointing out here that the determination of $\Psi_1, \cdots, \Psi_4$ from Ψ_0 seems to be a natural first step in this continuation problem. Other quantities such as σ or certain metric variables can be used equally as alternative initial data, but the choice of Ψ_0 seems simpler and is apparently the natural analog for gravitation, of certain characteristic initial data that are appropriate for other fields.

The exponent -5 in (7.1) is in agreement with what one would expect from the linear theory of a radiating quadripole. Also, (7.1) holds for a general null hypersurface in Schwarzschild's solution. If the hypersurfaces u = const open out into the future (i.e., they are analogous to the future null cones given by constant advanced time) then the condition (7.1) would be expected to hold for an isolated system in the absence of incoming radiation, as is suggested by the linearized theory. In fact, even incoming radiation of sufficiently curtailed duration would not be expected to affect (7.1), (7.2), or (7.3).

We now proceed to prove (7.4) from our assumptions.[30] The proof of (7.4) for a particular null

[25] The meaning of the order symbols used here is that $f(r, u, x^i) = O[g(r)]$ means $|f(r, u, x^i)| < g(r)\, F(u, x^i)$ for some function F independent of r and for all large r, and $f(r, u, x^i) = o[g(r)]$ means

$$\lim_{r\to\infty} \frac{f(r, u, x^i)}{g(r)} = 0 \text{ for each } u, x^i.$$

[26] These assumptions, though stated in terms of a particular coordinate system appear to have a considerable amount of coordinate independence. For example, given a null geodesic with affine parameter r and tangent vector l_μ, if the r parameter of the original coordinate system can be so adjusted that

$$\bar{r} = r + o(r), \quad \bar{l}_\mu = l_\mu + O(r^{-1}),$$

then (7.4) implies that $\bar{\Psi}_0 = O(r^{-5})$ also, where $\bar{\Psi}_0$ is the complex Riemann tensor component associated with $\bar{l}_\mu$. However, additional global assumptions appear to be necessary to ensure that r can always be so chosen.

[27] This may be a fairly strong restriction. It is, of course, stronger than just local analyticity in r since, for example, $r^{-n} \ln r$ cannot be expanded in negative powers of r.

[28] More properly, the quantity $D\Psi_0 - 5\rho\Psi_0$ may be the most significant one to specify on the hypersurface.

[29] R. Penrose (to be published).

[30] The necessity of (7.3) for the deduction of (7.4) and of ruling out the "asymptotically plane" case can be illustrated by considerations of certain plane waves. Plane waves can also be used to show that, for example, a local assumption merely of $\Psi_4 = O(r^{-1})$ or even $R_{\mu\nu\rho\sigma} = O(r^{-1})$ is quite inadequate for obtaining (7.4).

geodesic u, x^2, x^3 = const will depend on (7.1), (7.2), (7.3) only along this geodesic and its neighborhood within the hypersurface u = const. The order of procedure will be to obtain the r dependence of first ρ, σ and then the various x^i derivatives ($i = 3, 4$) of ρ, σ up to third order. Next, α, β, ξ^i, ω, Ψ_1, are similarly obtained, followed by their x^i derivatives. Then λ, μ, Ψ_2, are treated correspondingly, followed by Ψ_3, Ψ_4. The r dependence of the remaining quantities τ, γ, ν, X^i, U and hence g^{ij} may also be obtained if desired.

Writing

$$P = \begin{bmatrix} \rho & \sigma \\ \bar{\sigma} & \rho \end{bmatrix}, \qquad Q = \begin{bmatrix} 0 & \Psi_0 \\ \bar{\Psi}_0 & 0 \end{bmatrix}$$

(6.11a, b) become

$$DP = P^2 + Q. \tag{7.5}$$

This equation may be solved by

$$P = -(DY)Y^{-1}, \tag{7.6}$$

where

$$Y = \begin{bmatrix} y_1 & y_2 \\ \bar{y}_1 & \bar{y}_2 \end{bmatrix} \tag{7.7}$$

is a nonsingular solution (for given P) of

$$DY = -PY \tag{7.8}$$

and so satisfies

$$D^2Y = -QY. \tag{7.9}$$

The asymptotic behavior of the solutions to (7.9) when $\int r\,|\Psi_0|\,dr = O(1)$, is[31]

$$DY = F + o(1) \tag{7.10}$$

$$Y = rF + o(r) \tag{7.11}$$

where F is a constant matrix. We can improve on this here since $Q = O(r^{-5})$. From (7.9) and (7.11) we get

$$D^2Y = -rQF + o(r^{-4}) = O(r^{-4}).$$

Hence, integrating[32] twice and comparing with (7.10), we get

$$DY = F + O(r^{-3}), \tag{7.12}$$

$$Y = rF + E + O(r^{-2}), \tag{7.13}$$

where E is another constant matrix. The solution (7.6) for P can now be used giving

$$P = -r^{-1}I + r^{-2}EF^{-1} + O(r^{-3}) \tag{7.14}$$

provided F is nonsingular. If F is singular, the asymptotic behavior of P is quite different. The case $|F| = 0$, $F \neq 0$, gives the "asymptotically cylindrical" case and P becomes asymptotically proportional to a singular matrix, with $\rho = -\frac{1}{2}r^{-1} + O(r^{-2})$. If $F = 0$, we get the "asymptotically plane" case and $P = O(r^{-3})$. [In each case, E must be such that there are two linearly independent columns among those of E, F. Otherwise it follows that in fact $|Y| = 0$ for all r so we do not get a solution of (7.5) for P.] These two exceptional cases are to be ruled out by assumption. For any given null geodesic u, x^2, x^3 = const the two types of exceptional behavior can always be avoided by an arbitrarily small change in the coordinate system which changes the relevant hypersurface u = const into a slightly different one through this null geodesic. Such exceptional solutions of the Eq. (7.5) do not occur for general choices of initial values for ρ and σ.

From (7.14) we get

$$\rho = -r^{-1} + O(r^{-2}), \qquad \sigma = O(r^{-2}). \tag{7.15}$$

In fact, a lot more can be obtained about the asymptotic behavior of ρ and σ, but (7.15) is all that will be needed here.

In order to proceed further, we shall require the following lemma:

Lemma. Let the complex $(n \times n)$ matrix B and the complex column n vector b be given functions of r where

$$B = O(r^{-2}), \qquad b = O(r^{-2}). \tag{7.16}$$

Let the $(n \times n)$ matrix A be independent of r and have no eigenvalue with a positive real part. Then all of the solution of

$$Dy = (Ar^{-1} + B)y + b \tag{7.17}$$

are bounded as $r \to \infty$, y being a complex column n vector function of r.

Proof. Put $r = e^l$, then (7.17) can be rewritten:

$$\frac{d}{dl}\begin{pmatrix} y \\ 1 \end{pmatrix} = \left\{ \left[\begin{array}{c|c} A & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \\ \hline 0 \cdots 0 & 0 \end{array}\right] + \left[\begin{array}{c|c} C & c \\ \hline 0 \cdots 0 & 0 \end{array}\right] \right\} \begin{pmatrix} y \\ 1 \end{pmatrix} \tag{7.18}$$

[31] E. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill Book Publishers Inc., New York, 1955), p. 103.

[32] It is permissible to integrate order symbols formally but not to differentiate them.

where

$$C(l) = e^l B(e^l), \qquad c(l) = e^l b(e^l). \tag{7.19}$$

Now, the solutions ($z = \{\exp Al\}z_0$, $\zeta = \zeta_0$) of

$$\frac{d}{dl}\begin{pmatrix} z \\ \zeta \end{pmatrix} = \left[\begin{array}{ccc|c} & & & 0 \\ & A & & \vdots \\ & & & 0 \\ \hline 0 & \cdots & 0 & 0 \end{array}\right]\begin{pmatrix} z \\ \zeta \end{pmatrix}$$

are all bounded. Also, by (7.16) and (7.19) it follows that the integrals with respect to l of the moduli of the elements of C and of c are bounded as $l \to \infty$. Hence by a theorem of N. Levinson,[33] the solutions of (7.18) are also all bounded [with $y = \{\exp Al\}y_0 + O(1)$]. This proves the lemma.[34]

Suppose, now, that B, b, and y are also functions of x^3, x^4. Then, differentiating (7.17) with respect to x^i we get

$$D(d_i y) = (Ar^{-1} + B)(d_i y) + \{(d_i B)y + d_i b\}, \qquad (i = 3, 4)$$

which is again of the form (7.17) provided that

$$d_i B = O(r^{-2}), \qquad d_i b = O(r^{-2}).$$

If this is the case, it follows from the lemma that $d_i y$ must also be bounded. Repeating this, we get the correspondiag results for higher derivatives.

