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On the Dimensionality of the Real World

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The "strength" of systems of field equations is defined following a procedure due to Einstein. For an arbitrary dimension number, the strength of Einstein's field equations and of Maxwell's equations are calculated, and it is shown that only in four dimensions do the two systems of field equations determine their respective fields equally strongly. In addition, in four dimensions, Weyl's equation exhibits the same strength as the Einstein or Maxwell fields. The results are used to show that a necessary condition for a unified field-theoretic description of gravity and electromagnetism is that the world be four dimensional. If one also demands that the neutrino field be determined as strongly as the Einstein and Maxwell fields, one must have a two-component neutrino, rather than a four-component neutrino.

I. INTRODUCTION

IN the present analysis, we hope to present a "raison d'être" for the observed dimensionality ($n = 4$) of the physical world. Obviously, it is a trivial matter to find *ad hoc* postulates which will "demand" that the world exhibit the observed dimensionality, so that our analysis can be of interest only if the postulates which we adopt are compelling in their simplicity. We hope to show that such is the case.

Before proceeding to the details of our analysis, we wish to point out several observations of the structure of mathematical physics which indicate that the dimension number $n = 4$ is preferred.

Lanczos[1] has noted that Maxwell's equations for free space, viz.,

$$F^{\mu\nu}{}_{|\nu} = 0, \tag{1}$$

$$*F^{\mu\nu}{}_{|\nu} = 0, \tag{2}$$

have a symmetry which is revealed only in four dimensions. Furthermore, it happens that for $n = 4$ and only for $n = 4$ can one form a dual tensor from the Riemann tensor by the same operation used in forming the dual of $F_{\mu\nu}$. The dual tensor thus formed has the same symmetry properties and number of components as the original Riemann tensor.[1]

Next, we note that, by definition, the Dirac equation as normally used is valid only in four dimensions.

Lastly, one may consider Einstein's equations for empty space,

$$R_{\mu\nu} = 0, \tag{3}$$

which, it is easily shown, imply flat space

$$R_{\mu\nu\lambda\rho} = 0 \tag{4}$$

if the dimension of the space is less than four.

Many further examples exist to show that the apparatus used in describing our physical world shows preference for the four-dimensional world. We need not elaborate further, except to note that the most compelling reason for the observed dimensionality of the world was observed in passing by Einstein[2] in 1954. Einstein noted "that the gravitational equations for empty space determine their field just as strongly as do Maxwell's equations."

[1] C. Lanczos, Rev. Mod. Phys. 34, 379 (1962).

[2] A. Einstein, *The Meaning of Relativity*, (Princeton University Press, Princeton, New Jersey, 1956), 5th ed., p. 133.

It is this last remark which we wish to emphasize in the present analysis.

We will proceed to develop our results inductively, which is more natural in the present context.

II. THE STRENGTH OF FIELD EQUATIONS

To examine the field equations of mathematical physics, it is useful to employ a criterion which may indicate how strongly a set of equations determine a field. Einstein[2] used such a criterion in his analysis of the nonsymmetric Riemann field. Since the technique is our main tool, and is not commonly used, we wish to give a simple example.

Consider a real analytic function of two variables, satisfying

$$\partial\varphi/\partial x + \partial\varphi/\partial y = 0. \tag{5}$$

Obviously, the solution to the field equation is

$$\varphi = F(x - y), \tag{6}$$

where F is an arbitrary function. Let us, however, solve the problem in a different way.

Suppose φ expanded in a Taylor series about some point (x_0, y_0) as follows:

$$\varphi = \varphi^0 + \frac{1}{1!}[\varphi^0_x x + \varphi^0_y y] + \frac{1}{2!}[\varphi^0_{xx}x^2 + 2\varphi^0_{xy}xy + \varphi^0_{yy}y^2] + \cdots, \tag{7}$$

where the subscripts x or y denote partial derivatives and the superscript 0 implies evaluation at (x_0, y_0).

We insert our expansion into the field equation, and demand that coefficients of like powers of the variables vanish, thereby obtaining

$$\varphi^0_x + \varphi^0_y = 0, \tag{8a}$$

$$\varphi^0_{xx} + \varphi^0_{xy} = 0, \tag{8b}$$

$$\varphi^0_{xy} + \varphi^0_{yy} = 0, \tag{8c}$$

and so on. Therefore, our Taylor expansion reduces to

$$\varphi = \varphi^0 + (1/1!)\varphi^0_x(x - y) + (1/2!)\varphi^0_{xx}(x - y)^2 + \cdots \tag{9}$$

and φ is indeed an arbitrary function of $(x - y)$.

The criterion for the strength of field equations is a generalization of the above procedures using Taylor expansions. We define the strength of a set of field equations in terms of the number of nth-order Taylor coefficients remaining free. For our example, we define[2] the "weakness," z, as the number of coefficients of nth order remaining free in the Taylor expansion, which we readily calculate to be

$$z = (n + 1) - (n) = 1. \tag{10}$$

The result follows because in the nth term of the expansion there are $(n + 1)$ coefficients. The field equation gives n relations among the nth order coefficients.

With the above example in mind, we proceed to examine the strength of Einstein's and Maxwell's equations, following Einstein's procedures.[2]

III. STRENGTH OF MAXWELL'S EQUATIONS

We consider Maxwell's equations for free d-dimensional space:

$$F^{\mu\nu}{}_{|\nu} = 0, \qquad F_{\mu\nu,\rho} + F_{\nu\rho,\mu} + F_{\rho\mu,\nu} = 0. \tag{11}$$

First, we note that the equations are not all independent, since we have the *identities*

$$F^{\mu\nu}{}_{|\nu\mu} \equiv 0, \tag{12a}$$

$$H_{\mu\nu\rho,\lambda} - H_{\nu\rho\lambda,\mu} + H_{\rho\lambda\mu,\nu} - H_{\lambda\mu\nu,\rho} \equiv 0, \tag{12b}$$

where we have defined

$$H_{\mu\nu\rho} \equiv F_{\mu\nu,\rho}. \tag{13}$$

Now $F_{\mu\nu}$ is antisymmetric, so that there are $\frac{1}{2}(d^2 - d)$ independent field components. For each field component, we suppose a Taylor expansion. There are $\binom{d}{n}$ expansion coefficients of nth order, where

$$\binom{d}{n} \equiv (d + n - 1)!/(d - 1)!n! \tag{14}$$

for each field component.

The expansion coefficients would be independent, were it not for the field equations. However, we have d field equations of the first order from the vanishing of the divergence of $F_{\mu\nu}$, which provide $d\binom{d}{n-1}$ conditions. These conditions are not all independent because of Eq. (12a), however, which reduces the number of determining conditions by $\binom{d}{n-2}$.

Similarly, the cyclic field equations constitute $\binom{d-2}{3}$ equations which are not all independent. The identity, Eq. (12b), constitutes $\binom{d-3}{4}$ second-order differential equations, each of which reduces the number of independent field equations by $\binom{d}{n-2}$.

Finally, the number of free nth-order coefficients in the Taylor expansion is

$$z_m = \left[\frac{d^2 - d}{2}\right]\binom{d}{n} - \left[d\binom{d}{n-1} - \binom{d}{n-2} + \binom{d-2}{3}\binom{d}{n-1} - \binom{d-3}{4}\binom{d}{n-2}\right], \tag{15}$$

which we rewrite as follows:

$$z_m = \binom{d}{n}\left[z_{0m} + \frac{z_{1m}}{n} + \cdots\right], \tag{16}$$

where

$$z_{0m} = \frac{d^2 - d}{2} - (d - 1) - \frac{d!}{3!(d-3)!} + \frac{d!}{4!(d-4)!}, \tag{17a}$$

$$z_{1m} = (d - 1)\left[(d - 2) + \frac{d!}{3!(d-3)!} - \frac{2d!}{4!(d-4)!}\right]. \tag{17b}$$

We have expanded z asymptotically for large values of n. The coefficient z_{1m} is called[2] the "coefficient of freedom," and is larger the weaker the system of equations. The coefficient z_{0m}, if nonzero, indicates whether the system of equations leaves free any arbitrary functions of all d variables.

By simple algebra, we easily find that

$$z_{0m} = \tfrac{1}{24}(d - 1)(d - 2)(d - 3)(d - 4), \tag{18a}$$

$$z_{1m} = \tfrac{1}{12}(d - 1)(d - 2)[12 - d(d - 1)(d - 5)]. \tag{18b}$$

IV. STRENGTH OF EINSTEIN'S EQUATIONS

Here we must realize that only *equivalent* fields must be considered. Thus, fields arising from one another by coordinate transformation are the same field. Our field functions are the $\frac{1}{2}(d^2 + d)$ metric components of the symmetric $g_{\mu\nu}$. If

$$g'_{\mu\nu} = (\partial x^\alpha/\partial x^{\mu'})(\partial x^\beta/\partial x^{\nu'})g_{\alpha\beta} \tag{19}$$

then $g'_{\mu\nu}$ is equivalent to $g_{\alpha\beta}$. Thus the requirement of general covariance requires that we subtract $d\binom{d}{n+1}$ from the total number of nth-order coefficients.

To see this, suppose $g_{\alpha\beta}$ is expanded in a Taylor series. Then $g'_{\mu\nu}$ has a Taylor series with the nth-order term of its expansion containing all of the $(n + 1)$th derivatives of the d functions x. However, the numbers which are the evaluation of these functions do not characterize the field, hence we must not count them.

The field equations are

$$R_{\mu\nu} = 0 \qquad g_{\mu\nu,\rho} - g_{\alpha\nu}\Gamma^\alpha_{\mu\rho} - g_{\mu\beta}\Gamma^\beta_{\rho\nu} = 0 \tag{20}$$

and are not independent because of the identity

$$(R^{\mu\nu} - \tfrac{1}{2}Rg^{\mu\nu})_{|\nu} \equiv 0. \tag{21}$$

Now there are $\binom{d}{n}$ nth-order coefficients for each of the $g_{\mu\nu}$. This number is reduced by the necessity for general covariance as mentioned above. The number of free coefficients is further reduced by the $\frac{1}{2}(d^2 + d)$ field equations, each of which gives $\binom{d}{n-2}$ relations since the field equations are of second order. The Bianchi identities, of third order, provide $d\binom{d}{n-3}$ identical relations which reduce the degree of determinacy of the field equations.

Finally, we have the number of free nth-order coefficients in the Taylor expansions of the $g_{\mu\nu}$,

$$z_E = \frac{d^2 + d}{2}\binom{d}{n} - d\binom{d}{n+1} - \left[\frac{d^2 + d}{2}\binom{d}{n-2} - d\binom{d}{n-3}\right], \tag{22}$$

which we rewrite as

$$z_E = \binom{d}{n}\left[z_{0E} + \frac{z_{1E}}{n} + \cdots\right], \tag{23}$$

where

$$z_{0E} = 0, \tag{24a}$$

$$z_{1E} = d(d - 1)(d - 3). \tag{24b}$$

The vanishing of z_{0E} independently of d indicates that Einstein's field equations leave no free arbitrary functions aside from the freedom of general coordinate transformations, for any dimension.

V. UNIQUENESS OF FOUR DIMENSIONS

We are now in a position to show that in four dimensions and *only* in four dimensions do the Maxwell equations determine the Maxwell field as strongly as Einstein's equations determine the metric.

First of all, we note that z_{0m} vanishes only for the dimension numbers 1, 2, 3, or 4. Further, the coefficients of freedom for each set of field equations, z_{1m} and z_{1E} are equal when

$$d(d - 1)(d - 3) = \tfrac{1}{12}(d - 1)(d - 2)[12 - d(d - 1)(d - 5)]. \tag{25}$$

Solving, we have that z_{1m} equals z_{1E} when the dimension number is either *one* or *four*. The remaining possible roots satisfy

$$d^3 - 4d^2 + 13d - 6 = 0, \tag{26}$$

which has no integral roots.

Obviously, the dimension number *one* is absurd as a possible world because $F_{\mu\nu}$ does not exist therein, and hence *only* in *four dimensions* do the respective field equations determine their fields equally strongly. This result is the central point of the present analysis.

For four dimensions we have

$$z_{0E} = z_0 = 0, \tag{27a}$$

$$z_{1E} = z_{1m} = 12, \tag{27b}$$

which are measures of the strength of the field equations.

VI. THE NEUTRINO

It is of interest to examine the strength of the field equations for the neutrino. In keeping with experimental findings, we describe the free neutrino by Weyl's equation,[3]

$$(\bar{\sigma}\cdot\nabla + i\partial_4)\varphi = 0. \tag{28}$$

The function φ consists of four real functions. The field equations give four, real, first-order differential equations; hence the strength of the system is determined by

$$z_N = 4\binom{4}{n} - 4\binom{4}{n-1}, \tag{29}$$

which gives

$$z_N = \binom{4}{n}\left[0 + \frac{12}{n} + \cdots\right]. \tag{30}$$

Thus we find that the Weyl equation determines the neutrino field equally as strongly as do the Einstein equations and Maxwell's equations, for four dimensions. It is interesting that the massless Dirac equation *does not* exhibit the same strength as the simpler "parity-violating" Weyl equation.[4]

VII. MEANING OF THE RESULTS

In the previous sections, we have shown that only in four dimensions do the field equations of gravitation, electromagnetism, and neutrinos determine their fields equally strongly. Aside from being an interesting observation, this result permits us to understand the reason for the dimensionality of our physical world.

The world as observed physically consists of concentrated islands of matter, with a vast "empty" space constituting most of the realm. In the empty space as we know it, the principal physical phenomena occurring are described by the three, massless, long-range "particles" of Einstein, Maxwell, and Weyl.

If one believes in a unified field theory which links the phenomena of gravitation, electromagnetism, and neutrinos, then one may see that a necessary condition for the existence of such a theory is that the three fields be determined equally strongly, and therefore can occur only if the world is four dimensional.[5]

To see this more clearly, we may use the following argument. Suppose a given region of space contains an electromagnetic field, for example. Let us also suppose that the region is surrounded by an empty region, wherein Einstein's field equations are valid. If Maxwell's equations do not determine the metric representing the Maxwell field in the interior region as strongly as Einstein's equations determine the geometry in the exterior region, then, within the region which is occupied by the electromagnetic field, the geometry may be altered while still satisfying Maxwell's equations. But, then, the geometry outside of the region is fixed more strongly than the geometry inside.

At an interface of the boundary, then, one could alter the metric itself discontinuously. While it may be permissible that the derivatives of the $g_{\mu\nu}$ be discontinuous, it is unthinkable that the metric itself be discontinuous.

In the above argument, we have restricted ourselves to the assumption that Einstein's empty-space field equations are correct. Actually, we need not restrict ourselves that severely to prove the point, but there seems little reason to argue on more general grounds, at present. However, we wish to remark that considerations of the Cauchy initial-value problem for each field would lead to the same conclusion.

Thus, we may state that the following result holds. *A necessary condition for the existence of a unified field theory embracing gravitation, electromagnetism, and neutrinos is that the world be four dimensional.*

To paraphrase our results in a deductive manner, we may invent two postulates which are compelling in their simplicity, and which allow one to deduce the dimensionality. Our postulates would be as follows:

Postulate I. The physical theories of gravitation and electromagnetism are correctly described by the Einstein and Maxwell theories.

[3] P. Roman. *Theory of Elementary Particles* (Interscience Publishers, Inc., New York, 1961), 2nd ed., p. 107.

[4] Of course, we are aware that the Weyl theory of the free neutrino is not "parity-violated," as shown by J. McLennan, Phys. Rev. **106**, 821 (1957). Yet, it is true that the two-component description leads most naturally to the "parity violations" of interactions.

[5] We are adopting the incredibly naive view that the massive sources of our massless fields can be understood in principle in terms of the massless fields alone. Thus, whether our conclusions hold in our world or not depends upon whether or not the free fields account for mass, perhaps through the nonlinearities of Riemannian geometry.

Postulate II. A unified field theory exists which determines the phenomena of gravitation and electromagnetism as manifestations of the same phenomenon (e.g., in Ref. 6).

Finally, we wish to remark that one might also note that our results show that a neutrino theory of light would be possible only in four dimensions, with the neutrino described by the *two-component* Weyl equation, if at all possible. Apparently, the dimensionality of the world and the "parity violations" of weak interactions[4] are somehow linked.

VIII. CONCLUSIONS

However plausible the postulates which we have used may be, the fact remains that there is a mathematical reason for the world to be four dimensional. Indeed, only in four dimensions are the principal field equations of theoretical physics equally strong. Even if one denies the slightly metaphysical interpretation we have attempted to place upon this result, one must grant that the basic mathematical description of the most fundamental physical phenomena shows a remarkable proclivity for four dimensions.

The mathematical reasons for this proclivity have been demonstrated in the present analysis. Perhaps that is all of the "understanding" that is necessary.

[6] J. A. Wheeler, *Geometrodynamics* (Academic Press Inc., New York, 1962).

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Invariance and Conservation Laws in Classical Mechanics

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It is commonly supposed that, in classical mechanics, invariance of a physical system to coordinate translation implies conservation of linear momentum. "Invariance" may be defined in a number of ways. If it is defined to mean invariance of the equation of motion, it is shown that invariance of this equation with respect to coordinate translation does *not* imply conservation of linear momentum. The effects of scale transformation and coordinate inversion invariance are also investigated. Both the Lagrangian approach and Newton's (second) law approach are considered. It is shown that each of the above invariances implies a condition on the equation of motion, while a combination of these and time-inversion invariance is needed to obtain ordinary momentum conservation.

1. INTRODUCTION

IT is commonly supposed that, in classical mechanics, the invariance of a mechanical system to space displacement implies conservation of linear momentum, invariance to space rotation implies conservation of angular momentum, etc. The term "invariance" may be defined in various ways. When Hamilton's principle

$$\delta \int L\, dt = 0 \tag{1}$$

is used, and the Lagrangian L is assumed invariant under translation, the conservation of linear momentum, suitably defined, follows.

For example, consider the simple case of a single particle with one degree of freedom, described by a generalized coordinate q.[1] Let

$$L = L(q, \dot{q}, t), \tag{2}$$

where $\dot{q} = dq/dt$. Two types of translation can be considered:

(A) Geometrical. This corresponds to a translation of the coordinate system with respect to which

[1] Since q is a generalized coordinate, it need not be a displacement, but could be any quantity which gives the location of the particle. However, the fundamental nature of displacement is indicated by the fact that the definition of an acceptable set of generalized coordinates is that these coordinates give the *positions* of all the particles of the mechanical system.

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q is measured. As a fundamental postulate, it is assumed that such a translation cannot affect physical reality, i.e., the physical "trajectory" of the particle must be unchanged, although its description may be altered.

(B) Physical. This corresponds to an actual translation of the physical system, with the coordinate system fixed. Here the particle before and after the translation will not have the same physical trajectories. If the system should be invariant with respect to this translation on *physical* grounds, e.g., a free particle, then the two trajectories should be "equivalent." The definition of "equivalent" used here is that the physical translation has the same effect as an opposite translation of the coordinate system. Thus both types of translation become effectively the same in this case, and only (A) will be investigated here. If the particle is not free, the Lagrangian would have to contain other factors, e.g., specifying the location of a center of force.