Now consider the x^i derivatives of (6.11a, b) which can be put in the form

$$D\left\{r^2 d_i \begin{pmatrix} \rho \\ \sigma \\ \bar{\sigma} \end{pmatrix}\right\} = \begin{pmatrix} 2\rho + 2r^{-1} & \bar{\sigma} & \sigma \\ 2\sigma & 2\rho + 2r^{-1} & 0 \\ 2\bar{\sigma} & 0 & 2\rho + 2r^{-1} \end{pmatrix} \times r^2 d_i \begin{pmatrix} \rho \\ \sigma \\ \bar{\sigma} \end{pmatrix} + r^2 d_i \begin{pmatrix} 0 \\ \Psi_0 \\ \bar{\Psi}_0 \end{pmatrix}. \tag{7.20}$$

The lemma applies with $A = 0$, by (7.15), (7.3)', whence

$$d_i\rho = O(r^{-2}), \quad d_i\sigma = O(r^{-2}) \quad (i = 3, 4). \tag{7.21}$$

The lemma applies again to the next two x^i derivatives of (7.20) successively, whence

$$d_i\,d_j\rho,\ d_i\,d_j\sigma,\ d_i\,d_j\,d_k\rho,\ d_i\,d_j\,d_k\sigma = O(r^{-2}). \tag{7.22}$$

Next, using (6.9), we can apply the lemma to (6.12a), (6.11d, e), (6.10a, b), and their complex conjugates, y being the column vector

$$\{r^4\Psi_1, r^4\bar{\Psi}_1, r\alpha, r\bar{\alpha}, r\beta, r\bar{\beta}, r\xi^3, r\bar{\xi}^3, r\xi^4, r\bar{\xi}^4, \omega, \bar{\omega}\},$$

$b = 0$

and

$$A = \left[\begin{array}{ccc|cc} 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 \\ \hline & -a & & -1 & 0 \\ & & & 0 & -1 \end{array}\right],$$

$$a = \begin{bmatrix} 0&0&0&1&1&0&0&0&0&0 \\ 0&0&1&0&0&1&0&0&0&0 \end{bmatrix},$$

the elements of B being $O(r^{-2})$ expressions in r, ρ, σ, Ψ_0, $D\Psi_0$, and $d_i\Psi_0$. Hence

$$\Psi_1 = O(r^{-4}) \tag{7.23}$$

and

$$\alpha, \beta, \xi^3, \xi^4 = O(r^{-1}), \qquad \omega = 0(1). \tag{7.24}$$

Also, by (6.12a)

$$D\Psi_1 = O(r^{-5}). \tag{7.25}$$

Taking successive x^i derivatives and using (7.21), (7.22), and (7.3), the lemma also gives

$$d_i\Psi_1, \qquad d_i\,d_j\Psi_1, \qquad d_i\,d_j\,d_k\Psi_1 = O(r^{-4}),$$

$$d_i\alpha, \cdots, d_i\xi^4, \qquad d_i\,d_j\alpha, \cdots, d_i\,d_j\,d_k\xi^4 = O(r^{-1}),$$

$$d_i\omega, \cdots, d_i\,d_j\,d_k\omega = O(1)$$

and so by (6.12a)

$$d_i\,D\Psi_1, \qquad d_i\,d_j\,D\Psi_1 = O(r^{-5}).$$

Next consider (6.12b) and (6.11g, h). The lemma applies again with y as the column vector $\{r^3\Psi_2, r\lambda, r\mu\}$, with $A = 0$ and B, b as certain $O(r^{-2})$ expressions in r, ρ, σ, Ψ_0, α, Ψ_1, ω, $D\Psi_1$, ξ^i, $d_i\Psi_1$. Thus

$$\Psi_2 = O(r^{-3}) \tag{7.28}$$

$$\lambda, \mu = O(r^{-1}). \tag{7.29}$$

Hence,

$$D\Psi_2 = O(r^{-4}),$$

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[33] N. Levinson, Am. J. Math. **68**, 1 (1946).

[34] It may be seen from the proof to the lemma that conditions (7.16) are in fact, rather stronger than is necessary. They may be weakened to B, $b = O[f(r)]$ where $\int f\,dr = 0(1)$, $f > 0$. This enables condition (7.2) to be weakened to $D\Psi_0 = O(r^{-4}f(r))$ and (7.4) can still be obtained. Conditions (7.3) [and even (7.1)] can also be correspondingly weakened.

and continuing with the x^i derivatives we get

$$d_i\Psi_2, \quad d_id_j\Psi_2 = O(r^{-3});$$
$$d_i\lambda, \cdots, d_id_j\mu = O(r^{-1}); d_iD\Psi_2 = O(r^{-4}).$$

Similarly, the lemma applies to (6.12c) with $y = r^2\Psi_3$, then to its x^i derivative and then to (6.12d) with $y = r\Psi_4$ giving

$$\Psi_3 = O(r^{-2}) \tag{7.30}$$
$$d_i\Psi_3 = O(r^{-2}), \qquad D\Psi_3 = O(r^{-3})$$

and then

$$\Psi_4 = O(r^{-1}). \tag{7.31}$$

We may also continue the process and obtain

$$\tau = O(r^{-1}); \quad \gamma, \nu, X^3, X^4 = O(1); \quad U = O(r); \tag{7.32}$$

whence by (6.6)

$$g^{22} = O(r), \qquad g^{2i} = O(1), \qquad g^{ij} = O(r^{-2}),$$
$$(i, j = 3, 4). \tag{7.33}$$

It is possible to obtain a great deal more information about the asymptotic behavior of all these quantities by examining the above procedure a little more closely and then substituting the expressions obtained back into the equations. Also, by specializing the coordinate system further many simplifications can be obtained. (We have, in fact, not even used $\tau = \bar{\alpha} + \beta$ here.) This, together with the integration of the remainder of the Eqs. (6.10) and (6.11), will be discussed elsewhere.

VIII. CONCLUSIONS

In the last section we showed that under certain fairly general assumptions of approach to flatness at infinity that are to be expected in radiative empty spaces, the Riemann tensor exhibits a characteristic asymptotic behavior. This is given by (7.1), (7.23), (7.28), (7.30), and; (7.31); namely

$$\Psi_n = O(r^{-5+n}) \qquad (n = 0, 1, \cdots, 4).$$

We may thus, in general, break the space up into five regions; namely, a near zone, where all terms are important; three transition zones, where Ψ_0, Ψ_1, Ψ_2 become negligible in turn; and finally the radiation zone, where only Ψ_4 remains important and the Riemann tensor is essentially null. The fourth zone is, of course, generally essentially type III and the third is essentially "algebraically special" or usually type II.[5,13] The second zone is essentially a region in which there are "goedesic rays" in the terminology of Sachs[12] and the first zone is of "general" type.[6] Thus, as we move backwards from infinity along a suitable null geodesic the principal null directions "peel off" one by one from the (outgoing) radial direction. This behavior was first observed by Sachs by considering the linear theory.[6] (It must be pointed out, however, that in many particular cases the actual positions of the principal null directions and the Petrov types encountered may not, in fact, agree with the above in detail since some of the Ψ's may be fortuitously small in some regions.)

The analogy between the above and the case of electrodynamics is striking. In the latter case there are three regions to consider, namely, the near zone where r^{-3} terms are important, the transition zone where r^{-2} terms are important and the radiation zone where the field goes essentially as r^{-1} and is null. The two electromagnetic principal null directions exhibit, in the general case, the same characteristic "peeling off" as in the gravitational case.

An interesting further question to consider will be the corresponding "peeling off" theorem for the Einstein-Maxwell theory. The relevant spin coefficient equations are given in an appendix. Another question of importance here is that of the extent to which the assumptions made here are coordinate independent.