The invariance requirement on L is defined as follows. If $q' = q + b$ is the coordinate after translation, L is to have the same *value*, expressed as a function of q', as it did as the same function of q. Thus, for all b,

$$L(q, \dot{q}, t) = L(q', \dot{q}', t). \tag{3}$$

But $\dot{q}' = \dot{q}$, so that

$$L(q + b, \dot{q}, t) - L(q, \dot{q}, t) = 0, \qquad \text{for all } b, \tag{4a}$$

and

$$(1/b)[L(q + b, \dot{q}, t) - L(q, \dot{q}, t)] = 0, \quad b \neq 0. \tag{4b}$$

If q, $\dot{q}$, and t were independent variables, then (4a) would imply that L cannot be a function of q. However, since the variables $\dot{q}$ and q are related, the possibility exists that (4a) holds for some *particular* $q(t)$. That L cannot be a function of q is shown as follows. Taking the limit as $b \to 0$, (4b) becomes

$$\partial L/\partial q = 0. \tag{5}$$

Two interpretations for (5) are possible. The first follows from the fact that (5) can be regarded as an ordinary differential equation, and could imply that q is to be its solution. This interpretation is not valid, however, as the physical equation of motion is taken as a necessary condition for (1), and (1) implies Lagrange's equation of motion

$$\partial L/\partial q - (d/dt)(\partial L/\partial \dot{q}) = 0. \tag{6}$$

However, (6) is second order, while (5) is first order. Therefore they cannot in general have the same set of solutions,[2] and thus (5) must be regarded as implying

$$L = L(\dot{q}, t). \tag{7}$$

If the canonical momentum p is defined by

$$p = \partial L/\partial \dot{q}, \tag{8}$$

then the invariance of L with respect to translation does imply conservation of the momentum p.

This argument is given in detail because similar methods will be used in what follows, and because the emphasis here is on tracing rigorously the implications of invariance requirements.

The usual argument[3] is simply that, if space is homogeneous, L cannot be a function of q. The same result is obtained here, but there are three major parts to the proof. First, one assumes that invariance of the physical system implies the corresponding invariance of L. Secondly, invariance must be precisely defined, and, thirdly, the effects of this requirement must be deduced.

Concerning the first point, it is not clear that the invariance of the physical *system* implies invariance of L. Invariance properties may be induced from experiment, or assumed as postulates of a theory. In any case, the results must be compared with experiment. To start by assuming that L should not contain q makes this invariance part of its definition. While this is sufficient for momentum conservation (if p is defined as $\partial L/\partial \dot{q}$), it is not necessarily the most fundamental approach. Invariance of a system should refer to the invariance of physical observables, i.e., measurable quantities. While it is conceivable that one could devise methods for measuring L directly, such methods do not appear as direct as, for example, measurements of the displacement q. In any case, requiring invariances in L is not *more* fundamental than requiring them in other properties of the system, though it may be more convenient. Therefore, in this paper, the effects of certain invariance requirements on q will be investigated, in particular, coordinate translation, coordinate stretching (scale transformation), and coordinate inversion. The effects of these requirements on the equation of

[2] There are cases where the solutions of second- and first-order ordinary differential equations are identical. If a constant of the motion C exists for (6), as $g(q, \dot{q}, t) = C$, then the solution of this equation is equivalent to a solution of (6). However, C is a function of the initial or boundary conditions of the problem, as is the complete solution of (6). But (5) does not contain any boundary conditions, and thus its solution can contain only one of a pair of conditions, and therefore cannot be the general solution.

[3] L. D. Landau and E. M. Lifshitz, *Mechanics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1960), p. 5.

motion and (where possible) on the Lagrangian L will be shown.

2. COORDINATE TRANSLATION INVARIANCE

The dynamical law governing a single particle with one degree of freedom is obtained from

$$\delta \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt = 0, \tag{9}$$

where $q(t_1)$ and $q(t_2)$ are known. The dynamical law is then (6). Another observer, using the translated coordinate $q' = q + b$, finds the appropriate equation of motion by applying (9) in terms of his coordinates. Thus it is assumed that Hamilton's principle is *covariant*, i.e., it has the same *form* for both observers. Then

$$\delta \int L'(q', \dot{q}', t)\, dt = 0, \tag{10}$$

where L' is taken as the same function of q', $\dot{q}'$, and t as L is of q, $\dot{q}$, and t, i.e., the covariance of L is also assumed. Therefore, if (6) is written as

$$F(q, \dot{q}, \ddot{q}, t) = 0, \tag{11}$$

for coordinate q, an observer using coordinate q' will obtain from (10)

$$F'(q', \dot{q}', \ddot{q}', t) = 0, \tag{12}$$

where F' is the same function of q', $\dot{q}'$, $\ddot{q}'$, and t that F is of q, $\dot{q}$, $\ddot{q}$, and t respectively. Then (12) can be written

$$F(q + b, \dot{q}, \ddot{q}, t) = 0. \tag{13}$$

In using (10) and thus (13), the appropriate boundary conditions must be used, i.e., $q'(t_1)$ and $q'(t_2)$ must be given, where $q'(t_1) = q(t_1) + b$, etc. These boundary conditions, with (13), will yield the same physical trajectory as the solution of (11) with $q(t_1)$ and $q(t_2)$ given.

Combining (11) and (13), one has,[4] for all b,

$$F(q + b, \dot{q}, \ddot{q}, t) - F(q, \dot{q}, \ddot{q}, t) = 0, \quad \text{whenever } F = 0, \tag{14}$$

i.e., (14) is 0 only for q which satisfy (11). Dividing (14) by b, and taking the limit as $b \to 0$,

$$\partial F/\partial q = 0, \quad \text{whenever } F = 0. \tag{15}$$

From (6), F is linear in $\ddot{q}$, and may be written

$$F = G - \alpha\ddot{q},$$

where $\alpha(q, \dot{q}, t) = \partial^2 L/\partial\dot{q}^2$, and $G = G(q, \dot{q}, t)$. Then

$$\alpha(\partial F/\partial q) - F(\partial\alpha/\partial q) = \alpha(\partial G/\partial q) - G(\partial\alpha/\partial q). \tag{16}$$

But the left side of (16) is 0 whenever F is 0; thus

$$\alpha(\partial G/\partial q) - G(\partial\alpha/\partial q) = 0, \quad \text{whenever } F = 0. \tag{17}$$

However, (17) is an ordinary differential equation of *first* order, and therefore cannot, by our previous arguments, have all the solutions of $F = 0$. Therefore (17) must be an identity, or

$$\alpha(\partial G/\partial q) - G(\partial\alpha/\partial q) \equiv 0, \tag{18a}$$

and,

$$\alpha(\partial F/\partial q) - F(\partial\alpha/\partial q) \equiv 0. \tag{18b}$$

Then if $\alpha \not\equiv 0$,[5]

$$(\partial/\partial q)(F/\alpha) \equiv 0, \tag{19a}$$

and

$$(\partial/\partial q)(G/\alpha) \equiv 0. \tag{19b}$$

From (19b), $G/\alpha = r(\dot{q}, t)$, where r is an arbitrary function of $\dot{q}$ and t. Then

$$F = \alpha(r - \ddot{q}) = 0, \tag{20}$$

and since $\alpha \not\equiv 0$, the resultant equation of motion is of the form

$$\ddot{q} = r(\dot{q}, t). \tag{21}$$

Thus, if Lagrange's equation of motion is to be invariant with respect to q translation, it *must* be of the form (21). The sufficiency of (21) for translational invariances is obvious. If L does not contain t, or $r(\dot{q}, t) = f(\dot{q})g(t)$, then (21) implies a conservation law, since

$$\int d\dot{q}/f(\dot{q}) - \int dt\, g(t) = C. \tag{22}$$

The general physical significance of C is not known, but if $r = 0$, one obtains the usual result that $\dot{q}$ is conserved.[13]

It can be shown that, if $r \not\equiv 0$, the Lagrangian L must be a function of both $\dot{q}$ and q in order to produce the translation-invariant equation of motion (21). Since (21) is necessary and sufficient for translation invariance of the equation of motion, and implies

[4] The mathematical techniques used here are similar to those used by B. Podolsky and the author in a paper which appeared in Math. Comp. 18, 441 (1964). Some of these results can be obtained by the application of continuous groups to ordinary differential equations, but it is thought that these methods will be understood by a larger audience, as well as having an intrinsic interest.

[5] Only the case $\alpha \not\equiv 0$ is considered, as L is normally quadratic in $\dot{q}$. If $\alpha \equiv 0$, L is linear in $\dot{q}$, and no equation of motion results.

(if $r \neq 0$) that L is a function of q, the momentum $\partial L/\partial \dot{q}$ will not in general be conserved. Also, from (20), L must satisfy the partial differential equation

$$\frac{\partial L}{\partial q} - \frac{\partial^2 L}{\partial q \partial \dot{q}}\dot{q} - \frac{\partial^2 L}{\partial t \partial \dot{q}} = \frac{\partial^2 L}{\partial \dot{q}^2} r(\dot{q}, t).$$

If L is assumed of the form

$$L(q, \dot{q}, t) = g(q)h(\dot{q}, t), \tag{23}$$

Lagrange's equation becomes

$$h\frac{dg}{dq} - \frac{dg}{dq}\frac{\partial h}{\partial \dot{q}}\dot{q} - g\frac{\partial^2 h}{\partial \dot{q}^2}\ddot{q} - g\frac{\partial^2 h}{\partial t \partial \dot{q}} = 0. \tag{24}$$

From (19b),

$$\frac{\partial}{\partial q}\left\{\frac{(dg/dq)[h - (\partial h/\partial \dot{q})\dot{q}]}{g(\partial^2 h/\partial \dot{q}^2)} - \frac{\partial^2 h/\partial t \partial \dot{q}}{\partial^2 h/\partial \dot{q}^2}\right\} \equiv 0. \tag{25}$$

But this implies $g^{-1}dg/dq$ is not a function of q, so that

$$L = Ae^{\beta q}h(\dot{q}, t), \tag{26}$$

where A and β are constants.

If L is of the form

$$L = g(q) + h(\dot{q}, t), \tag{27}$$

a similar argument yields $g = \gamma q$, where γ is a constant, and

$$L = \gamma q + h(\dot{q}, t). \tag{28}$$

Thus if L is separable in the forms (23) and (27), the specific forms (26) and (28) are obtained, and $p = \partial L/\partial \dot{q}$ is *not* a constant of the motion in either case, although the equations of motion are invariant with respect to space displacement. The result (28) corresponds to a uniform field, where it is obvious the equation of motion should be translation invariant.

3. SCALE TRANSFORMATION INVARIANCE

It appears desirable to investigate also the implications of scale transformation invariance, i.e., the assumption that physical phenomena should be unchanged by a different choice of units. Greenberger[6] has investigated such effects in field theories, assuming invariance of the action function, but the approach here is again to examine the implications on the equation of motion, and, if possible, on L.

Following Sec. 2, let $q' = kq$, where $k > 0$. Then (12) becomes

$$F(kq, k\dot{q}, k\ddot{q}, t) = 0. \tag{29}$$

[6] D. M. Greenberger, Ann. Phys. (N. Y.) **25**, 290 (1963).

Letting $k = 1 + \epsilon$, and subtracting (11),

$$F(q + \epsilon q, \dot{q} + \epsilon\dot{q}, \ddot{q} + \epsilon\ddot{q}, t) - F(q, \dot{q}, \ddot{q}, t) = 0, \quad \text{whenever} \quad F = 0.$$

Dividing by ϵ and taking the limit as $\epsilon \to 0$,

$$q(\partial F/\partial q) + \dot{q}(\partial F/\partial \dot{q}) + \ddot{q}(\partial F/\partial \ddot{q}) = 0, \quad \text{whenever} \quad F = 0. \tag{30}$$

As before, let

$$F = \alpha[(G/\alpha) - \ddot{q}], \qquad \alpha \neq 0. \tag{31}$$

Then (30) yields

$$\left(\frac{G}{\alpha} - \ddot{q}\right)\left(q\frac{\partial \alpha}{\partial q} + \dot{q}\frac{\partial \alpha}{\partial \dot{q}} + \ddot{q}\frac{\partial \alpha}{\partial \ddot{q}}\right) + \alpha\left(q\frac{\partial}{\partial q} + \dot{q}\frac{\partial}{\partial \dot{q}}\right)\frac{G}{\alpha} = \alpha\ddot{q},$$

whenever $F = 0$. But when $F = 0$, $G/\alpha = \ddot{q}$, and thus

$$\left(q\frac{\partial}{\partial q} + \dot{q}\frac{\partial}{\partial \dot{q}}\right)\frac{G}{\alpha} = \frac{G}{\alpha}. \tag{32}$$

It can be shown that (32) is an identity, so that G/α must be *homogenous* of degree 1 in q and $\dot{q}$, or $G/\alpha \equiv 0$. From (31), F/α is homogeneous of degree 1 in q, $\dot{q}$, and $\ddot{q}$.[7]

The equation of motion then reduces to

$$\ddot{q} = H_1(q, \dot{q}, t), \tag{33}$$

where H_1 is homogenous of degree 1 in q and $\dot{q}$, or 0. If $H_1 \neq 0$, and assuming that H_1 does not depend explicitly on t, we have

$$H_1(kq, k\dot{q}) = kH_1(q, \dot{q}).$$

Since k is arbitrary, let $k = 1/q$. Then

$$H_1(1, \dot{q}/q) = (1/q)H_1(q, \dot{q}).$$

Let $z = \dot{q}/q$. Then

$$\ddot{q} = q(\dot{z} + z^2),$$

and (33) can be written

$$\dot{z} + z^2 = H_1(1, z),$$

or

$$dz/dt = H_1(1, z) - z^2.$$

Thus

$$\int \frac{dz}{[H_1(1, z) - z^2]} = t + C',$$

[7] This condition is also obviously sufficient for scale transformation invariance of the equation of motion.

where C' is a constant of the motion which is due to scale transformation invariance alone.

4. COORDINATE INVERSION INVARIANCE

If coordinate inversion ($q' = -q$) invariance of the equation of motion (11) is required, since geometrically this corresponds only to an interchange of labels on the $+q$ and $-q$ axes, (12) becomes

$$F(-q, -\dot{q}, -\ddot{q}, t) = 0. \tag{34}$$

Since F in (11) is linear in $\ddot{q}$, (11) and (34) can be written

$$\ddot{q} = f(q, \dot{q}, t), \tag{35a}$$

$$-\ddot{q} = f(-q, -\dot{q}, t). \tag{35b}$$

Adding,

$$f(q, \dot{q}, t) + f(-q, -\dot{q}, t) = 0, \tag{36}$$

whenever (35a) holds, and since (36) is an ordinary differential equation of lower order,

$$f(q, \dot{q}, t) \equiv -f(-q, -\dot{q}, t), \tag{37}$$

so that f must be an odd function in q and $\dot{q}$. The requirement of coordinate inversion invariance does not generate a conservation law.

5. SIMULTANEOUS INVARIANCES

If invariance of the equation of motion to coordinate translation, inversion *and* scale transformation is required, then from (21), (33) and (37), the equation of motion must have the form

$$\ddot{q} = a(t)\dot{q}. \tag{38}$$

This result implies the conservation law

$$\dot{q} \exp\left(-\int a\, dt\right) = \text{const.}$$

If L does not contain t explicitly, then a in (38) is a constant. Then if one adds, *ad hoc*, the requirement that (38) be time-inversion invariant, a must be 0, and the usual equation of motion for the free particle

$$\ddot{q} = 0 \tag{39}$$

is obtained.[8]

A necessary and sufficient condition that the equation of motion be (39) is that $L = L(\dot{q})$. The sufficiency is obvious (although if L is linear in $\dot{q}$, no equation of motion results). The necessity can be proven if L is assumed a function of q and $\dot{q}$ only. Then Lagrange's equation is

$$\partial L/\partial q - (\partial^2 L/\partial q \partial \dot{q})\dot{q} - (\partial^2 L/\partial \dot{q}^2)\ddot{q} = 0, \tag{40}$$

and if (39) holds,

$$\partial L/\partial q - (\partial^2 L/\partial q \partial \dot{q})\dot{q} = 0. \tag{41}$$

Equation (41) must be an identity, so that (39) implies

$$(\partial/\partial q)[L - (\partial L/\partial \dot{q})\dot{q}] \equiv 0,$$

or $L - (\partial L/\partial \dot{q})\dot{q}$ is a function of $\dot{q}$ only, say $s(\dot{q})$. Then one has

$$(\partial/\partial \dot{q})(L/\dot{q}) = -s/\dot{q}^2,$$

or

$$L = F(\dot{q}) + g(q)\dot{q}, \tag{42}$$

where g is an arbitrary function of q. However, the term $g(q)\dot{q}$ in L is an exact derivative, and therefore makes no contribution to the equation of motion. Therefore, if $\ddot{q} = 0$, L must be a function of $\dot{q}$ only (if such exact derivative terms are dropped).[9]

Thus, the ordinary free particle equation of motion and conservation of momentum are generated by the *combined* invariances of the equation of motion to coordinate translation and scale transformation (which here also imply coordinate inversion invariance), plus no explicit t dependence in L and time-inversion invariance.

6. NEWTON'S LAW APPROACH

If one starts with an equation of motion (as Newton's second law), instead of Hamilton's principle, and this equation is assumed of second order, it may be expressed by

$$\ddot{q} = r(q, \dot{q}, t). \tag{43}$$

To investigate the implications of the invariances discussed earlier, the methods of Secs. 2, 3, 4, and 5 may be applied directly to (43). Thus translational invariance requires that $r = r(\dot{q}, t)$, scale transformation invariance requires that r be homogenous of degree 1 in q and $\dot{q}$, and coordinate inversion invariance that r be an odd function of q and $\dot{q}$. The first of these conditions implies the conservation law (22) if r does not contain t, or if $r = f(\dot{q})g(t)$. Again the general physical significance of this con-

[8] The author is indebted to Professor Paul Weiss of Wayne State University for making this point.

[9] An interesting special case is $L = \dot{q} \ln \dot{q} + \gamma q$, which yields an equation of motion having both translation and scale transformation invariance ($\ddot{q} = \gamma\dot{q}$), but L is *not* invariant to either translation or scale transformation. However, for $q' = kq$, $L' = kL + k \ln k\dot{q}$, and both L and L' give the same equation of motion.

servation law is not known.[10] But in this case there is the additional problem of the definition of momentum. One can, of course, take p proportional to $\dot{q}$, but it is not clear that this is the only acceptable, or the best, definition. Also, if r does not contain t, scale transformation invariance implies a conservation law.

7. DISCUSSION

The implications of the assumptions of coordinate translation, scale transformation, and inversion invariances on the equation of motion of a one-dimensional classical particle,[11] obtained from Hamilton's principle or starting from Newton's second law, have been deduced. For the general case $L = L(q, \dot{q}, t)$ or $\ddot{q} = r(q, \dot{q}, t)$, translational invariance of the equation of motion does *not* seem to generate conservation of momentum,[10] contrary to the usual expectation.[12] If $L = L(q, \dot{q})$, or $r = f(\dot{q})g(t)$, a conserved quantity is found, but it does not appear to be related always to the momentum. Scale-transformation invariance requires homogeneity of the equation of motion, and also generates a conservation law if r does not contain t. Coordinate-inversion invariance requires only that the acceleration be an odd function of q and $\dot{q}$, which does not imply a conservation law.[13] This last is perhaps understandable, since, while translation and scale transformation are associated with one-parameter continuous groups, coordinate inversion is associated with a group of order 2.

However, the coupling of invariances leads to strong conditions on the equation of motion, and it was shown that ordinary momentum conservation is obtained, if L is not explicitly time dependent, under translation and scale transformation (which includes inversion), with the addition of time-inversion invariance.

From the above results, it seems likely that time-translation invariance alone does not generate conservation of energy. This and a number of other points will be discussed in a later paper.

8. ACKNOWLEDGMENTS

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[10] More generally, if (21) holds, and letting $\dot{q} = v$, the first-order equation $\dot{v} = r(v, t)$ is obtained. This implies the existence of a constant of the motion $G(v, t)$ if, and only if, $r = (\partial G/\partial t)/(\partial G/\partial v)$. This constant may be regarded as associated with the translational invariance of the equation of motion, and that the conservation of G is generated by coordinate translation invariance alone. The relationship between G and linear momentum is not clear, in general.

[11] The generalized coordinate q used here need not be Cartesian. However, if it is, then the invariances discussed would all be appropriate for a free particle. It is also apparent that, if q is the angle describing the rotation of a free rigid rotator about a fixed axis, these invariances should also hold. However, even for a free particle, one can choose q such that the invariances discussed are not applicable in that coordinate system. The decision that a certain invariance principle should hold can only be made on physical grounds. But if such an invariance is applicable, its effects on the equation of motion can then be found by the above methods.

[12] D. M. Greenberger, Ref. 6, p. 290; C. N. Yang, Science **127**, 565 (1958); E. P. Wigner, Progr. Theoret. Phys. (Kyoto) **11**, 437 (1954).

[13] The fact that not all invariances generate conservation laws has been stressed by Wigner (private communication; also Ref. 12).

Electromagnetic Field inside a Current-Carrying Region*

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The improper integrals, appearing in the course of evaluating the vector potential **A** and the electric field **E** inside a current-carrying region, are carefully examined. It is found that the integrals exist and have a well-defined meaning only when the current density function satisfies a Hölder condition. A definite and precise way of evaluating them is derived and **A**, **E** are shown to satisfy the usual inhomogeneous equations.

I. INTRODUCTION

THE electric field due to a volume current density distribution $\mathbf{J}(\mathbf{r})$ in a volume V can be compactly expressed at points exterior to V by means of a Green's dyadic as[1-3]

$$\mathbf{E}(\mathbf{r}_0) = \iiint_V j\omega\mu\mathbf{J}(\mathbf{r})\cdot\mathbf{G}(\mathbf{r}\mid\mathbf{r}_0)\,dV, \tag{1}$$

where

$$\mathbf{G}(\mathbf{r}\mid\mathbf{r}_0) = -\frac{1}{4\pi}\left(\mathbf{I}+\frac{1}{k^2}\nabla\nabla\right)\phi = \frac{1}{4\pi k^2}\nabla\times\nabla\times\phi\mathbf{I};$$

$$\phi = e^{-ikR}/R; \qquad R = |\mathbf{r}-\mathbf{r}_0|. \tag{2}$$

In the above, $\mathbf{I}$ is the identity dyadic and the harmonic time dependence $e^{j\omega t}$ has been assumed. At points exterior to V the integral in (1) is well defined and, as in potential theory,[4] it may be proved that $\mathbf{E}(\mathbf{r}_0)$ is an analytic (differentiable any number of times) function of x_0, y_0, z_0. When $\mathbf{r}_0$ is an interior point of V, ϕ and its derivatives have a singularity at $\mathbf{r}_0$ and the integral becomes improper. Its existence, let alone its continuity and differentiability, and, consequently, the existence of the function $\mathbf{E}(\mathbf{r}_0)$ on the left of Eq. (1) are at stake and must be carefully investigated. Situations of the same nature appear in potential theory and the rigorous theory of the improper integrals involved is given in detail in Ref. 4, pp. 17–21 and Chap. VI, in particular. In the following continuous reference will be made to the precise definitions and results of Ref. 4, since rigor, as will become apparent, is indispensable in situations of this kind. Despite the mathematical undertones of the development, its practical interest in connection with the theory of scattering, plasmas, electron beams, etc., needs no overstressing.

II. THE ELECTRIC FIELD AT INTERIOR POINTS

Consider a closed region V bounded by the surface S, both regular in accordance with the definitions in Chap. IV of Ref. 4. The Cartesian components J_x, J_y, J_z of the volume current density $\mathbf{J}(\mathbf{r})$ are considered to be piecewise continuous functions[4] of x, y, z in V. At the moment no further assumptions are made about them. The surfaces S_i in V at which $\mathbf{J}(\mathbf{r})$ is discontinuous are regular, by the definition of piecewise continuity.[4]

A point $\mathbf{r}$ is said to be an interior/exterior point of V provided it is the center of a sphere all/none of whose points belong to V[4]. At any exterior point $\mathbf{r}_0$, the volume integral in (1) defines an analytic function $\mathbf{E}(\mathbf{r}_0)$ of x_0, y_0, z_0. Consider now a point $\mathbf{r}_0$ interior to V. At such a point $\mathbf{E}(\mathbf{r}_0)$ may be expressed in terms of the scalar and vector potentials satisfying the Lorentz condition, namely

$$\mathbf{E}(\mathbf{r}_0) = -j\omega\mathbf{A} - \nabla_0\varphi = -j\omega\mathbf{A} + (1/j\omega\epsilon\mu)\nabla_0\nabla_0\cdot\mathbf{A}. \tag{4}$$

This expression is a direct consequence of Maxwell's Equations. It is also found that **A** satisfies the inhomogeneous vector wave equation

$$\nabla^2\mathbf{A} + k^2\mathbf{A} = -\mu\mathbf{J} \tag{5}$$

with general solution

$$A_u(\mathbf{r}_0) = \frac{\mu}{4\pi}\iiint_V J_u(\mathbf{r})\phi(R)\,dV; \qquad \phi = e^{-ikR}/R; \quad u = x, y, z. \tag{6}$$

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[1] R. D. Kodis, J. Soc. Indust. Appl. Math. 2, 89 (1954).
[2] J. Van Bladel, IRE Trans. on Ant. and Prop. 9, 563 (1961).
[3] J. Van Bladel, *Electromagnetic Fields* (McGraw-Hill Book Company, Inc., New York, 1964), Chap. 7, pp. 220–222.
[4] O. D. Kellogg, *Foundations of Potential Theory* (Dover Publications, Inc., New York, 1953).

The last integral is again improper and, in it, $J_u(\mathbf{r})$ is a piecewise continuous function of $\mathbf{r}$. However, the integral is convergent and defines the function $A_u(\mathbf{r}_0)$ throughout V. The definition of convergent improper integrals and certain lemmas on them are given in Ref. 4. [Let $f(\mathbf{r})$ become infinite at a single point $\mathbf{r}_0$ of the region V of integration. Then the integral

$$I = \iiint_V f(\mathbf{r})\, dV$$

is said to be convergent, or to exist, provided

$$\lim_{\delta \to 0} \iiint_{V-v} f(\mathbf{r})\, dV$$

exists, where v is a variable regular region subject to the sole restrictions that it shall have $\mathbf{r}_0$ in its interior, and that its maximum chord shall not exceed δ. The value of the convergent integral is defined to be this limit. It may also be proved that if I is convergent, the integral $\iiint_v f(\mathbf{r})\, dV$ approaches 0 with the maximum chord of v. Additional lemmas are given in Ref. 4, pp. 147–150.] Further, it is there proved that the so defined function $A_u(\mathbf{r}_0)$ is continuous and, even further, differentiable throughout V. This last property amounts to saying that $\partial A_u/\partial u_0 (u_0 = x_0, y_0, z_0)$ can be obtained by differentiating under the sign of integration. With this in mind it is possible to rewrite (4) in the form[2,3]

$$\mathbf{E}(\mathbf{r}_0) = -\frac{j\omega\mu}{4\pi} \iiint_V \mathbf{J}(\mathbf{r})\phi(R)\, dV - \frac{1}{4\pi j\omega\epsilon} \nabla_0 \iiint_V \mathbf{J}(\mathbf{r}) \cdot \nabla\phi\, dV \qquad (7)$$

in which the improper integrals are convergent.[4] Returning to the vector potential as defined by (6), we go one step further and inquire about the existence of the second derivatives of $\mathbf{A}(\mathbf{r}_0)$. As will become apparent, and in analogy with potential theory,[4] the mere continuity of $J_u(\mathbf{r}_0)$ does not suffice to guarantee even the existence of second derivatives. This is ensured only when the current density satisfies a so-called Hölder condition at $\mathbf{r}_0$, this being equivalent to the statement that there exist three positive constants c, B, α such that

$$|J_u(\mathbf{r}) - J_u(\mathbf{r}_0)| \leq BR^\alpha, \quad R = |\mathbf{r} - \mathbf{r}_0|; \quad u = x, y, z \qquad (8)$$

for all points $\mathbf{r}$ for which $R \leqq c$. Some plots and pertinent comments clarifying the meaning of this condition in one dimension will be given later. Notice that now $\mathbf{r}_0$ cannot belong to either S or S_i on which $\mathbf{J}(\mathbf{r})$ is discontinuous. Nevertheless, at such points, at least certain second derivatives of a continuous solution of (5) must be discontinuous, as is indicated by (5); i.e., if the density jumps by $\mathbf{J}_1$ in crossing such a surface, $\nabla^2\mathbf{A}$ must jump by $-\mu\mathbf{J}_1$.

Let now Σ be a sphere about $\mathbf{r}_0$ of radius a, lying in V. Then $\mathbf{A} = \mathbf{A}_1 + \mathbf{A}_2$, where $\mathbf{A}_1$ is the potential of the current density inside Σ and $\mathbf{A}_2$ the potential of the remaining current density distribution. As $\mathbf{r}_0$ is exterior to this latter distribution, the potential $\mathbf{A}_2$ has derivatives of all orders at $\mathbf{r}_0$ and satisfies $\nabla^2\mathbf{A}_2 + k^2\mathbf{A}_2 = 0$ there.

Consider next $\mathbf{A}_1$. If the density $\mathbf{J}(\mathbf{r})$ is constant in Σ then at each interior point $\mathbf{r}_1$ of Σ using (6) we may obtain (see also Fig. 1)

$$A_{1u}(\mathbf{r}_1) = \frac{\mu J_u}{k^2}\left[\frac{\sin k\,|\mathbf{r}_1 - \mathbf{r}_0|}{k\,|\mathbf{r}_1 - \mathbf{r}_0|} \times e^{-jka}(1 + jka) - 1\right]; \qquad u = x, y, z. \qquad (9)$$

We see that, at interior points, $A_{1u}(\mathbf{r}_1)$ exists and turns out to be differentiable any number of times with respect to x_1, y_1, z_1. In addition

$$\nabla_1^2 A_{1u} + k^2 A_{1u} = -\mu J_u, \qquad (10)$$

i.e., for constant $\mathbf{J}$, Eq. (5) is satisfied in the interior of Σ.

Setting now

$$\mathbf{J}(\mathbf{r}) = [\mathbf{J}(\mathbf{r}) - \mathbf{J}(\mathbf{r}_0)] + \mathbf{J}(\mathbf{r}_0),$$

we see that the potential of a sphere with continuous current density at $\mathbf{r}_0$ is the sum of the potentials of the sphere with vanishing density at $\mathbf{r}_0$ and of a sphere with constant density, equal to $\mathbf{J}(\mathbf{r}_0)$, of the given sphere. It remains to evaluate the contribution

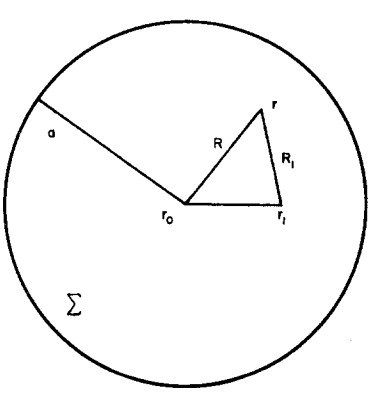

FIG. 1. The sphere Σ excluded around $\mathbf{r}_0$.

from the "excess" density $\mathbf{J}'(\mathbf{r})$ in the sphere, which was supposed to satisfy a Hölder condition. Assuming $a \leq c$, this means that

$$|J'_u(\mathbf{r})| \leq BR^a; \qquad R = |\mathbf{r} - \mathbf{r}_0|. \tag{11}$$

Under this condition, differentiation under the sign of integration is still possible. In fact, for two typical second derivatives we have

$$D_1 = \left[\iiint_\Sigma J'_u(\mathbf{r}) \frac{\partial^2 \phi(R)}{\partial x^2}\, dV\right]_{\mathbf{r}_0} = -\iiint_\Sigma J'_u(\mathbf{r}) \frac{e^{-jkR}}{R^3}$$

$$\times \left[1 + jkR - jkx^2 \frac{3 + jkR}{R} - \frac{3x^2}{R^2}\right] dV, \tag{12}$$

$$D_2 = \left[\iiint_\Sigma J'_u(\mathbf{r}) \frac{\partial^2 \phi(R)}{\partial x\, \partial y}\, dV\right]_{\mathbf{r}_0}$$

$$= \iiint_\Sigma J'_u(\mathbf{r}) \frac{xy}{R^5} e^{-jkR}[3 + jkR(3 + jkR)]\, dV, \tag{13}$$

where the origin was taken at $\mathbf{r}_0$ with $R = |\mathbf{r} - \mathbf{r}_0| = (x^2 + y^2 + z^2)^{\frac{1}{2}}$; the integrals involved are convergent by virtue of (11) and since, also, $|x| \leq R$, $|y| \leq R$, etc.[4]

The fact that the integrals are convergent and define D_1 and D_2 is not in itself enough to establish the identification, for instance, of D_1 with $(4\pi/\mu)(\partial^2 A_u/\partial x^2)_{\mathbf{r}_0}$. In order to achieve that, we resort to the definition of derivative and to the already established fact that for the first derivatives, differentiation under the sign of integration is permissible. If $\mathbf{r}_0$, $\mathbf{r}_1$, and $\mathbf{r}$ are the points (0, 0, 0), (h, 0, 0), and (x, y, z), respectively, we consider

$$I = \frac{4\pi}{\mu h}\left[\left(\frac{\partial A_u}{\partial x}\right)_{\mathbf{r}_1} - \left(\frac{\partial A_u}{\partial x}\right)_{\mathbf{r}_0}\right] - D_1 \tag{14}$$

for $h \neq 0$, where, with $R = (x^2 + y^2 + z^2)^{\frac{1}{2}}$ and $R_1 = [(x - h)^2 + y^2 + z^2]^{\frac{1}{2}}$, we obtain

$$I = \iiint_\Sigma J'_u(\mathbf{r})\left\{\frac{1}{h}\left[(x - h)e^{-jkR_1} \frac{1 + jkR_1}{R_1^3}\right.\right.$$

$$\left. - xe^{-jkR} \frac{1 + jkR}{R^3}\right] + \frac{e^{-jkR}}{R^3}$$

$$\left.\times \left[1 + jkR - jkx^2 \frac{3 + jkR}{R} - \frac{3x^2}{R^2}\right]\right\} dV. \tag{15}$$

The integral I is convergent for reasons similar to those for D_1 and with the use of the additional relations $|x - h| \leq R_1$, etc. It will be shown that I tends to 0 with h. Calling

$$g(h) = (x - h)e^{-jkR_1}(1 + jkR_1)/R_1^3 \tag{16}$$

it may be seen that the bracketed expression in the integrand of (15) is

$$\frac{g(h) - g(0)}{h} - g'(0) = g''(0)\frac{h}{2!}$$

$$+ g'''(0)\frac{h^2}{3!} + \cdots, \tag{17}$$

where a Maclaurin series in h was used to obtain the right-hand side. It is now obvious that the integral has a meaning for $h = 0$, in fact it is 0, since the integrand reduces then to 0. It remains to show that I is continuous in $\mathbf{r}_1$ at $\mathbf{r}_0$, so that it tends to 0 with h. It will then follow from (14) that the derivative $(4\pi/\mu)(\partial^2 A_u/\partial x^2)$ exists at $\mathbf{r}_0$ and equals D_1. The proof is based on the usual reasoning explained in Ref. 4: a small sphere σ about $\mathbf{r}_0$ is considered. With $\mathbf{r}_1$ interior to σ the integrand in (15) is continuous in $\Sigma - \sigma$, apart from the piecewise continuous density $J'_u(\mathbf{r})$. The contribution from $\Sigma - \sigma$ can, therefore, be made arbitrarily small, independently of σ, by restricting sufficiently h. Then I will be continuous if the integral over σ can be made arbitrarily small by sufficiently restricting the radius of σ, independently of the position of $\mathbf{r}_1$ in σ. Two infinities are now present in the integrand, those due to denominators containing R and those containing R_1. It is obvious that terms giving rise to convergent integrals [for instance those containing R in the denominator, because of (11)] can be discarded since they tend to 0 with σ, independently of $\mathbf{r}_1$. We then keep only the "most singular" terms. This immediately reduces the integrand to the corresponding one of potential theory (Ref. 4, pp. 154–155) and the rest of the proof can be found in Ref. 4. Thus I is continuous and the desired result

$$(4\pi/\mu)[\partial^2 A_u/\partial x^2]_{\mathbf{r}_0} = D_1 \tag{18}$$

is obtained. The same procedure applies to D_2 and to $\partial^2 A_u/\partial x \partial y$. In particular, forming $\nabla_0^2 A_u$ from (12), by interchanging x, y, z, adding and using (6), we find for the pontential due to $J'_u(\mathbf{r})$:

$$\nabla^2 A_u = -k^2 A_u. \tag{19}$$

Adding the potential of the rest of the distribution, inside and outside Σ, we see that all second derivatives of $\mathbf{A}$ exist and that (5) is satisfied.

Returning to the electric field and Eq. (4), it may be concluded that, as long as $\mathbf{J}$ satisfies a Hölder condition at $\mathbf{r}_0$, the equation is valid and that it can be expressed in terms of convergent integrals. Evaluation of $\mathbf{E}$ is based on Eqs. (4), (9) and on the possibility of differentiating under the sign of integration for the rest of the contribution. More explicitly, Eq. (1) becomes

$$\mathbf{E}(\mathbf{r}_0) = \iiint_{V-\Sigma} j\omega\mu \mathbf{J}(\mathbf{r})\cdot \mathbf{G}(\mathbf{r} \mid \mathbf{r}_0)\, dV + \iiint_{\Sigma} j\omega\mu[\mathbf{J}(\mathbf{r}) - \mathbf{J}(\mathbf{r}_0)]\cdot \mathbf{G}(\mathbf{r} \mid \mathbf{r}_0)\, dV + \frac{\mathbf{J}(\mathbf{r}_0)}{j\omega\epsilon}\left[\tfrac{2}{3}e^{-jka}(1 + jka) - 1\right]. \tag{20}$$

The integral over Σ is convergent. Notice that Σ can be any finite region around $\mathbf{r}_0$, not necessarily a sphere, as long as it lies in V and in it (11) is satisfied (i.e., max $|\mathbf{r} - \mathbf{r}_0| \leq c$). This would modify the form of Eq. (9) and the last term in (20), which, for a sphere, assume their simplest and more explicit form. However, the field may be evaluated at all points $\mathbf{r}_1$ interior to $\Sigma(\mathbf{r}_0)$, not only at its center. This is equivalent to using as excluded region for $\mathbf{r}_1$ a sphere with center at the nearby point $\mathbf{r}_0$, in accordance with the preceding remark. The general formula reads

$$\mathbf{E}(\mathbf{r}_1) = \iiint_{V-\Sigma(\mathbf{r}_0)} j\omega\mu \mathbf{J}(\mathbf{r})\cdot \mathbf{G}(\mathbf{r} \mid \mathbf{r}_1)\, dV + \iiint_{\Sigma(\mathbf{r}_0)} j\omega\mu[\mathbf{J}(\mathbf{r}) - \mathbf{J}(\mathbf{r}_1)]\cdot \mathbf{G}(\mathbf{r} \mid \mathbf{r}_1)\, dV + \frac{1}{j\omega\epsilon}\left[1 + \frac{1}{k^2}\nabla_1\nabla_1\right] \cdot \mathbf{J}_1\left[\frac{\sin k\,|\mathbf{r}_1 - \mathbf{r}_0|}{k\,|\mathbf{r}_1 - \mathbf{r}_0|}\, e^{-jka}(1 + jka) - 1\right], \tag{21}$$

where $\mathbf{J}_1 = \mathbf{J}(\mathbf{r}_1)$ is a constant vector, not operated upon by ∇_1. It is obvious that in all cases the inhomogeneous equation $\nabla \times \nabla \times \mathbf{E} - k^2\mathbf{E} = -j\omega\mu\mathbf{J}$ is satisfied.