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APPENDIX

In the spin coefficient notation Maxwell's equations take the form

$$\begin{aligned} D\Phi_1 - \bar{\delta}\Phi_0 &= (\pi - 2\alpha)\Phi_0 + 2\rho\Phi_1 - \kappa\Phi_2 \\ D\Phi_2 - \bar{\delta}\Phi_1 &= -\lambda\Phi_0 + 2\pi\Phi_1 + (\rho - 2\epsilon)\Phi_2 \\ \delta\Phi_1 - \Delta\Phi_0 &= (\mu - 2\gamma)\Phi_0 + 2\tau\Phi_1 - \sigma\Phi_2 \\ \delta\Phi_2 - \Delta\Phi_1 &= -\nu\Phi_0 + 2\mu\Phi_1 + (\tau - 2\beta)\Phi_2 \end{aligned} \tag{A1}$$

with

$$\Phi_0 = F_{\mu\nu}l^\mu m^\nu, \qquad \Phi_1 = \tfrac{1}{2}F_{\mu\nu}(l^\mu n^\nu + \bar{m}^\mu m^\nu),$$
$$\Phi_2 = F_{\mu\nu}\bar{m}^\mu n^\nu.$$

If the Ricci tensor is proportional to the Maxwell stress tensor, so that

$$\Phi_{mn} = k\Phi_m\bar{\Phi}_n \qquad (m, n = 0, 1, 2) \tag{A2}$$

then the Bianchi identities become (choosing $k = 1$ for convenience)

$$
\begin{aligned}
&(\delta - \tau + 4\beta)\Psi_4 - (\Delta + 2\gamma + 4\mu)\Psi_3 + 3\nu\Psi_2 \\
&\qquad = \bar{\Phi}_1\,\Delta\Phi_2 - \bar{\Phi}_2\,\bar{\delta}\Phi_2 + 2(\bar{\Phi}_1\Phi_1\nu - \bar{\Phi}_2\Phi_1\lambda - \bar{\Phi}_1\Phi_2\gamma + \bar{\Phi}_2\Phi_2\alpha), \\
&(\delta - 2\tau + 2\beta)\Psi_3 + \sigma\Psi_4 - (\Delta + 3\mu)\Psi_2 + 2\nu\Psi_1 \\
&\qquad = \bar{\Phi}_1\,\delta\Phi_2 - \bar{\Phi}_2\,D\Phi_2 + 2(\bar{\Phi}_1\Phi_1\mu - \bar{\Phi}_2\Phi_1\pi - \bar{\Phi}_1\Phi_2\beta + \bar{\Phi}_2\Phi_2\epsilon), \\
&(\delta - 3\tau)\Psi_2 + 2\sigma\Psi_3 - (\Delta - 2\gamma + 2\mu)\Psi_1 + \nu\Psi_0 \\
&\qquad = \bar{\Phi}_1\,\Delta\Phi_0 - \bar{\Phi}_2\,\delta\Phi_0 + 2(\bar{\Phi}_1\Phi_0\gamma - \bar{\Phi}_2\Phi_0\alpha - \bar{\Phi}_1\Phi_1\tau + \bar{\Phi}_2\Phi_1\rho), \\
&(\delta - 4\tau - 2\beta)\Psi_1 + 3\sigma\Psi_2 - (\Delta - 4\gamma + \mu)\Psi_0 \\
&\qquad = \bar{\Phi}_1\,\delta\Phi_0 - \bar{\Phi}_2\,D\Phi_0 + 2(\bar{\Phi}_1\Phi_0\beta - \bar{\Phi}_2\Phi_0\epsilon - \bar{\Phi}_1\Phi_1\sigma + \bar{\Phi}_2\Phi_1\kappa), \qquad \text{(A3)} \\
&(D + 4\epsilon - \rho)\Psi_4 - (\bar{\delta} + 4\pi + 2\alpha)\Psi_3 + 3\lambda\Psi_2 \\
&\qquad = \bar{\Phi}_0\,\Delta\Phi_2 - \bar{\Phi}_1\,\bar{\delta}\Phi_2 + 2(\bar{\Phi}_0\Phi_1\nu - \bar{\Phi}_1\Phi_1\lambda - \bar{\Phi}_0\Phi_2\gamma + \bar{\Phi}_1\Phi_2\alpha), \\
&(D + 2\epsilon - 2\rho)\Psi_3 + \kappa\Psi_4 - (\bar{\delta} + 3\pi)\Psi_2 + 2\lambda\Psi_1 \\
&\qquad = \bar{\Phi}_0\,\delta\Phi_2 - \bar{\Phi}_1\,D\Phi_2 + 2(\bar{\Phi}_0\Phi_1\mu - \bar{\Phi}_1\Phi_1\pi - \bar{\Phi}_0\Phi_2\beta + \bar{\Phi}_1\Phi_2\epsilon), \\
&(D - 3\rho)\Psi_2 + 2\kappa\Psi_3 - (\bar{\delta} + 2\pi = 2\alpha)\Psi_1 + \lambda\Psi_0 \\
&\qquad = \bar{\Phi}_0\,\Delta\Phi_0 - \bar{\Phi}_1\,\delta\Phi_0 + 2(\bar{\Phi}_0\Phi_0\gamma - \bar{\Phi}_1\Phi_0\alpha - \bar{\Phi}_0\Phi_1\tau + \bar{\Phi}_1\Phi_1\rho), \\
&(D - 2\epsilon - 4\rho)\Psi_1 + 3\kappa\Psi_2 - (\bar{\delta} + \pi - 4\alpha)\Psi_0 \\
&\qquad = \bar{\Phi}_0\,\delta\Phi_0 - \bar{\Phi}_1\,D\Phi_0 + 2(\bar{\Phi}_0\Phi_0\beta - \bar{\Phi}_1\Phi_0\epsilon - \bar{\Phi}_0\Phi_1\sigma + \bar{\Phi}_1\Phi_1\kappa).
\end{aligned}
$$

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The Solution of a Transition Problem in a Superconducting Strip*

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The isothermal transition of a strip of superconducting material from the superconducting state to the normal state, under the influence of a supercritical external magnetic field, is studied on the basis of the London theory of superconductivity. The problem can be formulated as a free boundary problem with parabolic differential equations which is solved mainly by numerical methods; an analytical solution in the form of series expansions is given for the early part of the transition.

It is found that, in the beginning, the transition in the strip behaves almost like the transition in a half-space. However, the two differ quite drastically as the transition nears completion. It is pointed out that to predict the total transition time for the strip by extrapolating from the analytical solution for the half-space is incorrect. The results show that such an estimate for the transition time would be much too small.

I. INTRODUCTION

THE transition of a superconducting material from the superconducting state to the normal state has been considered in several recent papers. The problem has an obvious application in the use of superconductors in computer elements such as the cryotron. All of the work published thus far has been concerned with the case where the superconducting material fills an infinite half-space. For example, Ittner[1] and Duijvestijn[2] have considered the effects of latent heat and eddy currents on

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[1] W. B. Ittner, III, Phys. Rev. **111**, 1483 (1958).
[2] A. W. Duijvestijn, IBM J. Research Develop. **3**, 132 (1959).

then the Bianchi identities become (choosing $k = 1$ for convenience)