III. ILLUSTRATIONS AND CONCLUSIONS

The following comments are addressed to the engineer and applied physisist, rather than to the mathematician. In order to illustrate the Hölder condition two functions are given

$$f_1(x) = -1/\log x, \quad x > 0; \qquad f_1(x) = 1/\log |x|, \quad x < 0; \qquad f_1(0) = 0, \tag{22}$$

$$f_2(x) = x^{\frac{1}{2}}, \quad x > 0; \qquad f_2(x) = -|x|^{\frac{1}{2}}, \quad x < 0; \qquad f_2(0) = 0. \tag{23}$$

The profile of their plot versus x, around $x = 0$, is shown in Fig. 2. They are both continuous at $x = 0$, they even have "continuously turning" tangent at $x = 0$, but they are not differentiable at $x = 0$. The second satisfies a Hölder condition at $x = 0$ with

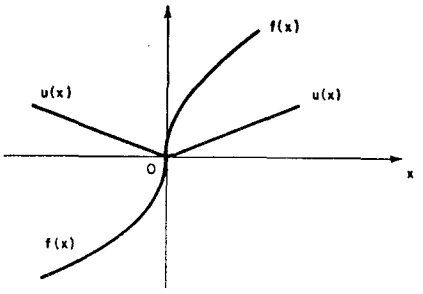

FIG. 2. Illustration of the Hölder condition.

$\alpha \leq \frac{1}{2}$, the first does not. The somewhat loose statement that a Hölder condition is stronger than continuity but weaker than differentiability if $\alpha < 1$, is illustrated by $f_2(x)$. Another example is $u(x) = |Bx|$, for which $\alpha \leq 1$.

In conclusion, a definite and precise way of evaluating the field at the interior points of a current-carrying region has been derived. At the same time attention has been drawn to the necessity of exercising special care in dealing with improper integrals. In particular, differentiation under the sign of integration (i.e., interchange of differential and integral operators) requires the utmost care. Moreover, it is not permissible, in general, to let the finite volume v, excluded from V, approach 0, unless a proof can be provided that

$$I_1 = \lim_{v\to 0} \iiint_{V-v} F(\mathbf{r})\, dV$$

exists. In fact, this limit will not exist, unless

$$I = \iiint_{V} F(\mathbf{r})\, dV$$

is a convergent integral, which is equivalent to saying[4] that

$$I_2 = \lim_{v\to 0} \iiint_{v} F(\mathbf{r})\, dV = 0.$$

[In this connection consider Eq. (20) for $\mathbf{J}(\mathbf{r}) = \mathbf{J}$ = constant throughout V. It is not permissible to let $\Sigma \to 0$ in this equation since

$$\lim_{\Sigma\to 0} \iiint_{\Sigma} \mathbf{J}\cdot \mathbf{G}(\mathbf{r} \mid \mathbf{r}_0)\, dV$$

does not exist and, therefore, does not approach 0. Then, neither does

$$\lim_{\Sigma\to 0} \iiint_{V-\Sigma} \mathbf{J}\cdot \mathbf{G}\, dV$$

exist.]

Relativistic Three-Particle SU_3 States

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The scheme for classifying three-particle states according to SU_3 is extended to the relativistic domain. A discussion is also given of the basic group theory lying behind the scheme.

INTRODUCTION

IT has recently been shown that the set of states for three noninteracting and nonrelativistic spinless particles can be put into a one-to-one correspondence with the set of irreducible representations of SU_3.[1] The SU_3 states followed uniquely from three requirements:

(i) The total 4-momentum Q, the total angular momentum J, and its third component J_z should be diagonal.

(ii) All three particles should be treated on an equal footing.

(iii) There should be easy passage between momentum and position representations.

In this note, the SU_3 states will be generalized to the relativistic case. Our method is based on the recent work of Halpern and is essentially an application of his technique to the problem at hand.[2] Section 1 is devoted to a simple mathematical exercise which contains the essence of the problem. The insight gained there is applied to the actual problem in Sec. 2. A final section discusses the underlying group-theoretical reasons for the success of the SU_3 classification scheme.

1. MATHEMATICAL PRELIMINARIES

Let S_c denote the surface of a cube in three-dimensional Euclidean space, and F the set of all continuous functions f defined on this surface. F is evidently a vector space under the operations of ordinary addition of functions and scalar multiplication. In addition, F can be given a scalar product by the rule

$$(f_1, f_2) = \int \bar{f}_1 f_2 \, dA, \tag{1.1}$$

where $\int dA$ denotes integration over the surface area of the cube. In this context we pose and answer the following question: How can one simply choose a complete orthonormal basis for F?

We notice that the surface of a cube is topologically equivalent to S^2, the surface of a sphere. (Here we ignore the corners and edges of the cube, or first round them off.) In fact, S_c can be mapped onto S^2 by a simple radial projection. That is, we can think of S_c as a surface obtained by taking a unit sphere and making radial deformations which vary from point to point.

Using the projection mapping, the scalar product (1.1) can be written in the equivalent form

$$(f_1, f_2) = \int W(\Omega) \bar{f}_1 f_2 \, d\Omega, \tag{1.2}$$

where the integral is now over S^2, and $W(\Omega)$ is a positive weight function arising from the change of variables. The answer to our question is now immediate. A simple complete orthonormal set, denoted by f_{lm}, can be had by writing

$$f_{lm} = W^{-\frac{1}{2}}(\Omega) Y_{lm}(\Omega) \tag{1.3}$$

where the Y_{lm} are the familiar spherical harmonics.

There are important observations to be drawn from our simple exercise. The Y_{lm} are famous for their simple transformation properties under the action of the generators of the rotation group. Denoting these generators by L_i, we see that the f_{lm} have the same properties under operators L_i' defined by

$$L_i' = W^{-\frac{1}{2}} L_i W^{\frac{1}{2}}. \tag{1.4}$$

Since the L_i are Hermitian with respect to the usual scalar product, the L_i' are Hermitian with respect to the scalar product (1.2). The L_i' also obey the same commutation rules as the L_i. Passing from the generators to the group itself, we know that

$$U_R Y(\Omega) = Y(R^{-1}\Omega), \tag{1.5}$$

where U_R denotes the unitary operator generated

[1] A. J. Dragt, J. Math. Phys. 6, 533 (1965) and hereafter referred to as (I).
[2] F. R. Halpern, Phys. Rev. 137, B1587 (1965).

by the L_i and corresponding to the rotation R. In the primed case, one has

$$U'_R f(\Omega) = W^{-\frac{1}{2}}(\Omega) W^{\frac{1}{2}}(R^{-1}\Omega) f(R^{-1}\Omega). \quad (1.6)$$

Finally, the U'_R satisfy the usual group properties,

$$U'_{R_1} U'_{R_2} = U'_{R_1 R_2}, \quad (1.7)$$

and are unitary with respect to the scalar product (1.2).

We conclude that, even though S_0 itself is not rotationally invariant, the space of functions F can nevertheless be completely decomposed with the aid of Hermitian operators L'_i related to the usual L_i through a simple similarity transformation Clearly, the same argument will go through for any manifold topologically equivalent to S^2. The surface S_0 merely served as a simple example.

2. RELATIVISTIC STATES

Let $|k\rangle$ denote a single-particle plane-wave state having 4-momentum k. The Lorentz group will act according to the rule

$$U(L)\ |k\rangle = |Lk\rangle, \quad (2.1)$$

where L is the ordinary 4×4 Lorentz transformation matrix. For U to be unitary, the scalar product must be of the form

$$\langle k \mid k' \rangle = (\omega\omega')^{\frac{1}{2}} \delta_3(\mathbf{k} - \mathbf{k}'), \quad (2.2)$$

where $\mathbf{k}$ and ω denote the space and time components of k. Three-particle plane-wave states are obtained by taking the tensor product $|k_1\rangle\ |k_2\rangle\ |k_3\rangle$ which will be written more briefly as $|k_1 k_2 k_3\rangle$.

The states which we seek will be superpositions of plane-wave states written in the form

$$|Q\mu\rangle = \int \prod_{i=1}^{3} \omega_i^{-1}\, d^3\mathbf{k}_i\ \delta(k_1 + k_2 + k_3 - Q) \times f_\mu(k_1 k_2 k_3)\ |k_1 k_2 k_3\rangle. \quad (2.3)$$

The state $|Q\mu\rangle$ has total 4-momentum Q and a set of discrete quantum numbers $\{\mu\}$. From now on we shall work directly in the center-of-momentum (CM) frame and pass to arbitrary frames by Lorentz velocity transformations. That is, we define

$$|Q\mu\rangle = U(L)\ |Q_0\mu\rangle, \quad (2.4)$$

where

$$Q = LQ_0, \quad (2.5)$$

$$Q_0 = (0, 0, 0, M), \quad (2.6)$$

and L is a pure velocity transformation.

The scalar product $\langle Q\mu | Q_0\nu\rangle$ can be calculated using Eq. (2.2),

$$\langle Q\mu |\ Q_0\nu\rangle = \delta(Q - Q_0) \int \prod_i \omega_i^{-1}\, d^3\mathbf{k}_i \times \delta_3(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3)\ \delta(\omega_1 + \omega_2 + \omega_3 - M) \bar{f}_\mu f_\nu. \quad (2.7)$$

For the moment we restrict ourselves to the case where all particles have the same mass m. As in (I), we introduce relative momenta defined by the relations

$$\begin{aligned} \mathbf{p}^{(1)} &= 2^{-\frac{1}{2}}(\mathbf{k}_2 - \mathbf{k}_1), \\ \mathbf{p}^{(2)} &= 6^{-\frac{1}{2}}(2\mathbf{k}_3 - \mathbf{k}_1 - \mathbf{k}_2), \\ \mathbf{p}^{(3)} &= 3^{-\frac{1}{2}}(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3). \end{aligned} \quad (2.8)$$

Using the new variables transforms the integral to the simpler form

$$3^{-\frac{1}{2}} \int d^3\mathbf{p}^{(1)}\, d^3\mathbf{p}^{(2)} (\omega_1\omega_2\omega_3)^{-1}\ \delta(\textstyle\sum \omega_i - M) \bar{f}_\mu f_\nu. \quad (2.9)$$

In this form it is clear that we are dealing with an integration over a certain five-dimensional manifold P (phase space) embedded in six-dimensional Euclidean space. In the low-energy limit, the argument of the delta function takes the form

$$\begin{aligned} &\textstyle\sum \omega_i - M \\ &\quad = (2m)^{-1}(\mathbf{p}^{(1)2} + \mathbf{p}^{(2)2}) + 3m - M. \end{aligned} \quad (2.10)$$

Thus at low energies (and up to a scale transformation), P is essentially S^5, the five-dimensional surface of a sphere in six-dimensional space. This circumstance suggests that we radially project P onto S^5 just as we projected S_0 onto S^2 in Sec. 1. Or equivalently, we should view $\mathbf{p}^{(1)}$ and $\mathbf{p}^{(2)}$ collectively as the components of a six-dimensional vector $\mathbf{p}$,

$$\mathbf{p} = (\mathbf{p}^{(1)}, \mathbf{p}^{(2)}). \quad (2.11)$$

Employing the projection mapping, the integral takes the final form

$$\int \prod_i \omega_i^{-1}\, d^3\mathbf{k}_i\ \delta(\textstyle\sum k_i - Q_0) \bar{f}_\mu f_\nu = \int d\Omega W(\Omega) \bar{f}_\mu f_\nu, \quad (2.12)$$

where $d\Omega$ denotes integration over S^5. The weight is given by

$$W = [\theta(p) 3^{-\frac{1}{2}} (\omega_1\omega_2\omega_3)^{-1} p^5 (\partial H/\partial p)^{-1}]|_{p=p_0}, \quad (2.13)$$

where

$$H(\Omega, p) = \textstyle\sum \omega_i - M \quad (2.14)$$

and $p_0(\Omega)$ is defined by the relation

$$H(\Omega, p_0) = 0. \tag{2.15}$$

More specifically,

$$W(\Omega) = (m_1 m_2 m_3)^{\frac{1}{3}}(\sum m_i)^{-\frac{1}{3}}(\omega_1\omega_2\omega_3)^{-1} \times (\sum \omega_i^2 m_i^{-1} - m_i)^3(M - \sum m_i^2\omega_i^{-1})^{-1}. \tag{2.16}$$

The quantities ω_i and M are to be evaluated in the CM frame. The term $\theta(p_0)$ is actually unnecessary since p_0 as defined by Eq. (2.15) is always positive. In other words, P is always topologically equivalent to S^5 even at high energies.

The rule for constructing covariant three-particle states satisfying conditions (i) and (ii) [and (iii) in the limit of low energy in the CM frame] is now apparent. We observe that the SU_3 functions found in (I) form a complete orthonormal set over S^5. Consequently, we simply write

$$f_\mu(\Omega) = W^{-\frac{1}{2}}(\Omega)g_\mu(\Omega) \tag{2.17}$$

to obtain the required orthonormal set over P with the scalar product (2.12). Here $g_\mu(\Omega)$ denotes an SU_3 function,

$$g_\mu(\Omega) = g(n_a n_b jm\omega; \alpha\beta\gamma\rho\phi). \tag{2.18}$$

The index μ collectively embraces the quantum numbers $(n_a n_b jm\omega)$. The coordinates of a point Ω in S^5 are given by the three Euler angles α, β, γ, and the two Dalitz–Fabri coordinates ρ, ϕ. Since the relationship between these coordinates and the point Ω depends only on the geometry of S^5, the Dalitz–Fabri plot as defined in (I) remains circular at all energies. This is in contrast to the usual definition where the shape of the plot is energy dependent.[3] The price that has been paid for this convenience is the appearance of the weight W.

The functions g_μ are characterized by their transformation properties under an SU_3 group having eight generators which, in analogy with Sec. 1, will again be denoted by L_i. In particular, the g_μ are eigenfunctions of certain operators O, built up from the L_i. Consequently, the f_μ will be eigenfunctions (with the same eigenvalues) of operators O_i' obtained by the similarity transformation (1.4). Now among the O_i are J^2 and J_z where $\mathbf{J}$ denotes the total angular momentum in the CM frame. But since W is rotationally invariant, we have $\mathbf{J}' = \mathbf{J}$ so that the f_μ are also angular momentum eigenfunctions. Finally, since W is a symmetric function of the momenta of the three particles, the operators L_i' and O_i' treat all particles on an equal footing. We conclude that the prescription (2.17) satisfies all the necessary requirements.

This completes our discussion on the construction of covariant SU_3 states in the equal-mass case. For the unequal-mass case, it is necessary to replace the definitions of $p^{(1)}$ to $p^{(3)}$ given in Eq. (2.8) with those given in the Appendix of (I) to assure that P is again essentially S^5 at low energies. When this is done, Eq. (2.16) also holds for the unequal-mass case.

3. DISCUSSION

In (I) it was implicitly assumed that the SU_3 functions formed a complete set over S^5. We now sketch a proof. To begin, we need two facts about the SU_3 functions which can easily be verified from their method of construction. They are that the functions $p^\lambda g_\mu$ are solutions of the six-dimensional Laplace equation and are homogeneous polynomials in the variables p_i ($i = 1$ to 6) of order $\lambda = n_a + n_b$. See Eqs. (6.4), (6.7), (6.57) of (I). Consequently, each SU_3 function is a spherical harmonic polynomial.

The completeness of the spherical harmonics can be easily proved by using the Weierstrass approximation theorem.[4] Let f be an arbitrary continuous function defined on S^5. We extend f to a continuous function $\hat{f}$ defined in the cube $-1 \leq p_i \leq 1$ by the rule

$$\hat{f}(\mathbf{p}) = p^2 f\left(\frac{\mathbf{p}}{p}\right), \quad p \neq 0; \qquad \hat{f}(0) = 0. \tag{3.1}$$

It follows from the Weierstrass theorem that $\hat{f}$ can be uniformly approximated by polynomials in the variables p_i constructed from monomials of the form $p_1^{n_1}p_2^{n_2}\cdots p_6^{n_6}$. But on S^5 these monomials can be re-expressed in terms of the spherical harmonics. Therefore, the spherical harmonics form a complete set over S^5.

It remains to be shown that the SU_3 polynomials comprise all of the spherical harmonics. The simplest thing to do is to count. The number of spherical harmonics of order λ on S^5 is given by[5]

$$N(\lambda) = (\lambda + 2)(\lambda + 3)!/12\lambda!. \tag{3.2}$$

[3] E. Fabri, Nuovo Cimento 11, 479 (1954).

[4] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1953), p. 65 ff.

[5] A. Erdelyi, *The Bateman Manuscript Project, Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 2, p. 237.

An SU_3 polynomial of order λ arises from representations having $n_a + n_b = \lambda$. The dimension of an SU_3 representation is given by[6]

$$d(n_a, n_b) = \tfrac{1}{2}(n_a + 1)(n_b + 1)(n_a + n_b + 2). \quad (3.3)$$

One easily checks that

$$N(\lambda) = \sum_{n_a+n_b=\lambda} d(n_a, n_b). \quad (3.4)$$

There is also a more group-theoretical derivation of the relation between SU_3 and S^5. It is based on the observation that S^5 is topologically equivalent to the cosets of SU_3 with respect to an SU_2 subgroup.[7] Let A and B be 3×3 SU_3 matrices and let H denote the SU_2 subgroup of SU_3 consisting of all matrices of the form[8]

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cdots & \cdots \\ 0 & \cdots & \cdots \end{bmatrix}.$$

Then A and B are in the same SU_2 coset provided $A^{-1}B \in H$. It is easily checked that A and B will be in the same coset if and only if they have the same first column (a_1, a_2, a_3). Since the matrices are unitary,

$$\sum |a_i|^2 = 1. \quad (3.5)$$

Also, given any set of a_i satisfying Eq. (3.5), it is possible to construct an SU_3 matrix having the a_i as a first column by suitably adjusting the other two columns. Consequently, the cosets of SU_3 with respect to H are in one-to-one correspondence with triplets of complex numbers obeying Eq. (3.5). Writing out Eq. (3.5) in real and imaginary parts gives S^5. We write this result symbolically as

$$SU_3/SU_2 \approx S^5. \quad (3.6)$$

In this form it is clear how SU_3 acts on S^5. It acts by the left multiplicative action of the group on its SU_2 cosets.[9]

The set F of continuous functions on S^5 can be viewed as continuous maps of SU_3/SU_2 onto C, the complex numbers. SU_3 now provides a family of mappings U of F onto itself by the rule

$$U_g : f \to f \circ g^{-1}; \qquad f \in F, \qquad g \in SU_3. \quad (3.7)$$

This is just Eq. (1.5) in disguise. Since F is a vector space, we get in this way a representation of SU_3. The representation is unitary since it preserves a scalar product similar to Eq. (1.1). Our problem is to determine what irreducible SU_3 representations are carried by F and how often each occurs.