$$
\begin{aligned}
&(\delta - \tau + 4\beta)\Psi_4 - (\Delta + 2\gamma + 4\mu)\Psi_3 + 3\nu\Psi_2 \\
&\qquad = \bar{\Phi}_1\,\Delta\Phi_2 - \bar{\Phi}_2\,\bar{\delta}\Phi_2 + 2(\bar{\Phi}_1\Phi_1\nu - \bar{\Phi}_2\Phi_1\lambda - \bar{\Phi}_1\Phi_2\gamma + \bar{\Phi}_2\Phi_2\alpha), \\
&(\delta - 2\tau + 2\beta)\Psi_3 + \sigma\Psi_4 - (\Delta + 3\mu)\Psi_2 + 2\nu\Psi_1 \\
&\qquad = \bar{\Phi}_1\,\delta\Phi_2 - \bar{\Phi}_2\,D\Phi_2 + 2(\bar{\Phi}_1\Phi_1\mu - \bar{\Phi}_2\Phi_1\pi - \bar{\Phi}_1\Phi_2\beta + \bar{\Phi}_2\Phi_2\epsilon), \\
&(\delta - 3\tau)\Psi_2 + 2\sigma\Psi_3 - (\Delta - 2\gamma + 2\mu)\Psi_1 + \nu\Psi_0 \\
&\qquad = \bar{\Phi}_1\,\Delta\Phi_0 - \bar{\Phi}_2\,\delta\Phi_0 + 2(\bar{\Phi}_1\Phi_0\gamma - \bar{\Phi}_2\Phi_0\alpha - \bar{\Phi}_1\Phi_1\tau + \bar{\Phi}_2\Phi_1\rho), \\
&(\delta - 4\tau - 2\beta)\Psi_1 + 3\sigma\Psi_2 - (\Delta - 4\gamma + \mu)\Psi_0 \\
&\qquad = \bar{\Phi}_1\,\delta\Phi_0 - \bar{\Phi}_2\,D\Phi_0 + 2(\bar{\Phi}_1\Phi_0\beta - \bar{\Phi}_2\Phi_0\epsilon - \bar{\Phi}_1\Phi_1\sigma + \bar{\Phi}_2\Phi_1\kappa), \qquad \text{(A3)} \\
&(D + 4\epsilon - \rho)\Psi_4 - (\bar{\delta} + 4\pi + 2\alpha)\Psi_3 + 3\lambda\Psi_2 \\
&\qquad = \bar{\Phi}_0\,\Delta\Phi_2 - \bar{\Phi}_1\,\bar{\delta}\Phi_2 + 2(\bar{\Phi}_0\Phi_1\nu - \bar{\Phi}_1\Phi_1\lambda - \bar{\Phi}_0\Phi_2\gamma + \bar{\Phi}_1\Phi_2\alpha), \\
&(D + 2\epsilon - 2\rho)\Psi_3 + \kappa\Psi_4 - (\bar{\delta} + 3\pi)\Psi_2 + 2\lambda\Psi_1 \\
&\qquad = \bar{\Phi}_0\,\delta\Phi_2 - \bar{\Phi}_1\,D\Phi_2 + 2(\bar{\Phi}_0\Phi_1\mu - \bar{\Phi}_1\Phi_1\pi - \bar{\Phi}_0\Phi_2\beta + \bar{\Phi}_1\Phi_2\epsilon), \\
&(D - 3\rho)\Psi_2 + 2\kappa\Psi_3 - (\bar{\delta} + 2\pi = 2\alpha)\Psi_1 + \lambda\Psi_0 \\
&\qquad = \bar{\Phi}_0\,\Delta\Phi_0 - \bar{\Phi}_1\,\delta\Phi_0 + 2(\bar{\Phi}_0\Phi_0\gamma - \bar{\Phi}_1\Phi_0\alpha - \bar{\Phi}_0\Phi_1\tau + \bar{\Phi}_1\Phi_1\rho), \\
&(D - 2\epsilon - 4\rho)\Psi_1 + 3\kappa\Psi_2 - (\bar{\delta} + \pi - 4\alpha)\Psi_0 \\
&\qquad = \bar{\Phi}_0\,\delta\Phi_0 - \bar{\Phi}_1\,D\Phi_0 + 2(\bar{\Phi}_0\Phi_0\beta - \bar{\Phi}_1\Phi_0\epsilon - \bar{\Phi}_0\Phi_1\sigma + \bar{\Phi}_1\Phi_1\kappa).
\end{aligned}
$$

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The Solution of a Transition Problem in a Superconducting Strip*

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The isothermal transition of a strip of superconducting material from the superconducting state to the normal state, under the influence of a supercritical external magnetic field, is studied on the basis of the London theory of superconductivity. The problem can be formulated as a free boundary problem with parabolic differential equations which is solved mainly by numerical methods; an analytical solution in the form of series expansions is given for the early part of the transition.

It is found that, in the beginning, the transition in the strip behaves almost like the transition in a half-space. However, the two differ quite drastically as the transition nears completion. It is pointed out that to predict the total transition time for the strip by extrapolating from the analytical solution for the half-space is incorrect. The results show that such an estimate for the transition time would be much too small.

I. INTRODUCTION

THE transition of a superconducting material from the superconducting state to the normal state has been considered in several recent papers. The problem has an obvious application in the use of superconductors in computer elements such as the cryotron. All of the work published thus far has been concerned with the case where the superconducting material fills an infinite half-space. For example, Ittner[1] and Duijvestijn[2] have considered the effects of latent heat and eddy currents on

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switching rates under the assumption of zero penetration depth. Cohen and Miranker[3] have investigated the effect of nonzero penetration depth for an isothermal switching process.

In the present paper, the process is again taken to be isothermal and the penetration depth nonzero, but the superconducting half-space is replaced by a finite strip and the combined effect of the finite boundary distances and the nonzero penetration depth is studied.

The introduction of the finite strip width brings with it rather serious mathematical difficulties. A similarity treatment can no longer be used and asymptotic methods are not applicable to the case of greatest interest in which the strip width is of the same order of magnitude as the penetration depth. The difficulties are overcome mainly by applying a numerical method based upon finite differences, although an analytical solution is also given.

The effect of combining nonzero penetration depth with finite strip width is shown graphically in Figs. 5 through 9 and discussed in detail in Sec. IV. It is found that in the beginning the transition in the strip almost coincides with the transition in the half-space, but later on it can be radically different. Unless the strip is very thin, its complete transition takes much more time than the transition in the half-space takes to reach the same distance from the surface, all other circumstances being the same. In particular, the results show that it is dangerous to predict the total transition time θ by extrapolating the analytical solution valid for small times all the way to the center of the strip.

The problem studied in the present paper can be formulated in the following manner: Consider a two-dimensional strip of superconducting material of width $2w$, and let z denote the distance from one of its surfaces measured across the strip (Fig. 1). Let an equal external magnetic field exist on both sides of the strip, perpendicular to the z-y plane. Assume the superconductor is kept at a constant subcritical temperature, $T < T_c$, and the critical magnetic field associated with T is H_c.

If at time $\tau = 0$ the external field is instantaneously raised from a subcritical value, $H_0 < H_c$, to a supercritical value, $H_e > H_c$, two normal conducting regions begin to form along the two surfaces, $z = 0$ and $z = 2w$, with a superconducting strip of reduced width in between. The two plane fronts separating the three regions move inward

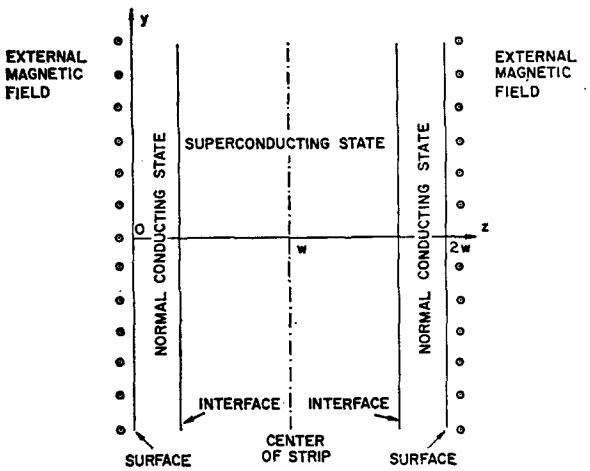

FIG. 1. Cross section of strip.

until, after the total transition time θ, they coincide at the center. Because of the symmetry with respect to $z = w$, it is enough to consider the transition in one half of the strip, say for $0 \leq z \leq w$.

The transition problem will be studied on the basis of the London theory of superconductivity. The amount of penetration is measured by the London penetration distance, $d = (\Lambda c^2/4\pi)^{\frac{1}{2}}$, where Λ is the London penetration constant and c the speed of light. At a given time τ the interface will be at a certain distance $\zeta(\tau)$ from the surface, where $\zeta(0) = 0$. The unknowns of the problem are $\zeta(\tau)$, as well as the field distributions $H^-(z, \tau)$ and $H^+(z, \tau)$ in the normal and superconducting regions, defined by $0 < z < \zeta(\tau)$ and $\zeta(\tau) < z \leq w$, respectively. For the total transition time θ one has $\zeta(\theta) = w$.

The corresponding problem in a half-space ($w = \infty$) and with an external field on the left side only, has been solved analytically, for small times and for $t \to \infty$, by Cohen and Miranker.[3] These authors found it useful to employ dimensionless space and time variables, x and t, respectively, by letting

$$x = z/z_0, \tag{1}$$

where z_0 is a convenient distance scale, and

$$t = \tau/\tau_0, \tag{2}$$

with

$$\tau_0 = 4\pi\sigma^- z_0^2/c^2, \tag{3}$$

where σ^- denotes the ohmic conductivity in the normal region. Furthermore, let

$$\alpha = z_0^2/d^2 \tag{4}$$

and $\beta = \sigma^+/\sigma^-$, where d is defined above and σ^+

[3] H. Cohen and W. L. Miranker, J. Math. Phys. **2**, 575 (1961).

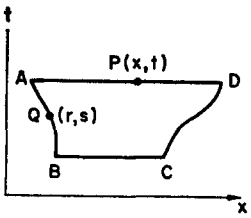

FIG. 2.

is the ohmic conductivity in the superconducting region. Finally, let

$$a = w/z_0 \tag{5}$$

$$\xi(t) = \zeta(\tau)/z_0, \tag{6}$$

and

$$\delta = \theta/\tau_0. \tag{7}$$

Then, $\xi(0) = 0$ and $\xi(\delta) = a$.

Mathematically, the transition of the strip, from the superconducting to the normal state, is described by the following free boundary problem (in which $0 < t$):

$$H^-_{xx} = H^-_t, \qquad [0 < x < \xi(t)], \tag{8}$$

$$H^+_{xx} = \alpha H^+ + \beta H^+_t, \qquad [\xi(t) < x < a, \quad t < \delta] \tag{9}$$

$$H^-(0, t) = H_e, \tag{10}$$

$$H^+_x(a, t) = 0, \qquad (t < \delta) \tag{11}$$

$$H^+(\xi(t), t) = H^-(\xi(t), t) = H_c, \qquad (t < \delta) \tag{12}$$

$$H^+_x(\xi(t), t) - \beta H^-_x(\xi(t), t) = -\alpha \int_{\xi(t)}^{a} H^+(x, t)\, dx, \qquad (t < \delta) \tag{13}$$

$$H^+(x, 0) = H_0 \cosh [\sqrt{(\alpha)}(a - x)]/\cosh [\sqrt{(\alpha)}a], \qquad (0 \leq x \leq a). \tag{14}$$

The diffusion and London equations, (8) and (9), boundary condition (10), and continuity relation (12) are equivalent with Eqs. (14), (15), (17), and (16) of reference 3, respectively. Relation (11) is a symmetry condition replacing (19) of reference 3. Interface condition (13) replaces (20) of reference 3 and is derived in the same way but using the fact that the supercurrent j^+ vanishes at the center $x = a$ of the strip. Finally, initial condition (14) says that, at $t = 0$, the subcritical field distribution is stationary [relation (14) is the solution of (9), with $H^+_t = 0$, which satisfies (11) and $H^+(0, 0) = H_0$].

In Sec. II of the present paper, the transition problem defined above is solved analytically for small times by expansions in powers of $\sqrt{t}$. In Sec. III, a numerical method is described which gives an approximate solution over the full time interval $0 \leq t \leq \delta$. Finally, in Sec. IV, the numerical and analytical results are discussed and compared with each other for various sets of parameter values.

II. ANALYTICAL APPROACH

1. Solution for Small Times

The problem defined in Sec. I can be solved analytically, for small times, using a Green's formula for the diffusion equation. However, the calculations involved are somewhat tedious. Therefore, the method will be explained in principle but only the more important relations, as well as the final result will be given in the following.

Consider a domain such as the one shown in Fig. 2, and assume $u(x, t)$ satisfies diffusion equation $u_{xx} = u_t$ in this domain. Then the following Green's theorem holds (reference 4, p. 311):

$$u(x, t) = \int_{ABCD} \{K(x, t; r, s)[u(r, s)\, dr + u_r(r, s)\, ds] - K_r(x, t; r, s)u(r, s)\, ds\}, \tag{15}$$

where the point $P(x, t)$ is between A and D, in the proper sense, $Q(r, s)$ is on the boundary $ABCD$, and

$$K(x, t; r, s) = \exp [-(x - r)^2/4(t - s)]/2(\pi)^{\frac{1}{2}}(t - s)^{\frac{1}{2}} \tag{16}$$

is the fundamental solution of $u_{rr} = u_s$, associated with $P(x, t)$. The segment BC is allowed to shrink to a point.

In this section, it will be assumed that $\beta = 1$; this amounts to passing to a *new* time variable, called t again, which is the old one divided by β. One can introduce new dependent variables,

$$u = H^- - H_e, \tag{17}$$

$$v = e^{\alpha t}H^+, \tag{18}$$

both of which satisfy diffusion equation (8), u being defined in the normal region and v in the superregion (Fig. 3). Let $0 < t < \delta$ and let $Q(r, s)$ be a

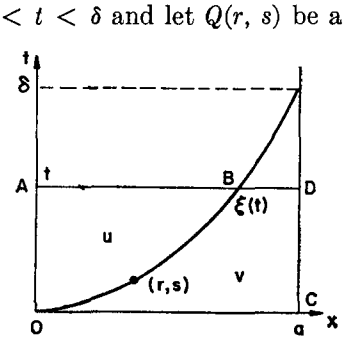

FIG. 3. (schematic).

[4] E. Goursat, *Cours d'analyse mathematique* III, (Gauthier-Villars, Paris, 1942), p. 287 *et. seq.*

point on the boundaries of the normal region, AOB, or of the super-region, $BOCD$. In terms of u and v, conditions (10) through (14) become

$$u(0, s) = 0 \tag{19}$$

$$v_r(a, s) = 0, \tag{20}$$

$$u(\xi(s), s) = -(H_e - H_c); v(\xi(s), s) = H_c e^{\alpha s}, \tag{21}$$

$$e^{-\alpha s} v_r(\xi(s), s) - u_r(\xi(s), s) = -\alpha e^{-\alpha s} \int_{\xi(s)}^{a} v(\rho, s)\, d\rho, \tag{22}$$

$$v(r, 0) = v_0(r) = H_0 \cosh [\sqrt{(\alpha)}(a - r)]/\cosh [\sqrt{(\alpha)}a], \tag{23}$$

respectively. The following notations will be used: $u_r(0, s) = f(s)$, $u_r(\xi(s), s) = g(s)$, $v_r(\xi(s), s) = h(s)$, and $v(a, s) = p(s)$. Formula (15) can be applied to both u and v. Noticing that $dr = 0$ along OA and CD, $ds = 0$ along OC, $dr = \dot{\xi}(s)ds$ on OB, and using the boundary and initial conditions, except (22), one gets

$$u(x, t) = -\int_0^t K(x, t; 0, s) f(s)\, ds + \int_0^t \{K(x, t; \xi(s), s)[g(s) - (H_e - H_c)\dot{\xi}(s)] + K_r(x, t; \xi(s), s)(H_e - H_c)\}\, ds, \tag{24}$$

and

$$v(x, t) = -\int_0^t \{K(x, t; \xi(s), s)[H_c e^{\alpha s}\dot{\xi}(s) + h(s)] - K_r(x, t; \xi(s), s) H_c e^{\alpha s}\}\, ds + \int_0^a K(x, t; r, 0) v_0(r)\, dr - \int_0^t K_r(x, t; a, s) p(s)\, ds. \tag{25}$$

If x passes to the limits 0 and $\xi(t)$ in (24), and to $\xi(t)$ and a in (25), four integral equations for $f(s)$, $g(s)$, $h(s)$, $p(s)$, and $\xi(s)$ are obtained. A fifth equation derives from (22). These equations will be called $I_1, I_2, \cdots I_5$, respectively. They can be solved for small t by expanding the unknown functions into powers of $\sqrt{t}$. The following steps must be carried out to achieve this.

Let $\psi(s)$ be a boundary of a domain, such as, e.g., OA, OB, or CD in Fig. 3, and let $x \to \psi(t) \pm$ denote the fact that x passes to the limit $\psi(t)$ from right (+) or left (−). As $x \to 0+$ and $\xi(t)-$ in (24), and $x \to \xi(t)+$ and $a-$ in (25), certain relations are needed for treating single- and double-layer integrals. Denote these two types of integrals by

$$S^{\psi}[q](x, t) = \int_0^t K(x, t; \psi(s), s) q(s)\, ds,$$

$$D^{\psi}[q](x, t) = \int_0^t K_r(x, t; \psi(s), s) q(s)\, ds,$$

respectively. Then, in passing to the limit, the following relations hold (reference 5, pp. 6, 7):

$$\lim_{x \to \psi(t)\mp} S^{\psi}[q](x, t) = S^{\psi}[q](\psi(t), t),$$

$$\lim_{x \to \psi(t)\mp} D^{\psi}[q](x, t) = D^{\psi}[q](\psi t), t) \pm q(t)/2.$$

Equation I_5 corresponding to (22) contains expressions such as $S_x^{\xi}[q]$ and $D_x^{\xi}[q]$. According to reference 5, (p. 7) they can be transformed as follows:

$$S_x^{\xi}[q] = -D^{\xi}[q],$$

$$D_x^{\xi}[q] = -\frac{q(0)}{2\sqrt{(\pi t)}} \exp(-x^2/4t) - D^{\xi}[q\dot{\xi}] - S^{\xi}[\dot{q}],$$

using the fact that $\xi(0) = 0$.