A little reflection shows that our problem is a specific example of a more general problem: given a compact group G and a closed subgroup H, what representations of G are carried by the vector space F of maps of G/H onto C? As another example, consider SU_2. It is easy to check that $SU_2/U_1 \approx S^2$, where U_1 is the one-dimensional unitary subgroup of rotation about the z axis. Again, for SU_2 itself one has $SU_2 \approx S^3$. The question is: what representations of SU_2 are carried by functions defined on S^2 and S^3, and how often does each representation occur?

The answer to the general problem is given by the Frobenius reciprocity theorem.[10] Take a specific irreducible representation Γ^α of G. Then Γ^α also provides a representation of the subgroup H. In general, when viewed as a representation of H, Γ^α is reducible. See how many times Γ^α when restricted to H contains the identity representation of H. Call this number ν_α. Then F carries the representation Γ^α of G exactly ν_α times.

We first apply the theorem to the case $G = SU_2$. Representations of SU_2 are labeled by a single index j. For the case in which $H = U_1$, we have to ask: for what values of j does Γ^j have a vector with $j_z = 0$? Obviously j must be integral; in which case there is one and only one vector with $j_z = 0$. Therefore only the integral spin representation of SU_2 occur for S^2, and each integral representation occurs once. The representations are given, of course, by the Y_{lm}. For the case of SU_2 itself, H is the identity element. We therefore have to ask how many times the identity representation of the identity element occurs in Γ^j. The answer is $2j + 1$ times, the dimension of Γ^j. Therefore, the functions defined on S^3 carry all irreducible representations of SU_2, and each representation occurs $2j + 1$ times. The representations are given by the $D^j_{mm'}(\alpha\beta\gamma)$

[6] J. J. de Swart, Rev. Mod. Phys. **35**, 916 (1963).

[7] H. Weyl, *The Classical Groups* (Princeton University Press, Princeton, New Jersey, 1961), p. 268.

[8] This is an SU_2 of the "X" type in the terminology of (I).

[9] It can be shown in general that if a group G acts transitively on a manifold M, then $M \approx G/H$, where H is some subgroup of G. M is called a homogeneous space. See L. Pontrjagin, *Topological Groups* (Princeton University Press, Princeton, New Jersey, 1958), p. 291; or see R. L. Bishop and R. J. Crittenden, *Geometry of Manifolds* (Academic Press Inc., New York, 1964), p. 38.

[10] G. W. Mackey, Ann. Math, **55**, 101 (1952). See Theorem 8.2. The representations we are dealing with are special cases of "induced" representations in which the "inducing representation" of H is one dimensional. See also A. Weil, *L'integration dans les groupes topologiques et ses applications*, Actualities Scientifique et Industrielles No. 869 (Hermann & Cie., Paris, 1940), p. 83. The completeness of the spherical harmonics discussed earlier can also be proved using the Frobenius theorem and the Peter–Weyl theorem.

functions. We get a representation for each of the $2j + 1$ values of m'.

We now apply the Frobenius theorem to the case of SU_3/SU_2. We need to know how many times the identity representation of SU_2 occurs in an irreducible representation $\Gamma(\lambda_1, \lambda_2)$ of SU_3. To use the language of unitary symmetry, we want to know how many particles with zero isotopic spin are contained within any given SU_3 multiplet. The answer is one, and only one.[11] Consequently, each irreducible representation of SU_3 occurs once and only once in the set of functions over S^5. The representations are given, of course, by the SU_3 wavefunctions found in (I). This is the underlying group-theoretical reason for the success of the SU_3 classification scheme.

[11] H. Boerner, *Representations of Groups* (North-Holland Publishing Company, Amsterdam, 1963), p. 160.

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Analytic Properties of the Elastic Unitarity Integral*

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In this paper, certain results concerning the singularities of holomorphic functions with integral representations are used to investigate the analytic properties of the elastic unitarity integral of the quantum theory of fields. In particular, it is shown that each of the Landau singularities of the scattering amplitude is an actual singularity. It is also shown that if the scattering amplitude is not identically zero it must have a natural boundary on the unphysical sheet.

I. INTRODUCTION

In a previous paper I[1] the present authors have studied certain generalizations of the Hadamard problem[2] and have given theorems concerning the location of the possible singularities of holomorphic functions (of several complex variables) determined by germs which are given by integrals with holomorphic integrands whose singularities lie on analytic sets. In this paper we illustrate the method by applying the theorems to the elastic unitarity integral of the quantum theory of fields.[3,4] We reproduce the results of Zimmermann[5] on the Landau singularities of the scattering amplitude in a way that makes clear the connection with Landau's[6] treatment of the singularities of the Feynman amplitudes. Furthermore the method provides new results which bear on the paper of Freund and Karplus[7] on the possibility of a natural boundary of the scattering amplitude on an unphysical sheet. In particular, we show that each of the Landau singularities is an actual singularity, not merely a possible singularity, of the scattering amplitude. It follows that the *natural boundary must be present* if the scattering amplitude is not identically zero.

The conclusion that the Landau singularities are actual singularities is interesting. A direct proof that the first Landau singularity is actually a singularity is quite complicated. Aks[8] has based a proof of the necessity of first allowed production process, in a quantum theory of fields with nonvanishing scattering amplitude, on the existence of the first Landau singularity. The result of the present paper suggests that all (nonforbidden) production processes occur with nonzero cross section.

In the main body of this paper, the "envelope method"[9] is used to study the locations of the singularities of the elastic unitarity integral. The "Hadamard approach"[9] to the problem of the location of the singularities of the elastic unitarity integral is illustrated in an Appendix.

2. THE ELASTIC UNITARITY INTEGRAL

As an illustration of our continuation theorems we consider the unitarity conditions in the quantum theory of fields. It is well known[10] that the elastic scattering amplitude $\phi(s; x)$ for bosons of mass m (spin and change zero) and energy $s^{\frac{1}{2}}$ satisfies the unitarity condition

$$\phi(s; x) - \phi^*(s; x) = \frac{i}{8}\left(\frac{s-4m^2}{s}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_{-1}^{+1} dx_2 \times \frac{\theta(1-x_1^2-x_2^2-x^2+2x_1x_2x)}{(1-x_1^2-x_2^2-x^2+2x_1x_2x)^{\frac{1}{2}}} \phi^*(s;x_1)\phi(s;x_2), \quad (2.1)$$

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[1] R. P. Gilbert, H. C. Howard, and S. Aks, J. Math. Phys. **6**, 1157 (1965), hereafter denoted by I.

[2] J. Hadamard, Acta Math. **22**, 55 (1898); also see I. Theorem 0, and R. P. Gilbert, Pacific J. Math. **10**, 1243 (1960).

[3] The elastic unitarity condition is a direct consequence of the unitarity of the S-matrix operator at energies below the first production threshold. For details see: S. Ø. Aks, Technical Note BN-363, Institute for Fluid Dynamics and Applied Mathematics, University of Maryland, College Park, Maryland. Also J. Math. Physics **6**, 516 (1965).

[4] Also see: S. Mandelstam, Nuovo Cimento **15**, 658 (1960).

[5] W. Zimmermann, Nuovo Cimento **21**, 268 (1961).

[6] L. D. Landau, Nuclear Phys. **13**, 181 (1959); Zh. Eksperim. i Teor. Fiz. **37**, 62 (1959) [English transl.: Soviet Phys.—JETP **10**, 45 (1960).]

[7] P. G. O. Freund and R. Karplus, Nuovo Cimento **21**, 519 (1961).

[8] See S. Ø. Aks, Ref. 3.

[9] For details see I[(1)], and R. P. Gilbert, J. Math. Phys. **5**, 983 (1964).

[10] See: S. Ø. Aks[3] and S. Mandelstam.[4]

where $\theta = \cos^{-1} x$ is the scattering angle in the center of momentum system, $(s; x) \in E \times I \equiv [4m^2, 16m^2) \times [-1, +1]$, and $\theta(\xi)$ is taken to be the characteristic function for the set $\{\xi > 0\}$. We remark that we are considering fields invariant under replacement by their negative, otherwise we would have (2.1) valid in $\tilde{E} \times I$ $[\tilde{E} \equiv [4m^2, 9m^2)]$ instead. We note that it is possible for us to write the unitarity condition (2.1) in the alternate form

$$\phi(s; x) - \phi^*(s; x) = \frac{i}{16}\left(\frac{s - 4m^2}{s}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \times \int_0^{2\pi} d\rho\, \phi^*(s; x_1)\, \phi(s; x\, x_1 + [(1 - x^2)(1 - x_1^2)]^{\frac{1}{2}} \cos \rho), \quad (2.2)$$

where $(s; x) \in E \times I$.

We may consider Eqs. (2.1) and (2.2) as integral equations for $\phi^*(s; x)$ with kernels

$$K_1(x, x_1; s) \equiv \int_{-1}^{+1} dx_2 \times \frac{\theta(1 - x_1 - x_2^2 - x^2 + 2x_1x_2x)}{(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x)^{\frac{1}{2}}} \phi(s; x_2), \quad (2.3)$$

and

$$K_2(x, x_1; s) \equiv \frac{1}{2} \int_0^{2\pi} d\rho\, \phi(s; x\, x_1 + (1 - x^2)^{\frac{1}{2}}(1 - x_1^2)^{\frac{1}{2}} \cos \rho), \quad (2.4)$$

respectively. These kernels are equivalent to within a change of parametric representation made by replacing ρ in (2.4) by

$$\arccos \{(x_2 - x\, x_1)[(1 - x^2)(1 - x_1^2)]^{-\frac{1}{2}}\}.$$

We note, however, that this change of parameter is not one-to-one at the end points of the x_2 integration, namely $x_2 = \pm 1$.

3. THE ELEMENTARY ANALYTIC PROPERTIES OF THE ELASTIC SCATTERING AMPLITUDE

Let us now assume that $\phi(s; x)$ is holomorphic (analytic and single valued) in the bi-cylinder $\bar{D}^+(E) \times \mathfrak{R}(I)$, where $\bar{D}^+(E)$ is compact and contains E as a part of its boundary and $D^+(E) \cap \{\text{Im } S < 0\} = 0$. We require that $\bar{D}^+(E)$ forms an upper semineighborhood for the set E (i.e., the points of E are accessible from $D^+(E) \cap \{\text{Im } S \geq 0\}$; we will also have occasion to use the lower semineighborhood $D^-(E)$ which is similarly defined. From the Schwarz inequality we have

$$|x\, x_1 + (1 - x^2)^{\frac{1}{2}}(1 - x_1^2)^{\frac{1}{2}} \cos \rho|^2 \leq (x^2 + [1 - x^2])(x_1^2 + [1 - x_1^2] \cos^2 \rho) \leq x_1^2 \sin^2 \rho + \cos^2 \rho \leq 1,$$

for $(x, x_1) \in (I \times I)$; hence it is clear that $K_2(x, x_1; s)$ is holomorphic (analytic and single valued) in the two complex variables,

$$(x, x_1) \in \mathfrak{R}^{(2)}(I \times I) \subset \mathfrak{R}(I) \times \mathfrak{R}(I).$$

From this we may conclude that, if there exists a function $\phi_2 \in L_2(I)$ for fixed $s \in \bar{D}^+(E)$, which satisfies the integral equation

$$\phi_2(s; x) = \phi(s; x) - \frac{1}{8}\left(\frac{s - 4m^2}{s}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1\, K_2(x, x_1; s)\phi_2(s, x_1), \quad (2.5)$$

then $\phi_2(s; x)$ is analytic in x for

$$x \in \mathfrak{R}(I) \cap \mathfrak{R}^{(2)}(I \times I)$$

and s such that $s \in \bar{D}^+(E)$.

The existence of a solution of (2.5) for each $s \in \bar{D}^+(E)$ is now considered under the previous assumptions. For each such fixed s, $K_2(x, x_1; s)$ is holomorphic, and therefore, bounded for $(x, x_1) \in (I \times I)$; hence $K_2(x, x_1; s)$ is an L_2 kernel,

$$\int_{-1}^{+1} dx \int_{-1}^{+1} dx_1\, |K_2(x, x_1; s)|^2 < \infty,$$

and (2.5) as well as the equations gotten from (2.5) by conjugating the kernel satisfy the Fredholm alternative.[11] We remember that for $s \in E$ $\phi^*(s, x)$ is assumed to satisfy the elastic unitarity condition (2.2) which, if regarded as an integral equation for $\phi^*(s, x)$, is the same as (2.5). It follows, providing our hypotheses are consistent regarding the analiticity requirements on $\phi(s; x)$, (which we assume to be the case in what follows) that (2.5) has a solution for each fixed $s \in E$. For s fixed in $D^+(E) - E$ (2.5) may not have a solution; however, since $K_2(s, s_1; s)$ is an L_2 kernel and holomorphic in the parameter s, such points are isolated and have no finite limit points. We conclude that for s fixed in in $D^+(E)$ [with the possible exception of a finite set contained in $D^+(E) - E$]$\phi_2(s; x)$ is analytic in x for $x \in \mathfrak{R}(I) \cap \mathfrak{R}^{(2)}(I \times I)$.

The analytic properties of $\phi_2(s; x)$ in s (for fixed x) are now discussed. We consider s as a parameter in (2.5) and note that both the kernel $K_2(x, x_1; s)$ and the inhomogeneous term $\phi(s; x)$ are holomorphic in the parameter for $(x, x_1) \in \mathfrak{R}^{(2)}(I \times I) \subset$

[11] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955), p. 170.

$\mathfrak{R}(I) \times \mathfrak{R}(I)$. As a consequence, for each fixed x, $\phi_2(s; x)$ is holomorphic in the parameter s for all points $s \in \tilde{D}^+(E)$ at which a solution of (2.5) exists. From what has already been said, $\phi_2(s; x)$ is, for each fixed $x \in \mathfrak{R}(I) \cap \mathfrak{R}^{(2)}(I \times I)$, holomorphic in $\tilde{D}^+(E) - F$ where $F \subset \tilde{D}^+(E)$ is the (finite) set of points on which (2.5) does not have a solution. Using Hartogs' theorem we have from the analycity in x (for fixed s) and s (for fixed x) that $\phi_2(s; x)$ is holomorphic in

$$(\tilde{D}^+(E) - F) \times \{\mathfrak{R}(I) \cap \mathfrak{R}^{(2)}(I \times I)\}.$$

We have so far made no restrictive assumptions about $\tilde{D}^+(E)$ [or the domain of analyticity of $\phi(s; x)$]. At this time we list the weakest assumptions made in this paper regarding the domain of analyticity of $\phi(s; x)$ (i.e., the smallest domain). (From time to time we shall strengthen these assumptions to obtain more specific results.) To this end we introduce the two sets Λ, Π, which are contained in $\mathbf{C}^{(2)}$,

$$\Lambda \equiv \{(s, x) \mid s \geq 4m^2; x \in \mathbf{C}^{(1)}\},$$

$$\Pi \equiv \{(s, x) \mid x = \pm[1 + 2t/(s - 4m^2)], \quad t \geq 4m^2; s \in \mathbf{C}^{(1)}\}, \tag{3.1}$$

and the complement of their union $\Omega^{(2)} \equiv \mathbf{C}^{(2)} - \Lambda \cup \Pi$. *We assume that* $\phi(s; x)$ *is holomorphic in* $\Omega^{(2)}$. We will show that $\Omega^{(2)}$ is *not* a holomorphy domain for functions satisfying (2.1); in other words if $\phi(s; x)$ is holomorphic in $\Omega^{(2)}$ and satisfies (2.1) it can be analytically continued to a domain which contains $\Omega^{(2)}$ as a proper subset.

From the previous discussion we have that on the surface $E \times I$, $\phi^*(s + i0; x) = \phi_2(s, x)$; furthermore, as a consequence of certain physical invariance properties we must have $\phi^*(s; x) = \phi(s^*; x)$ for $(s, x) \in \{\mathfrak{IC}_\phi \cap x = \text{real}\}$[12], where $\mathfrak{IC}_\phi$ is the *domain of holomorphy* for $\phi(s; x)$. (The domain of holomorphy of ϕ is the *germ space* generated by the holomorphic function ϕ.) Since a holomorphic function of several complex variables is completely determined by its values in a real environment[13] we realize that $\phi(s; x)$ and $\phi_2(s, x)$ are direct analytic continuations of one another across E. For instance, starting at the point $s^0 + ie(s^0 \in E)(x^0 \in \mathfrak{R}(I)$ and fixed) we may pass around $s = 4m^2$ in $\tilde{D}^+(E) - F$ in a counter clockwise manner to reach the point $(s^0 - i\epsilon, x^0)$. The value of the function $\phi(s; x)$ here is then $\phi(s^0 - i\epsilon; x^0) = \phi^*(s^0 + i\epsilon; x^0)$, and we use these values as $\epsilon \to 0$ to determine $\phi_2(s, x)$ on $E \times I$. $\phi_2(s; x)$ may then be continued to another "sheet" of the Riemann space by passing through the cut (or hypersurface) $E \times \mathbf{C}^1$. If we now continue $\phi_2(s; x)$ around the previous path encircling $s = 4m^2$ to the point $(s^0 - i\epsilon, x^0)$ we can show this value $\phi_2(s^0 - i\epsilon; x^0)$ approaches $\phi(s^0 + i\epsilon, x^0)$ as $\epsilon \to 0$ (ϕ_2 on the second sheet, ϕ on the first sheet).

We remember that [under our previous assumptions concerning $\phi(s; x)$] (2.5) as well as the equation obtained from (2.5) by conjugating the kernel satisfies the Fredholm alternative. We have also found that the (inhomogeneous) equation (2.5) has a solution for $s \in E$ [the same is true for the equation with conjugated kernel since this equation has as its solution $\phi(s; x)$ as is seen by conjugating each term of (2.2)] hence the homogeneous equations will only have the trivial solutions. We will use this to show that $\phi_2(s^0 - i\epsilon; x^0)$ approaches $\phi(s^0 + i\epsilon; x^0)$ as $\epsilon \to 0$. At the point $(s^0 - i\epsilon; x^0)$, (2.1) becomes

$$\begin{aligned}\phi^*(s^0 + i\epsilon; x^0) - \phi_2(s^0 - i\epsilon; x^0) &= \frac{1}{8}\left(\frac{s^0 - 4m^2}{s^0}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_{-1}^{+1} dx_2 \\ &\times \frac{\theta(1 - x_1^2 - x_2^2 - x^{0^2} + 2x_1x_2x^0)}{(1 - x_1^2 - x_2^2 - x^{0^2} + 2x_1x_2x^0)^{\frac{1}{2}}} \\ &\times \phi_2(s^0 - i\epsilon; x_1)\phi^*(s^0 + i\epsilon; x_2).\end{aligned} \tag{3.2}$$

After the change of variables $x_1 \leftrightarrow x_2$ and some simplification (2.1) is given by

$$\begin{aligned}\varphi(s^0 + i\epsilon; x^0) - \phi^*(s^0 + i\epsilon; x^0) &= \frac{1}{8}\left(\frac{s^0 - 4m^2}{s^0}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_{-1}^{+1} dx_2 \\ &\times \frac{\theta(1 - x_1^2 - x_2^2 - x^{0^2} + 2x_1x_2x^0)}{(1 - x_1^2 - x_2^2 - x^{0^2} + 2x_1x_2x^0)^{\frac{1}{2}}} \\ &\times \phi(s^0 + i\epsilon; x_1)\phi^*(s^0 + i\epsilon; x_2).\end{aligned} \tag{3.3}$$

Combining (3.2) and (3.3) gives

$$\begin{aligned}&\phi(s^0 + i\epsilon; x^0) - \phi_2(s^0 - i\epsilon; x^0) \\ &= \frac{1}{8}\left(\frac{s^0 - 4m^2}{s^0}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_{-1}^{+1} dx_2 \\ &\times \frac{\theta(1 - x_1^2 - x_2^2 - x^{0^2} + 2x_1x_2x^0)}{(1 - x_1^2 - x_2^2 - x^{0^2} + 2x\, x_2x^0)^{\frac{1}{2}}} \\ &\times \phi^*(s^0 + i\epsilon; x_2)\{\phi(s^0 + i\epsilon; x_1) - \phi_2(s^0 - i\epsilon; x_1)\},\end{aligned} \tag{3.4}$$

[12] This is a consequence of *PCT* invariance (for particles with zero spin and charge). For details, R. F. Streater and A. S. Wightman, *PCT, Spin & Statistics, and All That* (W. A. Benjamin, Inc., New York, 1964).

[13] S. Bochner and W. T. Martin, *Several Complex Variables* (Princeton University Press, Princeton, New Jersey, 1948), p. 34.

which, from the equivalence of (2.3) and (2.4), may be written as

$$\{\phi(s^0 + i\epsilon; x^0) - \phi_2(s^0 - i\epsilon; x^0)\}$$
$$= \frac{1}{8}\left(\frac{s^0 - 4m^2}{s^0}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1\, K_2^*(x^0, x_1; s^0)$$
$$\times \{\phi(s^0 + i\epsilon; x_1) - \phi_2(s^0 - i\epsilon; x_1)\}. \quad (3.5)$$

We have noted above that the homogenous equations with kernels $K_2(x, x_1; s)$ and $K_2^*(x, x_1; s)$ have only trivial solutions for $s \in E$ hence we conclude that $\{\phi(s^0 + i\epsilon; x^0) - \phi_2(s^0 - i\epsilon; x^0)\} = 0$ as $\epsilon \to 0$ with $s^0 \in E$ and it follows that ϕ_2 and ϕ approach each other in value on their respective sheets; hence the Riemann space appears locally in the s variable about $s = 4m^2$ as a square-root ramification.

Now returning to our investigation of the singularities of $\phi_2(s; x)$ in terms of $\phi(s; x)$ (i.e., determining analytic information about a direct continuation from information about the original branch), we introduce instead of (2.1) and (2.2) the relations

$$\phi(s; x) - \phi_2(s; x) = \frac{1}{8}\left(\frac{s - 4m^2}{s}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_{-1}^{+1} dx_2$$
$$\times \frac{\theta(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x)}{(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x)^{\frac{1}{2}}} \phi_2(s; x_1)\phi(s; x_2) \quad (3.6)$$

and

$$\phi(s; x) - \phi_2(s; x) = \frac{1}{16}\left(\frac{s - 4m^2}{s}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_0^{2\pi} d\rho$$
$$\times \phi_2(s; x_1)\, \phi(s; x\, x_1 + [(1 - x^2)(1 - x_1^2)]^{\frac{1}{2}} \cos \rho), \quad (3.7)$$

which we consider in $\Omega^{(2)}$. In the following we shall be concerned with the analytic continuation of $\phi_2(s; x)$ (the scattering amplitude on the second sheet of the square root ramification at $s = 4m^2$) starting from the domain of analyticity $[\bar{D}^+(E) - F] \times [\mathfrak{R}(I) \cap \mathfrak{R}^{(2)}(I \times I)]$ determined above.

4. SOME REMARKS ON THE METHOD OF ANALYTICALLY CONTINUING THE UNITARITY INTEGRAL

We note that the θ function in the integrand of (3.6) is not a holomorphic function. In fact there is ambiguity concerning just how it should be "continued"; however, we may remove it by considering the integral to be taken over a two-dimensional chain Γ_x, whose boundary is given by

$$\partial\Gamma_x \equiv \{(x_1, x_2) \mid 1 - x_1^2 - x_2^2 - x^2 + 2x_2x_1x$$
$$= 0; x_1, x_2 \text{ real}; x \text{ fixed}\}; \quad (4.1)$$

that is, we may replace (3.6) by,

$$\phi(s; x) - \phi_2(s; x) = \frac{1}{8}\left(\frac{s - 4m^2}{s}\right)^{\frac{1}{2}} \iint_{\Gamma_x} dx_1\, dx_2$$
$$\times \phi_2(s, x_1)\, \phi(s, x_2)/(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x)^{\frac{1}{2}}. \quad (4.2)$$

Holding *this* boundary fixed we may now deform $\Gamma_x \to \tilde{\Gamma}_x$ provided that no singularities of the integrand in (3.6) lie inside $\tilde{\Gamma}_x - \Gamma_x$. We may also vary $\partial\Gamma_x$ provided we do not sweep over singularities. To be more precise, let us hold x fixed and define $\partial\Gamma_x$ as follows: let x be real and

$$\partial\Gamma_x(\lambda) \equiv \{(x_1, x_2) \mid x_k = f_k(\alpha; \lambda, x),$$
$$(k = 1, 2); x, \lambda \text{ fixed}; \alpha \in [0, 1]\},$$

such that $f_k(\alpha; \lambda, x)$ is a smooth function of $(\alpha, x) \in [0, 1] \times [0, 1]$ and $f_k(\alpha; 0, x) \equiv x_k$. The set

$$\bigcup_{\lambda \in [0,1]} \{\partial\Gamma_x(\lambda)\}$$

is called the "homotopy cylinder" of this mapping from the curve $\partial\Gamma_x \equiv \partial\Gamma_x(0)$ to the curve $\tilde{\partial}\Gamma_x \equiv \partial\Gamma_x(1)$.

Now if no singularities of the integrand lie in the domain D bounded by

$$\{\tilde{\Gamma}_x - \bigcup_{\lambda \in [0,1]} [\partial\Gamma_x(\lambda)] - \Gamma_x\}$$

we may replace integration over the chain Γ_x by integration over the chain $\tilde{\Gamma}_x$ minus integration over the homotopy cylinder $\bigcup_{\lambda \in [0,1]} \partial\Gamma_x(\lambda)$. In the case where integration over each lamina $\partial\Gamma_x(\lambda)$ vanishes our result simplifies to invariance of the integral under the variation of integration domain $\Gamma_x \to \tilde{\Gamma}_x$. [We remark that this is the case if each $\partial\Gamma(\lambda)$ bounds a topological two-chain $\Gamma(\lambda) \subset Z^{(1)}(\lambda)$, where $Z^{(1)}(\lambda)$ is an analytic set of complex dimension one, and the integrand is holomorphic regular in $Z^{(1)}(\lambda)$.]

In the case we have, the integrand is singular, with a $\frac{1}{2}$ power, infinity at the points satisfying $\mathfrak{Q} \equiv \{1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x = 0\}$. By definition $\partial\Gamma_x(\lambda)$ coincides with this for $\lambda = 0$. If we further require that $\partial\Gamma_x(\lambda)$ meets $\mathfrak{Q}$ only at $\lambda = 0$, then this singularity is certainly integrable on the set ∂D given above. The only place difficulty may arise is if a boundary point coincides with a point on a double line of $\mathfrak{Q}$, i.e., for $x = \pm 1$ ($x_1 = \pm x_2$). We already know, however, that the integral is regular for x in a complex neighborhood of I, and this rules out this possibility.

Summarizing our discussion, we recall that from Theorem 3 of the paper I a fixed boundary could lead to singularities of the integral; however, from the above remarks we realize that it is possible to

deform the boundary (thereby changing the value of the integral) with the integral not becoming singular unless we pass over a nonintegrable singularity of the integrand.

We conclude therefore, that in our case no point (x_1, x_2) need contribute to a possible singularity of the integral unless we cannot deform the boundary away from it (in the sense of the theorems of the paper I). We may now proceed to extend our usual treatment to possible singularities which may correspond to boundary points, and we conclude that they are already counted by the envelope method. (The envelope method actually lists as possibly singularities those points which become infinite at least as fast as second order poles. Hence, if one of these points coincides with a boundary point the integral is singular.)

5. FURTHER PROPERTIES OF THE SCATTERING AMPLITUDE

At this point it is useful to make a small digression concerning the function $\phi(s; \cos\theta)$[14] where

$$\phi(s; \cos\theta) \equiv \phi(s - 2q^2[1 - \cos\theta]) \equiv \phi(s, t) \equiv \phi(s, t, u)\,|_{s+t+u=4m^2}. \quad (4.4)$$

For physical reasons[14], $\phi(s, t, u)$ is assumed to be invariant under all permutations of the variables s, t, and u; we refer to this property of the scattering amplitude as *crossing symmetry*.

The function $\phi(s, t, u)$ is to be considered as a holomorphic function of the three complex variables s, t, u in the cut domain

$$\left\{\mathbf{C}^{(3)} - \sum_{\mu=1}^{3} b_\mu^{[5]}\right\},$$

where

$$\begin{aligned} b_1^{[5]} &\equiv \{(s, t, u) \mid s \geq 4m^2; (t, u) \in \mathbf{C}^{(2)}\}, \\ b_2^{[5]} &\equiv \{(s, t, u) \mid t \geq 4m^2; (s, u) \in \mathbf{C}^{(2)}\}, \\ b_3^{[5]} &\equiv \{(s, t, u) \mid u \geq 4m^2; (t, s) \in \mathbf{C}^{(2)}\}. \end{aligned} \quad (5.1)$$

(We note that the superscripts in square brackets on the $b_\mu^{[5]}$ refer to the *real dimensionality* in contrast to the *ordinary* bracketed superscripts on the $\mathbf{C}^{(3)}$ which refers to the complex dimensionality.) We assume further *at least for the moment* that on the "cuts" $b_\mu^{[5]}$ the function $\phi(s, t, u)$ has singularities lying on "isolated" analytic sets, which may correspond to polar-type or branch-type singularities contained in sets of the form

$$\begin{aligned} a_{1,\nu}^{[4]} &\equiv \{(s, t, u) \mid s = \alpha_{1,\nu};\ (t, u) \in \mathbf{C}^{(2)}\}, \\ a_{2,\nu}^{[4]} &\equiv \{(s, t, u) \mid t = \alpha_{2,\nu};\ (s, u) \in \mathbf{C}^{(2)}\}, \\ a_{3,\nu}^{[4]} &\equiv \{(s, t, u) \mid u = \alpha_{3,\nu};\ (t, s) \in \mathbf{C}^{(2)}\}, \\ &\qquad (\nu = 1, 2, \cdots). \end{aligned} \quad (5.2)$$

This is to be expected, since with the exception of the boundary of a holomorphic domain (a natural boundary for at least one function in the family of holomorphic functions defined in that domain) the singularities of a holomorphic function lie on analytic sets.[15] This is to say, the only analytic sets contained in the "cuts" must be of complex dimension ≤ 2 and hence are contained in the $a_{\mu,\nu}^{[4]}$.

The restriction of the space on which $\phi(s, t, u)$ is defined, to the analytic plane

$$P^{(2)} \equiv \{(s, t, u) \mid s + t + u = 4m^2\}, \quad (5.3)$$

introduces restricted sets as the new singular sets. However, these new sets may be represented as the intersection of analytic sets and hence are of complex dimensions ≤ 2. We conclude from this that the only singularities of

$$\phi(s, t) \equiv \phi(s, t, u)\,|_{s+t+u=4m^2}$$

are contained in analytic sets which are isolated from one another. This result will be of importance in what follows.

6. CRITERIA FOR SINGULARITIES OF THE SCATTERING AMPLITUDE ON THE SECOND SHEET OF THE SQUARE-ROOT RAMIFICATION AT $s = 4m^2$ (SEE REF. 16)

Before proceeding we should like to mention that our basic attack on the problem of determining the singularities of $\phi_2(s; x)$ from information concerning the singularities of $\phi(s; x)$ will be as follows. We shall suppose that the singularities of $\phi(s; x)$ and $\phi_2(s; x)$ are contained in the sets $\mathfrak{S}$ and $\mathfrak{S}_2$, respectively. Then using the results of the previous section we shall determine the possible singularities of the right-hand side of (4.2). *These must be contained in the set* $\mathfrak{S} \cup \mathfrak{S}_2$, because of the equality of the function $\phi(s; x) - \phi_2(s; x)$ and the right-hand side of (4.2). We realize immediately by considering the coefficient of the integral that $(s = 0, 4m^2) \times \mathbf{C}^{(1)}$ will be a ramification set with square-root behavior in the s variable.

We now return to our consideration of the sin-

[14] See, for example: G. F. Chew, *S-Matrix Theory of Strong Interactions* (W. A. Benjamin, Inc., New York, 1961), p. 9.

[15] H. Behnke and H. Grauert, "Analysis of Non-Compact Complex Spaces" in *Analytic Functions* (Princeton University Press, Princeton, New Jersey, 1960), p. 11.

[16] An alternative discussion of the singularities of the scattering amplitude on the second sheet of the square-root ramification at $s = 4m^2$ is given in the Appendix.

gularities of the integral of (4.2). We wish to obtain first a representation for the singularity manifold of the integrand, and we note it should take into account the singularities of the kernel, and the two holomorphic function $\phi(s; x)$ and $\phi_2(s; x)$. The kernel clearly is singular whenever $1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x = 0$; let us assume that the function $\phi(s; x)$ may only be singular on the set

$$\mathfrak{S} \equiv \bigcup_{\nu \in I} \{(x, s) \mid x^2 = [1 + 2\beta_\nu/(s - 4m^2)]^2; \quad \beta_\nu \geq 4m^2; \quad s \in \mathbf{C}^{(1)}\},$$

where $I \equiv \{1, 2, 3, \cdots\}$ and let us explore this conjecture. The reader is directed to Chew's book[17] for the motivation in choosing $\mathfrak{S}$ as the singularity set of ϕ. Since no candidates for singularities can arise from applying the Hadamard condition to pairs

$$\left[x^2 - \left(1 + \frac{2\beta_\mu}{s - 4m^2}\right)^2\right] = 0,$$

$$\left[x^2 - \left(1 + \frac{2\beta_\nu}{s - 4m^2}\right)^2\right] = 0 (\mu \neq \nu),$$

we may consider each of these terms separately when computing the possible singular sets of the integral and then take the topological sum. If the situation should require it we can introduce the possibility of a natural boundary by considering a sequence of functions $\{\phi_{(\nu)}(s; x)\}$ each singular at a denumerable set

$$\mathfrak{s}_\nu \equiv \bigcup_{\mu \in I_\nu} \{(s, x) \mid x = 1 + 2\beta_{\mu,\nu}/(s - 4m^2); \quad \beta_{\mu,\nu} \geq 4m^2; \quad s \in \mathbf{C}^{(1)}\}$$

and such that the set of points $\beta_{\mu,\nu}$ becomes dense on the half-line $\beta \geq 4m^2$ as $\nu \to \infty$. In this way it is possible to apply our previous results to each individual function $\phi_{(\nu)}(s; x)$ in the sequence, and thereby extend these results to function singular on analytic hypersurfaces[18].

Following theorems of I, and letting $x_2^2 - [1 + 2\beta_\mu/(s - 4m^2)] \equiv A$, we determine the sets

$$\mathfrak{Q}_0^{(2)}(\beta_\mu) \equiv \{(x; x_1, x_2) \mid (1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) \times G_2(s; x_1)A = 0\}, \tag{6.1}$$

where $G_2(s; x_1) = 0$ is a representation of the singularities of $\phi_2(s; x_1)$,

$$\mathfrak{Q}_1^{(2)}(\beta_\mu) \equiv \left\{(x; x_1, x_2) \mid A\left[\frac{\partial G_2}{\partial x_1}(s; x_1) \times (1 - x_1^2 - x_2^2 + 2x_1x_2x) + 2G_2(s; x_1)(x_2x - x_1)\right] = 0\right\}; \tag{6.2}$$

$$\mathfrak{Q}_2^{(2)}(\beta_\mu) \equiv \{(x; x_1, x_2) \mid G_2(s; x_1)[x_2(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) + A(x_1x - x_2)] = 0\}. \tag{6.3}$$

According to theorems of the paper I by the present authors, the possible singularities of the integral (4.2) for the singularity of ϕ corresponding to β_μ lie on the set $\mathfrak{Q}_0^{(2)}(\beta_\mu) \cap \mathfrak{Q}_1^{(2)}(\beta_\mu) \cap \mathfrak{Q}_2^{(2)}(\beta_\mu)$.

There are many ways in which the three equations determining these sets can be satisfied, but not all solutions lead to singularities. The following is a list of solutions:

$$G_2(s; x_2) = A = (1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) = 0; \tag{6.4a}$$

$$G_2(s; x_1) = A = 0, \quad 1_1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x \neq 0; \tag{6.4b}$$

$$G_2(s; x_1) = (1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) = 0, \quad A \neq 0; \tag{6.4c}$$

$$(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) = A = 0, \quad G_2(s; x) \neq 0; \tag{6.4d}$$

$$(1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) = (x_2x - x_1) = (x_1x - x_2) = 0, \quad G_2(s, x_1) \neq 0, \quad A \neq 0; \tag{6.4e}$$

$$A = x_2 = 0; \quad (1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) \neq 0, \quad G_2(s; x_1) \neq 0; \tag{6.4f}$$

$$G_2(s; x) = \partial G_2(s; x_1)/\partial x_1 = 0; \quad (1 - x_1^2 - x_2^2 - x^2 + 2x_1x_2x) \neq 0, \quad A \neq 0. \tag{6.4g}$$

Equations (6.4e) yield as possible singularities $x = \pm 1$; however, we have already found that $\phi_2(s; x)$ is analytic in a complex neighborhood of $[-1, +1]$ for $s \in E$. Equations (6.4b, c, d) do not lead to singularities at all, and (6.4g) is independent of x. We note also that the points $s \in E$ do not satisfy these equations. In particular some points on the set $\{s \leq 0\}$ satisfy (6.4f). In addition as noted earlier there may exist isolated singularities in the s plane, independent of the x variable.

7. THE SINGULARITIES OF THE SCATTERING AMPLITUDE ON THE SECOND SHEET

Equation (6.4a) is the most interesting contributor to possible singularities, and we examine it in detail.

[17] G. F. Chew,[14] p. 3; following Chew's remarks we may expect $\beta_\nu = (2\nu m)^2$.

[18] S. Bergman, J. Anal. Math. 11, 249 (1963).

First we note that a singularity of the right-hand side of (4.2) must also be a singularity of the left-hand side, which in turn must be a singularity of $\phi(s; x)$ or $\phi_2(s; x)$ or both.