Let $K = K(x, t; r, s)$. With the help of relations

$$K_r = -K_x = K \cdot [(x - r)/2(t - s)]$$

$$K_{rr} = -K_{rx} = K \cdot \{[(x - r)^2/4(t - s)^2] - [1/2(t - s)]\},$$

derived from (16), one can rewrite all integrals in terms of K only.

In I_1 through I_5, it is useful to replace the integration variable s by $\sigma = s/t$, where $0 \leq \sigma \leq 1$. Also, new unknown functions can be defined by

$$\chi(s) = \xi(s)/\sqrt{s},$$

$$\phi(s) = \sqrt{(s)} f(s),$$

$$\gamma(s) = \sqrt{(s)} g(s),$$

$$\eta(s) = \sqrt{(s)} h(s).$$

Having made these transformations, the denominators of the integrands, the denominators of the exponents in the kernels, and the integration limits, of all integrals with respect to σ are independent of t (in I_5, in order to achieve this, one must also multiply all terms by $\sqrt{t}$).

In solving I_1 through I_5 for small t by power-series expansion, one can drop the unknown function $p(t)$ and Eq. I_4 (corresponding to $x \to a-$) for the following reasons. Equations I_1 and I_2 are free of

[5] I. I. Kolodner, Commun. Pure Appl. Math. 1, 1 (1956).

$p(s)$ to begin with. In I_3, the only term containing $p(s)$ is

$$\int_0^1 \frac{\exp\{-[\chi(t)-(a/\sqrt{t})]^2/4(1-\sigma)\}[\chi(t)-(a/\sqrt{t})]}{4\sqrt{\pi}\,(1-\sigma)^{\frac{3}{2}}} \times p(t\sigma)\,d\sigma.$$

Assuming $|p(s)|$ bounded for $0 \leq s \leq t$ and $\chi(t) = O(1)$ as $t \to 0$, this integral is smaller than any power of t as $t \to 0$. The same is true for the terms of I_5 containing $p(s)$. On the other hand, if one writes

$$\chi(s) = \sum_{j=0}^{\infty} \chi_j s^{j/2}, \tag{26}$$

and similar expansions for $\phi(s)$, $\gamma(s)$, and $\eta(s)$, and if the integrands are expanded with respect to σ and integrated term by term, most integrals of I_1, I_2, I_3, and I_5 have expansions in increasing powers of $\sqrt{t}$. Thus, one can neglect the terms containing $p(s)$ which do not contribute to any finite power of $\sqrt{t}$. As $p(t)$ itself is uninteresting for small t, one can drop I_4 and is left with four equations and four unknowns.

The only integrals in the new system of equations which are not taken with respect to σ are

$$\int_0^a K(x, t; r, 0)\begin{Bmatrix}\cosh\\ \sinh\end{Bmatrix}[\sqrt{(\alpha)}(a-r)]\,dr.$$

They can be evaluated in closed form using the normalized error function,

$$\Phi(y) = \frac{2}{\sqrt{\pi}}\int_0^y e^{-\nu^2}\,d\nu.$$

The values of y which occur are $O(1/\sqrt{t})$ as $t \to 0$. Thus, for small t one can use the asymptotic expression of $\Phi(y)$, which holds for large y's:

$$\Phi(y) = 1 - O(e^{-y^2}/y).$$

As terms $O(\sqrt{(t)}e^{-1/t})$ are dropped systematically in this small-time analysis, one simply has $\Phi(O(1\sqrt{t})) = 1$.

The solution has been calculated in zero-order approximation only. If χ_0 is for a moment assumed known, the zero-order approximations I_1^0, I_2^0, and I_3^0, of I_1, I_2, and I_3, respectively, form a linear algebraic system of equations for ϕ_0, γ_0, and η_0. The coefficients are transcendental expressions in χ_0 which can be evaluated in closed form by quadrature, using $\Phi(y)$ again. The solutions ϕ_0, γ_0, and η_0 can then be plugged into I_5^0, the zero-order approximation of I_5. This yields a transcendental equation for χ_0 which reduces to

$$\Phi(\chi_0/2) = \frac{H_e - H_c}{H_e - H_0}, \tag{27}$$

and from which χ_0 is obtained by inverse interpolation of the error function $\Phi(y)$ defined above. Equation (27) will be discussed in Sec. IV.

2. Remark on Final Part of Transition

Under certain conditions, one can predict that the transition in the strip should reach the center with infinite speed. In fact, assume

$$\lim_{t\to\delta}[H_x^+(\xi(t), t) - H_x^+(a, t)] = 0. \tag{28}$$

It is clear that

$$\lim_{t\to\delta}\int_{\xi(t)}^{a} H^+(x, t)\,dx = 0,$$

because H^+ is bounded and $[a - \xi(t)] \to 0$ as $t \to \delta$. Thus, from (11), (13), and (28) it follows that

$$\lim_{t\to\delta} H_x^+(\xi(t), t) = \lim_{t\to\delta} H_x^-(\xi(t), t) = 0. \tag{29}$$

Differentiating (12) with respect to time gives

$$dH^*(\xi(t), t)/dt = H_x^*(\xi(t), t)\dot{\xi}(t) + H_t^*(\xi(t), t) = 0. \tag{30}$$

Assume now that

$$\lim_{t\to\delta} H_t^+(\xi(t), t) \quad \text{and} \quad \lim_{t\to\delta} H_t^-(\xi(t), t)$$

do not vanish simultaneously. Then, it follows from (29) and (30) that $\dot{\xi}(t) \to \infty$ as $t \to \delta$, that is $\xi \to a$. The numerical solutions, obtained by the method described in Sec. III, seem to confirm this result (Figs. 7, 8, 9).

3. Limitations of Analytical Approach

As pointed out before, the analytical derivation of (27) requires tedious calculations. Furthermore, the result is disappointing because (27) is equivalent to the corresponding result for the half-space [reference 3, Eq. (65)]. This means that, if there is any substantial effect of the finiteness of the specimen upon the transition, this effect is not seen initially but must show up later.

In order to study the transition over the full time interval $0 \leq t \leq \delta$ it seems desirable to attack the problem numerically by reformulating it in terms of finite differences. Such an approach is described in Sec. III.

III. NUMERICAL SOLUTION

1. Finite Grid with Variable Time-Step

The moving-boundary problem formulated in Sec. I is to be solved approximately on a finite grid. The numerical field distributions will be denoted

by $H^*_{i,k} \approx H^*(x_i, t_k)$, with integers i, k, $0 \leq i \leq n$, $0 \leq k$. Let $x_0 = 0$; $x_i = ih$, $0 < i < n$; and $x_n = nh = a$. Applying a method used before by Douglas and Gallie,[6] a variable time step, l_j, $1 \leq j \leq n$, is to be determined in such a way that the interface passes through the mesh points (x_k, t_k), $0 \leq k \leq n$, where $t_0 = 0$, and

$$t_k = \sum_{j=1}^{k} l_j, \qquad k \geq 1.$$

This means $\xi(t_k)$ is approximated by $x_k = kh$, and δ by t_n (since $x_n = a$).

The advantage of this method is that one can classify the grid points *a priori* as left-hand, interface, and right-hand points ($i < k$, $i = k$, and $i > k$, respectively) and one knows exactly how and where to apply the various difference operators and boundary conditions.

Solving the free boundary problem numerically means determining all internal field values of both regions and at the right-hand boundary, $i = n$, as well as the unknown time steps. The solution is obtained by stepping forward in time. In the first ($k = 1$) and last ($k = n$) time steps the general procedure used for $2 \leq k \leq n - 1$ must be slightly modified.

2. General Procedure ($2 \leq k \leq n - 1$)

Assume $H_{i,j}$ and l_j known for all i, and for $j \leq k - 1$, $2 \leq k \leq n - 1$ (Fig. 4).