We assume at first that the singularities of $\phi_2(s; x)$ may be represented as a finite union of analytic sets

$$\left\{(s, x) \;\middle|\; \prod_{n=1}^{N} [x - g_n(s)] = 0\right\},$$

and we use the criteria of (6.4a) to determine the possible singularities of the integral (4.2). We conclude if $x = g_k(s)$, k fixed ($1 \leq k \leq N$) is a singularity of $\phi_2(s; x)$ then

$$x = f_k(s) \equiv \pm\left\{\left(1 + \frac{2\beta_\mu}{s - 4m^2}\right)g_k(s) \pm \left([g_k^2(s) - 1]\left[\frac{4\beta_\mu}{s - 4m^2} + \frac{4\beta_\mu^2}{(s - 4m^2)^2}\right]\right)^{\frac{1}{2}}\right\} \tag{7.1}$$

may also be a singularity of $\phi_2(s; x)$. Let us assume first that just one of the roots designated by $f_k(s)$ is identical to a certain $g_n(s)$, say $g_i(s)$. In this case we see that this term in the singularity representation appears on both sides of expression (4.2). More precisely, if $\mathfrak{S}$ and $\mathfrak{S}_2$ are representations for the singularity manifolds of $\phi(s; x)$ and $\phi_2(s; x)$, respectively, and

$$\mathfrak{S}_3 \equiv \{1 - x^2 - x_1^2 - x_2^2 + 2x x_1 x_2 = 0\} \cap \mathfrak{S} \cap \mathfrak{S}_2,$$

then the only possible singularities of $\phi_2(s; x)$ [as given by the representation (4.2) and (6.4a)] must lie in the set $(\mathfrak{S} \cup \mathfrak{S}_2) \cap \mathfrak{S}_3$. Under the above assumptions we must conclude that the only possible singularity is given by $x = g_i(s)$. However, if we proceed with *this new assumption, namely* $x = g_i(s)$ *is the only singularity* of $\phi_2(s; x)$ we find that $(\mathfrak{S} \cap \mathfrak{S}_2) \cap \mathfrak{S}_3 = \phi$, i.e., there are *no singularities* of this sort arising from Eq. (6.4a). This follows since all the singularities of $\phi_2(s; x)$ must be contained in the union of all intersections defined by $\{(s, x) | x - g_n(s) = x - f_m(s) = 0\}$ ($1 \leq n, m \leq N$). Each such intersection is itself a union of isolated points $\{(s_\rho, x_\rho)\}$ ($\rho = 1, 2, 3, \cdots$). Since the singularities of a function of two complex variables are not isolated points (they are contained on analytic sets) we conclude that these points are not singularities. This argument may now be extended to the case where several of the $g_n(s)$ correspond to $f_m(s)$ terms, by eliminating one-by-one terms which do not lie in *both* $\mathfrak{S}_3 \cap (\mathfrak{S} \cup \mathfrak{S}_2)$, and then by recomputing $\mathfrak{S}_3$ using the new $\mathfrak{S}_2$, i.e., $\mathfrak{S}_2$ minus those terms which did not appear in $\mathfrak{S}_3 \cap (\mathfrak{S} \cup \mathfrak{S}_2)$. We can repeat this process until no terms exist on either side. *We conclude that if we assume the singularities of* $\phi_2(s; x)$ *lie on a finite sum of analytic sets, then there are no possible singularities of* $\phi_2(s; x)$ *which arise from the Hadamard argument*, i.e., (6.4a).

However, we can show that $\phi_2(s; x)$ *is* singular on the analytic set

$$\mathcal{J} = \{(s; x) \mid x = \pm g_1(s) \equiv \pm[1 + 8m^2/(s - 4m^2)],\ s \in \mathbf{C}^{(1)}\} \tag{7.2}$$

corresponding to the points $t = 4m^2$ (s arbitrary); hence, it follows from what has been shown above that, under the assumption that the singularities of $\phi_2(s; x)$ lie on a union of analytic sets, $\phi_2(s; x)$ must be *singular on a union of infinitely many analytic sets*. We will investigate the singularities of the integral (4.2) arising from the criteria (6.4a), assuming that the singularities of $\phi_2(s; x)$ can be represented as a union of denumerably many analytic sets

$$\left\{(s; x) \;\middle|\; \prod_{n=1}^{\infty} [x - g_n(s)]e^{-P_n(s;x)} = 0\right\},$$

where the function $P_n(s; x)$ are polynomials which are introduced to ensure the convergence of the infinite product.

First we note that $\phi(s; x)$ is singular on the analytic set $\mathcal{J}$ given by (7.2). We have remarked above that $s = 4m^2$ is a square-root ramification, and it follows from the crossing symmetry of $\phi(s, t)[= \phi(t, s)]$ that $t = 4m^2$—or equivalently, the set $\mathcal{J}$— is also a square-root ramification [unless, of course, $\phi(s; x) \equiv 0$, which we assume is not the case]. Now either $\phi_2(s; x)$ is singular on $\mathcal{J}$, canceling the singularity of $\phi(s; x)$, or the integral (4.2) is singular on $\mathcal{J}$. In either case $\phi_2(s; x)$ must be singular, for if the integral (4.2) is singular on the set $\mathcal{J}$, then this singularity must arise under the criteria (6.4a) from a singularity of $\phi_2(s; x)$ on some other analytic set $\{(s; x) \mid x = g(s), s \in \mathbf{C}^{(1)}\}$. However, the existence of such a singularity will be seen to be *inconsistent with the known analytic properties of* $\phi_2(s; x)$; in particular, a solution $\phi_2(s; x)$ of (2.5) will be shown to be holomorphic at points satisfying $x = g(s)$.

To this end let us suppose at first that $\phi_2(s; x)$ is singular on the set determined by $x = g(s)$, and as a consequence the integral (4.2) is singular on the set $\mathcal{J}$; then $g(s)$ must satisfy

$$\pm\left(1 + \frac{8m^2}{s - 4m^2}\right) = \left(1 + \frac{2\beta_\mu}{s - 4m^2}\right)g(s) \pm \left\{[g^2(s) - 1]\left[\frac{4\beta_\mu}{s - 4m^2} + \frac{4\beta_\mu^2}{(s - 4m^2)^2}\right]\right\}^{\frac{1}{2}}, \tag{7.3}$$

where $1 + 2\beta_\mu/(s - 4m^2)$ is a singularity of $\phi(s; x)$. It follows that $g(s)$ is given by

$$\pm g(s) = \left(1 + \frac{8m^2}{s - 4m^2}\right)\left(1 + \frac{2\beta_\mu}{s - 4m^2}\right) \pm \left\{\left[\frac{16m^2}{s - 4m^2} + \frac{64m^4}{(s - 4m^2)^2}\right] \times \left[\frac{4\beta_\mu}{s - 4m^2} + \frac{4\beta_\mu^2}{(s - 4m^2)^2}\right]\right\}^{\frac{1}{2}}. \quad (7.4)$$

We assume for the moment that the + sign holds on the right-hand side of (7.4). Since $\beta_\mu \geq 4m^2$, we have, for $s > 4m^2$,

$$g(s) > 1 + \frac{2\beta_\mu}{s - 4m^2} \geq 1 + \frac{8m^2}{s - 4m^2} > 1.$$

Since $g(s) > 1$ we can rule out the plus sign on the right-hand side of (7.3). Alternatively, if the minus sign on the right of (7.4) holds we conclude from (7.3) that

$$1 + 2\beta_\mu/(s - 4m^2) \geq 2g^2(s) - 1.$$

But this is not consistent with the inequality

$$2g^2(s) - 1 \geq g(s), \qquad g(s) > 1 + 2\beta_\mu/(s - 4m^2)$$

and we conclude that the minus sign on the right-hand side of (7.3) does not hold. Since neither the plus nor the minus sign in (7.3) is consistent with a plus sign on the right in (7.4) we must have a minus sign on the right in (7.4), if there is to be a singularity of the form $x = g(s)$.

We remark furthermore that β_μ must be strictly greater than $4m^2$ if the minus sign on the right in (7.4) is to hold since $\beta_\mu = 4m^2$ gives $g(s) = \pm 1$, which is inconsistent with the analyticity of the solution $\phi_2(s; x)$ of (2.5) in a complex neighborhood of $I = [-1, +1]$. Actually, for $4m^2 \leq s < 16m^2$, the solution $\phi_2(s; x)$ of (2.5) is not singular in the interval $0 \leq x < 1 + 8m^2/(s - 4m^2)$ as an inspection of the integrand in (2.4) shows. This excludes the possibility that $\phi_2(s; x)$ is singular on $x = g(s)$ since we can show that $1 < g(s) < 1 + 8m^2/(s - 4m^2)$ for $s > 4m^2$ and sufficiently near $4m^2$. For $s > 4m^2$, $g(s) > 1$ follows immediately from (7.4) (with minus sign) and

$$1 + 2\beta_\mu/(s - 4m^2) > 1 + 8m^2/(s - 4m^2) > 1.$$

By straightforward computation using (7.4) (with minus sign) the inequality $g(s) < 1 + 8m^2/(s - 4m^2)$ is found to be equivalent to the inequality $2[1 + 8m^2/(s - 4m^2)]^2 - 1 \geq 1 + 2\beta_\mu/(s - 4m^2)$. This inequality is, for $s > 4m^2$, equivalent to

$$64m^2/(s - 4m^2) \geq (\beta_\mu - 16m^2),$$

which for any fixed β_μ, is satisfied for $s - 4m^2$ sufficiently small. Therefore, $\phi_2(s; x)$ cannot be singular on $x = g(s)$ for any choice of signs in (7.4).

To summarize, we recall that $\phi(s; x)$ was known to be singular on $\mathcal{J}$. Furthermore, it then followed that $\phi_2(s; x)$ *had* to be singular on either $\mathcal{J}$ or on $\{x = g(s)\}$ or on both. We have just shown by direct computation that $\phi_2(s; x)$ cannot be singular on $\{x = g(s)\}$; hence, it follows that $\phi_2(s; x)$ *must be* singular on $\mathcal{J}$.

We shall next consider the possibility of an infinite union of analytic sets, since in this case the arguments used for a finite union break down. Let us denote a singularity of $\phi_2(s; x)$ by $x = g_k(s)$ (k a positive integer); then it follows from (6.4a) that

$$x = g_{k+1}(s) \equiv \pm\left\{\left(1 + \frac{2\beta_\mu}{s - 4m^2}\right)g_k(s) \pm \left([g_k^2(s) - 1]\left[\frac{4\beta_\mu}{s - 4m^2} + \frac{4\beta_\mu^2}{(s - 4m^2)^2}\right]\right)^{\frac{1}{2}}\right\} \quad (7.5)$$

may also be a singularity of $\phi_2(s; x)$; in this way, starting from the singularity of $\phi_2(s; x)$ on $x = \pm g_1(s) = \pm[1 + 8m^2/(s - 4m^2)]$ we find by induction a sequence of possible singularities $x = \pm g_1(s)$, $x = \pm g_2(s)$, $\cdots$, $x = \pm g_n(s)$, $\cdots$ of $\phi_2(s; x)$. We remark that these are the only singularities consistent with the criteria (6.4a). Moreover, in the case $\beta_\mu = 4m^2$, we can show that $\phi_2(s; x)$ *is* singular on each of the sets of the sequence.

Let us assume that, although $x = \pm g_k(s)$, $k > 1$, is a possible singularity of $\phi_2(s; x)$, $\phi_2(s; x)$ is actually holomorphic on this set. From this assumption and (6.4a), it follows that $\phi_2(s; x)$ is holomorphic on $x = \pm g_{k+1}(s)$ since the integral (4.2) [hence $\phi_2(s; x)$] is singular on $x = \pm g_{k+1}(s)$ only if $\phi_2(s; x)$ is singular on $x = \pm g_k(s)$. Starting from the nonexistence of a singularity on $x = g_{k+1}(s)$, we find that $\phi_2(s; x)$ cannot be singular on $x = \pm g_{k+2}(s)$; it follows that the possible singularities of $\phi_2(s; x)$ are contained in the sets determined by $x = \pm g_1(s) = \pm[1 + 8m^2/(s - 4m^2)]$, $x = g_2(s)$, $\cdots$, $x = g_{k-1}(s)$. But this is not possible since it has already been shown that $\phi_2(s; x)$ may not be singular on a union of finitely many analytic sets of this type. In particular it would follow that $\phi_2(s; x)$ is not singular on $x = \pm g_1(s) = \pm[1 + 8m^2/(s - 4m^2)]$. Since we know that $\phi_2(s; x)$ *is* singular on the set determined by $x = \pm g_1(s) = \pm 1 + 8m^2/s - 4m^2)$ (if $\phi(s; x) \not\equiv 0$) we have reached a contradiction.

It follows that $\phi_2(s; x)$ *is singular on each of the sets determined by* $x = \pm g_1(s) = \pm[1 + 8m^2/(s - 4m^2)]$, $x = \pm g_2(s)$, $\cdots$, $x = \pm g_n(s)$, $\cdots$ *where* $g_{k+1}(s)$ *is*

obtained from $g_k(s)$ *using* (7.5). These singularities are well known as the Landau singularities[19,20] of the Feynman graphs of canonical field theory. It is at first surprising that we can prove that $\phi_2(s; x)$ is actually singular on the Landau singularities since the theorems on which the arguments are based give necessary (but not sufficient) conditions for the existence of a singularity. The sufficiency arises from the occurrence of $\phi_2(s; x)$ on both sides of (4.2).

8. THE NECESSITY OF A NATURAL BOUNDARY ON THE SECOND SHEET

Freund and Karplus[7] have shown that the points on the set $\mathfrak{L} = \{(s; x) \mid s \leq 0; x \in \mathbf{C}^{(1)}\}$ may consitutute a natural boundary of $\phi_2(s; x)$ and, therefore, of $\phi(s; x)$ on the second sheet of the square-root ramification at $s = 4m^2$. Their conjecture is based on the observation that in every neighborhood of a point $(s; x) \in \mathfrak{L}$ there is a point $(s'; x')$, and a positive integer k, such that $x' = \pm g_k(s')$; each point of $\mathfrak{L}$ is an accumulation point of points on the Landau singularities, hence $\mathfrak{L}$ may be a natural boundary of $\phi_2(s; x)$. Since we have shown that $\phi_2(s; x)$ must be singular on each of the Landau singularities, it follows that each point of $\mathfrak{L}$ is an accumulation point of singularities of $\phi_2(s; x)$ and is, therefore, a singular point of $\phi_2(s; x)$. We conclude that the set $\mathfrak{L}$ constitutes a natural boundary of $\phi_2(s; x)$, if $\phi_2(s; x) \not\equiv 0$.

APPENDIX

In the main body of the paper we treated the [standard form (3.6) of] the elastic unitarity integral, using Theorem 5 of the paper I by the present authors, and found, for the locations of the possible singularities of the integral, the criteria (3.4). In this appendix we illustrate Theorem 4 of that paper (the "Hadamard approach") by applying it to the alternative form of (3.7) of the elastic unitarity integral.

$$\phi(s; x) - \phi_2(s; x) = \frac{i}{16}\left(\frac{s - 4m^2}{s}\right)^{\frac{1}{2}} \int_{-1}^{+1} dx_1 \int_0^{2\pi} d\rho \times \Psi(s; x, x_1, \rho)\phi_2(s; x_1), \quad \text{(A1)}$$

where $\Psi(s; x, x_1, \rho) = \phi(s; x\,x_1 + [1 - x^2]^{\frac{1}{2}}[1 - x_1^2]^{\frac{1}{2}} \cos\rho)$, and determining criteria for the location of singularities.

We suppose that $\phi(s; x)$ and $\phi_2(s; x)$ satisfy all assumptions made in the main part of the paper; in particular, $\phi_2(s; x)$ is taken to be singular on a union (of denumerably many) analytic sets. In accordance with Theorem 4 we denote the singularity set of $\phi_2(s; x)$ by

$$\mathfrak{S}_{1,0}^{(3)} = \{(s; x, x_1, \rho) \mid G_2(s; x_1) = 0;\ (x, \rho) \in \mathbf{C}^{(2)}\},$$

while the singularity set of $\Psi(s; x, x_1, \rho)$ is denoted by

$$\mathfrak{S}_{2,0}^{(3)} = \{(s; x, x_1, \rho) \mid (x\,x_1 + [(1 - x^2) \times (1 - x_1^2)]^{\frac{1}{2}} \cos\rho)^2 - [1 + 2\beta_\mu/(s - 4m^2)]^2 = 0\}.$$

We also introduce the set

$$\mathfrak{H}_{1,2}^{(3)} = \{(s; x, x_1, \rho) \mid [\partial G_2(s; x_1)/\partial x_1] \times (xx_1 + [(1 - x^2)(1 - x_1^2)]^{\frac{1}{2}} \cos\rho) \times [(1 - x^2)(1 - x_1^2)]^{\frac{1}{2}} \sin\rho = 0\}$$

described in Theorem 4.

It follows from Theorem 4, that (for each β_μ) the possible singularities of the integral (A.1) are included in the set $\mathfrak{S}_{1,0}^{(3)} \cap \mathfrak{S}_{2,0}^{(3)} \cap \mathfrak{S}_{1,2}^{(3)}$. A point $(s; x) \in \mathbf{C}^{(2)}$ is contained in this intersection if it belongs to one of the sets determined by the following equations:

$$\sin\rho = 0, \quad \cos\rho = \pm 1; \quad G_2(s; x_1) = (x\,x_1 \pm [(1 - x^2)(1 - x_1^2)]^{\frac{1}{2}})^2 - [1 + 2\beta_\mu/(s - 4m^2)]^2 = 0\,, \quad \text{(A2a)}$$

$$1 - x^2 = G_2(s; x) = x^2 - [1 + 2\beta_\mu/(s - 4m^2)]^2 = 0\,, \quad \text{(A2b)}$$

$$1 - x_1^2 = G_2(s; x_1) = x^2 - [1 + 2\beta_\mu/(s - 4m^2)]^2 = 0\,, \quad \text{(A2c)}$$

$$x\,x_1 + [(1 - x^2)(1 - x_1^2)]^{\frac{1}{2}} \cos\rho = G_2(s; x_1) = 1 + 2\beta_\mu/(s - 4m^2) = 0, \quad \text{(A2d)}$$

$$\partial G_2(s; x_1)/\partial x_1 = G_2(s; x_1) = (x\,x_1 + [(1 - x^2) \times (1 - x_1^2)]^{\frac{1}{2}} \cos\rho)^2 - [1 + 2\beta_\mu/(s - 4m^2)]^2 = 0. \quad \text{(A2e)}$$

We remark that (A.2a) and (6.4a) determine the same set; it follows that Sec. 7 holds without change for the elastic unitarity condition in the form (A.1). No singularities are contributed by (A.2b) since we have found in connection with (3.5) that $\phi_2(s; x)$ is holomorphic at $x = \pm 1$; similarly (A2c) contributes no singularities. Condition (A2d) contributes points satisfying $s = 4m^2 - 2\beta_\mu < 0$, x arbitrary, while (A2e) relates to the possible singularities of $\phi_2(s; x)$ which depend on the s variable alone.

[19] D. Landau, Ref. 6.

[20] W. Zimmermann[6] using other methods has shown that (except for the isolated singularities which are x independent) the Landau singularities are the only possible singularities of $\phi_2(s; x)$ consistent with the assumption we have made.

Crossing Symmetric Regge Representation for the Invariant Scattering Amplitude*

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A crossing symmetric Regge representation for the invariant scattering amplitude is constructed which simultaneously exhibits *all* Regge poles in the three channels. It is assumed that the amplitude satisfies the Mandelstam representation, and that the usual Mandelstam–Sommerfeld–Watson transform exists. To achieve explicit crossing symmetry it is found necessary to work with the Legendre function of the second kind. Except for neglecting the influence of possible angular momentum cuts, the representation is exact for all s, t, and u, with no restriction on the location of the Regge poles. As an illustration of how it might be used in practice, the Chew–Jones formula for the amplitude of definite signature is derived in the strip approximation.