In passing to the k level one first has to let $H_{0,k} = H_e$ and $H_{k,k} = H_c$ because of (10) and (12), respectively. The diffusion equation (8) and London equation (9) can be replaced by the backward-difference equations

$$(H_{i+1,k} - 2H_{i,k} + H_{i-1,k})/h^2 = (H_{i,k} - H_{i,k-1})/l_k \qquad (1 \leq i \leq k - 1) \qquad (31)$$

and

$$(H_{i+1,k} - 2H_{i,k} + H_{i-1,k})/h^2 = \alpha H_{i,k} + \beta(H_{i,k} - H_{i,k-1})/l_k \qquad (k + 1 \leq i \leq n - 1), \qquad (32)$$

respectively. This yield as many equations as there are unknown internal field values.

There are two additional unknowns, $H_{n,k}$ and l_k, and two additional conditions, (11) and (13). As these conditions involve differentiation, it is useful to formulate (31) once more at P, using $h/2$ as space step and μ_k as time step (Fig. 4). An approximation for μ_k is obtained by drawing an arc of parabola through the points (k, k), $(k - 1, k - 1)$, and $(k - 2, k - 2)$ and determining the distance PQ accordingly. This yields $8\mu_k = 5l_k - l_{k-1}$. At Q the field is H_c. Similarly, Eq. (32) can be formulated at R and S, using the steps $h/2$ and l_k. The field values at A and B are obtained by interpolating the known distribution at the $(k - 1)$ level. For example: $8H_A = 3H_{k+1,k-1} + 6H_{k,k-1} - H_c$. In this way the quantities, H_P, H_R, and H_S can be expressed by field values in regular grid points and by l_k.

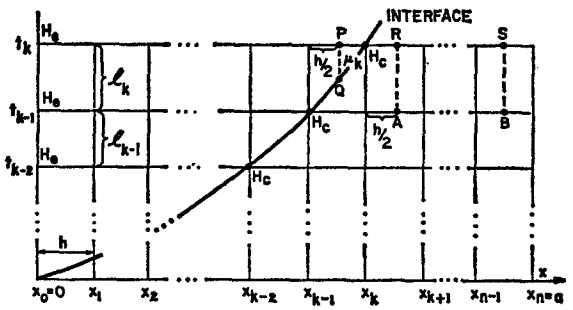

FIG. 4. Finite grid with variable time step.

The standard three-point forward and backward differentiation formulas (reference 7, p. 96) with the step $h/2$, and the trapezoidal rule (reference 7, p. 117) with the step h can now be used to write (11) and (13) in difference form:

$$3H_{n,k} - 4H_S + H_{n-1,k} = 0 \qquad (33)$$

and

$$(-3H_c + 4H_R - H_{k+1,k}) - \beta(3H_c - 4H_P + H_{k-1,k}) + (\alpha h^2/2)\left(H_c + 2\sum_{i=k+1}^{n-1} H_{i,k} + H_{n,k}\right) = 0, \qquad (34)$$

respectively. Relations (31) through (34) form a nonlinear algebraic system of n equations whose solution gives the $(n - 1)$ unknown field values and l_k.

The very nature of the nonlinearity suggests an iterative method for solving the equations. The system becomes linear if one replaces l_k by a given trial value, $l_k^{(1)}$. If (34) is dropped temporarily, the remaining linear system yields the trial field values $H_{i,k}^{(1)}$ associated with $l_k^{(1)}$. The $H_{i,k}^{(1)}$ are inserted into (34); this makes the left side of (34) equal to a residue $r_k^{(1)}$. By suitably choosing new trial values, $l_k^{(\nu)}$, $\nu = 2, 3, \cdots$, the quantity $|r_k^{(\nu)}|$ can be made

[6] J. Douglas, Jr., and T. M. Gallie, Jr., Duke Math. J. 22, 557 (1955).

[7] W. E. Milne, *Numerical Calculus* (Princeton University Press, Princeton, New Jersey, 1949).

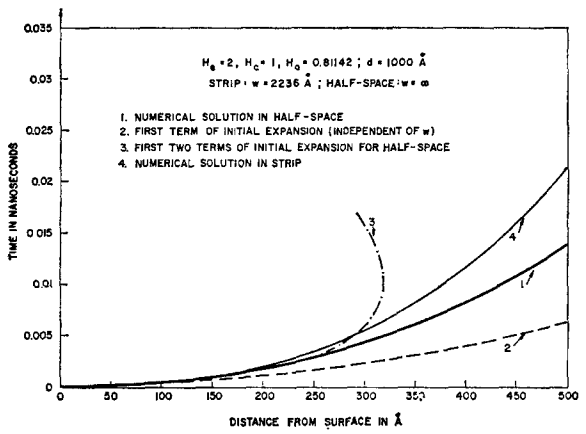

FIG. 5. Early part of transition.

smaller and smaller. The process stops when $|r_k^{(\nu)}| < \epsilon$ with a suitably small $\epsilon > 0$.

The solution $\lambda = l_k$ of $r_k(\lambda) = 0$ is first approached from below, by letting $l_k^{(\nu)} = \nu l_{k-1}/u$, $\nu = 1, 2, \cdots, \omega$, where u is, e.g., 5 or 10. In doing this, one assumes the solution is suitably smooth in terms of h so that l_k will not be too different from l_{k-1}. It can be expected that $r_k^{(\nu)}$ will change sign. Let ω be such that this happens when ν passes from $\omega - 1$ to ω. Then the correct l_k is trapped between $l_k^{(\omega-1)}$ and $l_k^{(\omega)}$ and the final approximation of it can be found by repeatedly using the rule of false position. This last approximation will be taken for l_k and the corresponding field values for $H_{i,k}$.

3. First and Last Integration Steps ($k = 1, n$)

For $k = 1$, $H_{0,1} = H_e$ and $H_{1,1} = H_c$. In lowest order approximation one has $\xi(t) = \chi_0\sqrt{t}$, where χ_0 is obtained from (27). This yields a guess $l_1^* = h^2/\chi_0^2$ of l_1 if one lets $\xi(l_1^*) = h$. Then, the trial values become $l_1^{(\nu)} = \nu l_1^*/u$. On the same basis one finds $\mu_1^{(\nu)} = 3l_1^{(\nu)}/4$. For $k = 1$, $H_{i,k-1} = H^+(ih, 0)$ in (32), using (14).

For $k = n$, relation (34) cannot be applied. Instead, one can use a finite difference analog, $3H_c - 4H_P + H_{n-1,n} = 0$, of (29b).

4. Modifications for $w = \infty$

In this case, (11) is to be replaced by Eq. (19) of reference 3:

$$H^+(x, t) \to 0, \qquad (x - \xi(t)) \to \infty. \tag{35}$$

The upper limit of the integral in (13) becomes ∞, and, instead of (14), one has [reference 3, (18)]:

$$H^+(x, 0) = H_0\, e^{-\sqrt{(\alpha)}x}, \qquad (x \geq 0). \tag{36}$$

Numerically, infinity is replaced by a sufficiently large finite distance from $\xi(t)$. That is, the right-hand distribution is calculated for $k < i < k + m$ by formulating (32) for all these values of i and letting $H^+_{k+m,k} = 0$ for all k, according to (35). Relation (33) must be dropped. A suitable integer m is chosen in consideration of α and h in such a way that $H^+_{m,0} = H_0 e^{-\sqrt{(\alpha)}mh}$ is sufficiently small. In (34), n must be replaced by $k + m$. A finite transition times does not exist in this case. Instead, the calculation is carried out for a prescribed number of time steps.

IV. RESULTS

The numerical method described in Sec. III, whose main feature is the use of variable time steps, was applied to the Stefan problem by Douglas and Gallie.[6] These authors proved that, in this case, the method is convergent and stable.

The transition problem considered here reduces to a Stefan problem only in the limiting case $\alpha \to \infty$, that is if the field is identically zero in the superconducting region. In order to test the numerical method for finite α this method was first applied to the problem in a half-space, that is with $w = \infty$, and the result compared with both the expansion for small times and the asymptotic solution for large times given for $w = \infty$ by Cohen and Miranker.[3] All calculations were done with $\beta = 1$ and $a = 1$,

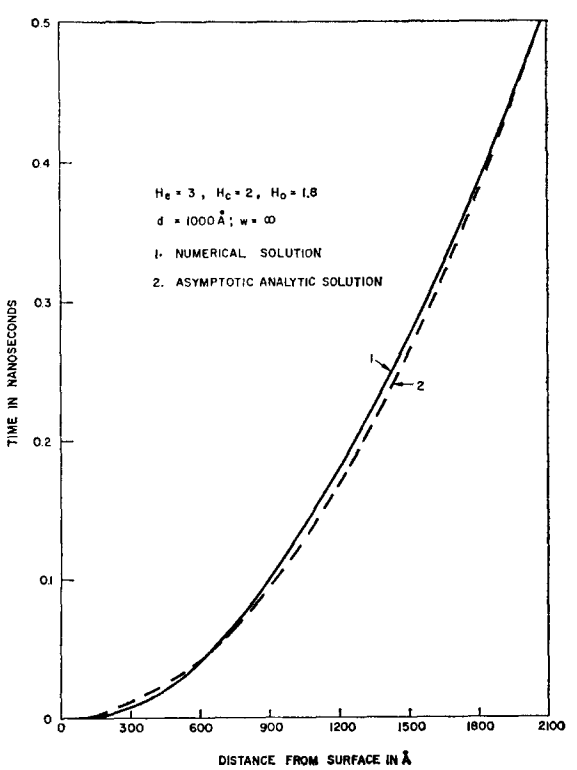

FIG. 6. Asymptotic behavior of transition in the half-space.

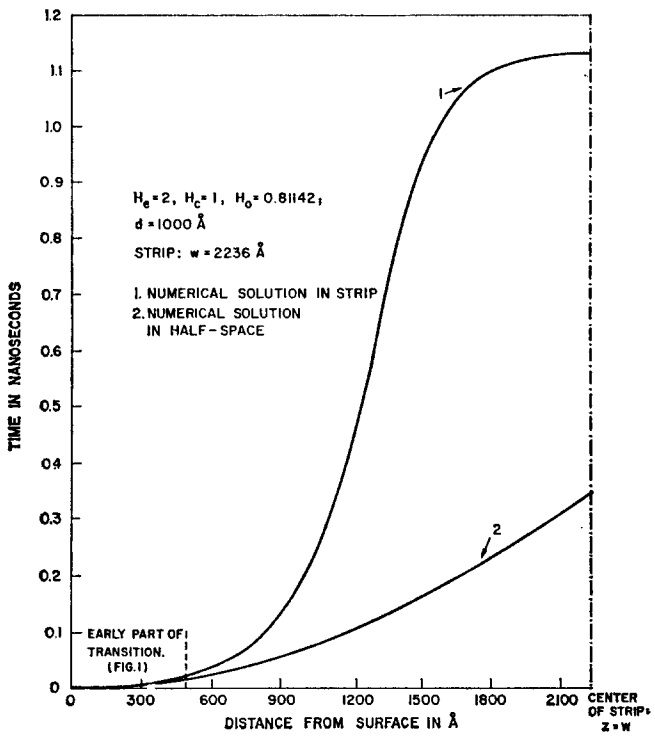

FIG. 7. Comparison between transition in strip and half-space.

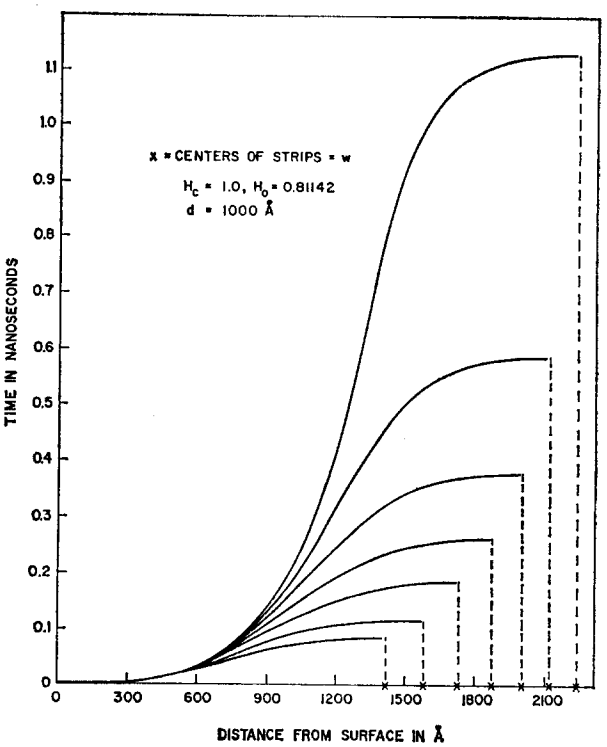

FIG. 8. Transition in strips of various widths, with driving field = two times critical field (numerical solutions).

and it was assumed that $4\pi\sigma^-/c^2 = 1$ cm^{-2}sec so that, numerically, formula (3) becomes $\tau_0 = z_0^2$, where z_0 is measured in cm. From $a = 1$ and Eqs. (4) and (5), it follows that $\alpha = w^2/d^2$. The computation of the complete solution of one transition problem using $n = 50$ required a few minutes on the IBM 7090. With $u = 5$ (defined in Sec. III.2), the total average number of iterations per time step was about 10.

The agreement between the numerical solution and the initial expansion was very good in all cases. An example is shown in Fig. 5. The agreement with the asymptotic expansion was good in those cases where the numerical solution was carried out sufficiently far in time (Fig. 6). There were no signs of numerical instability.

Passing to the finite strip and finite penetration, it is interesting to compare the numerical solution for this general case with the numerical and analytical solutions in the half-space, carried over $0 \leq z \leq w$. The lowest-order terms of the initial expansions of the interface in the half-space and the strip are identical, that is (27) is equivalent with Eq. (65) of reference 3. Thus, in the beginning, the transition is not much influenced by the width of the superconducting specimen. The numerical solutions confirm this result (Fig. 5). However, as Fig. 7 shows, the two transitions behave in an entirely

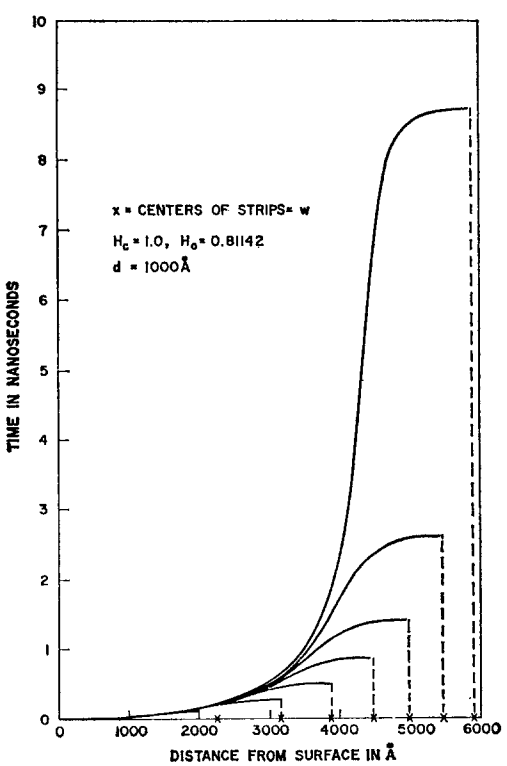

FIG. 9. Transition in strips of various widths, with driving field = five times critical field (numerical solutions).

different way later on. For not too thin strips, the total transition time θ is much larger than the time required for the transition in the half-space to reach the same distance. Thus, it is dangerous to try to estimate θ by extrapolating the analytical solution valid for small times and small distances as far as $z = w$. If with a given external field one increases the width of the strip, keeping all other parameters constant, the transition time increases very rapidly when the width reaches a certain critical range (Fig. 8). With a stronger external field, the same phenomenon is observed but for much wider strips (Fig. 9).

All interface curves calculated numerically for the strip seem to intersect the center line $x = a$ of the strip under a right angle. This seems to confirm the prediction, made under Sec. II.2., that $\dot{\xi}(t) \to \infty$ as $\xi \to a$.

Notice that this prediction was based upon relation (29), which in turn depends on assumption (28). One could think that, in using (29b) to determine l_n, according to Sec. III.3., one forces the numerical interface curves to become flat in the last step only. This is not the case; the numerical curves begin to flatten out well before reaching the grid-point (x_{n-1}, t_{n-1}), that is while the solution is still calculated according to the general procedure described in Sec. III.2.

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The author would like to express his gratitude to Hirsh Cohen for his important contributions to the formulation and solution of the problem considered in this paper, as well as to Willard L. Miranker and Farouk Odeh for their valuable suggestions.

ERRATUM: Ising Model and Excluded Volume Problem

M. F. Sykes
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