1. INTRODUCTION

IN this paper we construct a crossing symmetric Regge representation for the invariant scattering amplitude with the assumption that $A(s, t, u)$ satisfies the Mandelstam representation, and that the amplitudes of definite signature have an "ordinary" Mandelstam–Sommerfeld–Watson (MSW) representation (see Sec. 2). Furthermore, for our approach to make sense, we must require that the Regge poles recede into the left half angular momentum plane above a certain energy. The final expression for the amplitude will be exact to the extent that we have neglected any angular momentum cuts, if they exist[1]; such neglect is often justified. Concerning the Gribov–Pomeranchuk singularities,[2] we shall assume that they are absent on the angular momentum sheet of interest, and thus will not contribute directly to the asymptotic behavior. For certain cases Mandelstam has shown this to be true.[1]

Khuri[3,4] has proposed a crossing symmetric Regge representation using power series expansions in s, t, and u. As a consequence of this technique, the "Regge terms" in his expression contain poles which have no physical meaning; Chew and Jones,[5] on the other hand, choose to work with the Legendre function of the first kind; their expression, however, is strictly correct only if none of the trajectories lies in the left half angular momentum plane. In this paper we propose to construct a representation for the amplitude with neither one of the just-mentioned drawbacks; in return we must assume that $A^{\pm}(s, t)$ has a MSW representation. Rather than working with $P_l(z)$, we choose to work with the Legendre function of the second kind, $Q_l(z)$, since $P_l(z)$ has the undesirable property of diverging for $\mathrm{Re}\, l < -1$, as $|z| \to \infty$.

Since the MSW transform plays a dominant role in our calculation, we shall devote the following section to its brief examination. In Sec. 3 we then discuss the analytic continuation of the "Regge term" to arbitrary complex values of its argument, and in Sec. 4 we finally construct the crossing symmetric Regge representation. We conclude with Sec. 5, where we use the representation to extend the Chew–Jones form of the new strip approximation[5] to include trajectories lying in the left half angular momentum plane; in particular we shall recover their expression if we limit ourselves to those poles lying in the right half angular momentum plane.

2. THE MANDELSTAM–SOMMERFELD–WATSON (MSW) TRANSFORM

It is well known that the presence of exchange forces requires us to work with the amplitudes of definite signature; it is these amplitudes, $A^{\pm}(s, t)$, which (we assume) have a MSW representation[6,7]:

$$A^{\pm}(s, t) = -\frac{i}{2}\int_{-L-i\infty}^{-L+i\infty} dl(2l+1)a^{\pm}(l, s)\frac{Q_{-l-1}(-z_s)}{\pi\cos\pi l} + \sum_{\mathrm{Re}\,\alpha_j > -L} \beta_j(s)\frac{Q_{-\alpha_j(s)-1}(-z_s)}{\cos\pi\alpha_j(s)} + B^{\pm}(s, t), \quad (2.1)$$

where the summation extends only over trajectories of a given $(\pm)$ signature. Throughout this paper the subscript j will label a Regge trajectory of definite signature, and we shall suppress any $(\pm)$ super-

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[1] S. Mandelstam, Nuovo Cimento **30**, 1127, 1148 (1963).
[2] V. N. Gribov and I. Ya. Pomeranchuk, Proc. Intern. Conf. High Energy Phys. CERN, 1962, p. 522.
[3] N. N. Khuri, Phys. Rev. **132**, 914 (1963).
[4] R. J. Eden has constructed a modified representation by using Legendre transforms; see Phys. Rev. **132**, 912 (1963).
[5] G. F. Chew and C. E. Jones, Phys. Rev. **135**, B208 (1964).
[6] See, for example, E. J. Squires, *Complex Angular Momenta and Particle Physics* (W. A. Benjamin, Inc., New York, 1963), p. 10.
[7] To simplify the discussion we shall take all external masses to be equal; furthermore we will ignore spin complications.

script on $\alpha_j(s)$ and $\beta_j(s)$ if what is meant is clear from the context in which the expression appears. Here z_s is defined in terms of s and t as follows:

$$z_s = 1 + t/2q_s^2,$$
$$s = 4(q_s^2 + m^2),$$

and $a^{\pm}(l, s)$ is given by the Froissart–Gribov formula,[8]

$$a^{\pm}(l, s) = \frac{1}{\pi}\int_{t_0}^{\infty} \frac{dt'}{2q_s^2} Q_l\left(1 + \frac{t'}{2q_s^2}\right) \times [A_t(s, t') \pm A_u(s, \mathbf{u}')], \qquad (2.2)$$

for all l for which the integral converges, and is determined otherwise by analytic continuation; $A_t(s, t)$ and $A_u(s, u)$ are the absorptive parts of $A(s, t, u)$ in the t and u channels, respectively, with s, t, and u related by the equation $s + t + u = \sum_i m_i^2$, where m_i are the external particle masses; $\mathbf{u}$ (or $\mathbf{t}$) is obtained from u (or t) by making the substitution $z_s \to -z_s$; thus for the equal-mass case, $\mathbf{u} = t$ and $\mathbf{t} = u$. The quantities $\alpha_j(s)$ and $\beta_j(s)$ appearing in (2.1) are the jth Regge pole of $(\pm)$ signature, and the residue of $(2l + 1)a^{\pm}(l, s)$ at the jth Regge pole, respectively. The last term in (2.1) is defined as follows:

$$B^{\pm}(s, t) = \frac{1}{\pi}\sum_{l=1}^{N}(-1)^l 2l \times [a^{\pm}(l - \tfrac{1}{2}, s) - a^{\pm}(-l - \tfrac{1}{2}, s)]Q_{l-\frac{1}{2}}(-z_s) + \frac{1}{\pi}\sum_{l=N+1}^{\infty}(-1)^l 2l a^{\pm}(l - \tfrac{1}{2}, s)Q_{l-\frac{1}{2}}(-z_s), \quad -N - \tfrac{3}{2} < L < -N - \tfrac{1}{2}. \qquad (2.3)$$

Let us consider formula (2.1); we notice that the second term seems to have poles at the half integers of $\alpha(s)$; such singularities must, of course, be absent in the full amplitude. If, however, we assume that the Mandelstam reflection symmetry holds [i.e., that $a^{\pm}(-l - \frac{1}{2}, s) = a^{\pm}(l - \frac{1}{2}, s)$ for l integral], then one may readily verify, by letting $L \to \infty$ (thus extending the domain of analyticity in s of the second term in 2.1), that these poles will cancel pairwise in the sum, so that the sum itself has no such spurious singularities. The symmetry is known to hold for a large class of potential problems. In order to avoid these poles we shall assume henceforth that the partial-wave amplitudes satisfy the Mandelstam reflection symmetry; it then follows also that $A(s, t)$ is always dominated at large t by Regge poles. One final remark should be added here: it is essential that the second term in (2.1), hereafter referred to as the "Regge term," be an analytic function of s and t; this means that we must choose L sufficiently large so that *all* Regge trajectories will lie to the right of the integration contour; in particular we shall take L to be infinite.

[8] See Ref. 6, p. 46.

3. ANALYTIC CONTINUATION OF THE "REGGE TERM"

Expression (2.1), with $Q_{-\alpha-1}(-z_s)$ defined on the conventional sheet cut from $z_s = -1$ to $+1$, and from $z_s = +\infty$ to $+1$, does not equal $A^{\pm}(s, t)$ for all s and t, as can be seen by comparing their respective analytic structures. In fact, it follows from the definition of $A^{\pm}(s, t)$,

$$A^{\pm}(s, t) = \frac{1}{\pi}\int_{t_0}^{\infty} dt' \frac{A_t(s, t')}{t' - t} \pm \frac{1}{\pi}\int_{u_0}^{\infty} du' \frac{A_u(s, u')}{u' - \mathbf{u}}, \qquad (3.1)$$

and from the dispersion relations for the absorptive parts $A_t(s, t)$ and $A_u(s, u)$,

$$A_t(s, t) = \frac{1}{\pi}\int_{s_0}^{\infty} ds' \frac{\rho_{st}(s', t)}{s' - s} + \frac{1}{\pi}\int_{u_0}^{\infty} du' \frac{\rho_{tu}(t, u')}{u' - (\Sigma - s - t)},$$
$$A_u(s, u) = \frac{1}{\pi}\int_{s_0}^{\infty} ds' \frac{\rho_{su}(s', u)}{s' - s} + \frac{1}{\pi}\int_{t_0}^{\infty} dt' \frac{\rho_{tu}(t', u)}{t' - (\Sigma - s - u)}, \qquad (3.2)$$

that $A^{\pm}(s, t)$ is an analytic function of s and t with the s plane cut from threshold to $+\infty$ and from $\Sigma - u_0 - t_0$ to $-\infty$, and with the t plane cut from t_0 to infinity along the positive axis. As usual, s_0, t_0, and u_0 are the lowest thresholds in the s, t and u channels, respectively, and $\Sigma = s + t + u = 4m^2$. The analytic structure of $a^{\pm}(l, s)$, which enters into the background integral, may be obtained from the Froissart–Gribov definition, Eq. (2.2). Writing $b^{\pm}(l, s) = a^{\pm}(l, s)/(q_s^2)^l$, we find that $b^{\pm}(l, s)$ is an analytic function of s except for a right-hand cut starting at s_0, and two left-hand cuts extending to $-\infty$ from $s_0 - t_0$ and from $\Sigma - t_0 - u_0$, respectively. It should be noticed that $(q_s^2)^{-l}Q_l(1 + t/2q_s^2)$ has no discontinuity for $-t/4 < q_s^2 < 0$.

Next we consider the "Regge term" of the MSW transform:

$$R_j(s, t) = \gamma_j(s)(q_s^2)^{\alpha_j(s)} \times Q_{-\alpha_j(s)-1}(-1 - t/2q_s^2)/\cos \pi\alpha_j(s). \qquad (3.3)$$

Here we have written $\beta_j(s) = \gamma_j(s)(q_s^2)^{\alpha_j(s)}$, where

$\gamma_i(s)$ is the residue of $(2l+1)b^\sigma(l,s)$ at $l=\alpha_i(s)$; σ is the signature of the trajectory $\alpha_i(s)$.[9] Equation (3.3) has the desired threshold cut in s plus a number of other cuts arising from the argument of the Legendre function and the factor $(q_s^2)^\alpha$; comparing the right- and left-hand sides of (2.1), we conclude that the latter cuts must be absent in the full amplitude. For s physical (i.e., $s > s_0$), we notice that the cuts in t of $R_i(s,t)$ are consistent with those of $A^\pm(s,t)$: a right-hand cut beginning at $t=0$, and a finite left-hand cut extending from $t=0$ to $t=-4q_s^2$; both cuts are seen to move with s. Since the Legendre function contains the entire t dependence, and since $\gamma_i(s)$ and $\alpha_i(s)$ are assumed to have only the right-hand threshold cut, we conclude from the foregoing analysis that the desired continuation of $R_i(s,t)$ must leave the right-hand s and t cuts fixed. Consider the expression

$$(q_s^2)^\alpha \tilde{Q}_{-\alpha-1}\left(-1-\frac{t}{2q_s^2}\right) = -\frac{\sin\pi\alpha}{\pi}\int_0^\infty \frac{dt'}{t'-t}(q_s^2)^\alpha Q_{-\alpha-1}\left(1+\frac{t'}{2q_s^2}\right) + \frac{1}{2}\int_{-1}^{+1}\frac{dz'}{z'-(1+t/2q_s^2)}(q_s^2)^\alpha P_{-\alpha-1}(-z'), \quad \mathrm{Re}\ \alpha < 0; \tag{3.4}$$

for $\mathrm{Re}\,\alpha \geq 0$ it is defined by analytic continuation. Except for cuts, the rhs defines an analytic function of s and t. Now for s physical, $\tilde{Q}_{-\alpha-1}(-z_s) = Q_{-\alpha-1}(-z_s)$, since for $s > s_0$, (3.4) becomes the dispersion relation for the conventional Legendre function of the second kind, [for convenience we have multiplied both sides of the equation by the threshold factor $(q_s^2)^\alpha$]. It is clear that (3.4) is the desired continuation; its analytic structure in the t plane needs no comment. Concerning the cuts in s, we notice that the first integral on the rhs has a cut extending along the negative q_s^2 axis. The discontinuity across this cut is given by

$$\Delta_s\int_0^\infty \frac{dt'}{t'-t}(q_s^2)^\alpha Q_{-\alpha-1}\left(1+\frac{t'}{2q_s^2}\right) = -i\pi(-q_s^2)^\alpha\int_0^{-4q_s^2}\frac{dt'}{t'-t}P_{-\alpha-1}\left(-1-\frac{t'}{2q_s^2}\right), \quad -\infty < q_s^2 < 0. \tag{3.5}$$

Examination of the second integral, however, shows that it has a similar cut whose discontinuity is the negative of (3.5) [this is easily verified by using the relation

$$(q_s^2+i\epsilon)^\alpha - (q_s^2-i\epsilon)^\alpha = 2i(-q_s^2)^\alpha\sin\pi\alpha].$$

In conclusion, we therefore find that (3.4) defines an analytic function of s and t, with the t plane cut from $-4q_s^2$ to $t=0$, and from $t=0$ to $+\infty$, and with the q_s^2 plane cut from $q_s^2=0$ to $+\infty$ and from $q_s^2=-t/4$ to infinity in a radial direction. For future reference we state the formula for the analytically continued "Regge term":

$$R_i(s,t) = -\beta_i(s)\frac{\tan\pi\alpha_i}{\pi}\int_0^\infty\frac{dt'}{t'-t}Q_{-\alpha_i-1}\left(1+\frac{t'}{2q_s^2}\right) + \beta_i(s)\frac{1}{2\cos\pi\alpha_i}\int_{-1}^{+1}\frac{dz'}{z'-(1+t/2q_s^2)}P_{-\alpha_i-1}(-z'), \quad \alpha_i\equiv\alpha_i(s). \tag{3.6}$$

4. A CROSSING SYMMETRIC REGGE REPRESENTATION

Let us define the following set of variables:

$$z_s = 1+t/2q_s^2 = -1-u/2q_s^2, \tag{4.1a}$$

$$z_t = 1+s/2q_t^2 = -1-u/2q_t^2, \tag{4.1b}$$

$$z_u = 1+s/2q_u^2 = -1-t/2q_u^2; \tag{4.1c}$$

$$x = 4(q_x^2+m^2), \tag{4.1d}$$

where $x = s$, t, or u; in the physical regions of the s, t, and u reactions, z_s, z_t, and z_u are the cosines of the respective c.m. (center of mass) scattering angles, and s, t, and u are the squares of the respective c.m. energies. We now write down three alternative expressions for the amplitude $A(s,t,u)$ expressed in terms of the three possible pairs of independent variables: (s,z_s), (t,z_t), and (u,z_u); in fact, these expressions are the usual one-dimensional dispersion relations for $A(s,t,u)$, with s, t, and u held fixed in turn:

$$A(s,z_s) = \frac{1}{\pi}\int_{t_0}^\infty dt'\frac{A_t(s,t')}{t'-t(s,z_s)} + \frac{1}{\pi}\int_{u_0}^\infty du'\frac{A_u(s,u')}{u'-u(s,z_s)} = \tfrac{1}{2}\sum_\sigma[A^\sigma(s,z_s)+\xi_\sigma A^\sigma(s,-z_s)], \tag{4.2a}$$

$$A(t,z_t) = \frac{1}{\pi}\int_{s_0}^\infty ds'\frac{A_s(s',t)}{s'-s(t,z_t)} + \frac{1}{\pi}\int_{u_0}^\infty du'\frac{A_u(t,u')}{u'-u(t,z_t)} = \tfrac{1}{2}\sum_\eta[A^\eta(t,z_t)+\xi_\eta A^\eta(t,-z_t)], \tag{4.2b}$$

[9] Notice that the cut in q_s^2 of the function $(q_s^2)^{\alpha(s)}$ is not arbitrary, but is fixed by the choice of sheet for the Legendre function.

$$A(u,z_u) = \frac{1}{\pi}\int_{s_0}^{\infty} ds' \frac{A_s(s',u)}{s'-s(u,z_u)} + \frac{1}{\pi}\int_{t_0}^{\infty} dt' \frac{A_t(t',u)}{t'-t(u,z_u)} = \tfrac{1}{2}\sum_{\lambda}[A^{\lambda}(u,z_u) + \xi_{\lambda}A^{\lambda}(u,-z_u)]. \quad (4.2c)$$

Here σ, η, and λ equal $(\pm)$ depending on the signature, and $\xi_{\pm} = \pm 1$. The expression below each of the dispersion relations is readily obtained from the definition of $A^{\pm}(x, z_x)$; we construct $A^{\pm}(x, z_x)$ by attaching a $(\pm)$ sign to the second integral in the dispersion relation for $A(x, z_x)$, and by substituting $-z_x$ for z_x in the integrand. Thus, for example, (4.2a) is seen to follow from (3.1). Let us make a partial-wave expansion of $A^{\pm}(x, z_x)$:

$$A^{\pm}(x,z_x) = \sum_l (2l+1)a^{\pm}(l,x)P_l(z_x), \quad x = s, t, u, \quad (4.3)$$

where z_x is given in terms of s, t, and u by Eqs. (4.1 a–d); performing a MSW transformation on this series we obtain

$$A^{\sigma}(x,z_x) = -\frac{i}{2}\int_{-\infty-i\infty}^{-\infty+i\infty} dl(2l+1)a^{\sigma}(l,x)\frac{\tilde{Q}_{-l-1}(-z_x)}{\pi\cos\pi l} + \sum_j \beta_j(x)\frac{\tilde{Q}_{-\alpha_j(x)-1}(-z_x)}{\cos\pi\alpha_j(x)}, \quad (4.4)$$

where $\tilde{Q}_l(z)$ is defined by (3.4), and where the summation extends only over trajectories of a given signature. Next we consider the Mandelstam representation for the amplitude $A(s, t, u)$,[10]

$$A(s,t,u) = A_{12}(s,t) + A_{13}(s,u) + A_{23}(t,u), \quad (4.5)$$

where a typical term—say, $A_{12}(s, t)$—is given by

$$A_{12}(s,t) = \frac{1}{\pi^2}\int_{s_0}^{\infty}\int_{t_0}^{\infty} ds'\,dt' \frac{\rho_{st}(s',t')}{(s'-s)(t'-t)}. \quad (4.6)$$

We leave it understood that the necessary subtractions have been made. Our program is to extract explicitly that part of the amplitude which has Regge-type asymptotic behavior.[11] Accordingly, we shall split the various integrals in (4.5) into parts whose domains of integration correspond to the various double spectral regions shown in Fig. 1. Thus, for example,

$$A_{12}(s,t) = \frac{1}{\pi^2}\int_{s_0}^{s_1}\int_{t_0}^{t_1} ds'\,dt' \frac{\rho_{st}(s',t')}{(s'-s)(t'-t)} + \frac{1}{\pi^2}\int_{s_1}^{\infty}\int_{t_1}^{\infty} ds'\,dt' \frac{\rho_{st}(s',t')}{(s'-s)(t'-t)} + [A_{12}^{s_1}(s,t) + A_{12}^{t_1}(s,t)], \quad (4.7)$$

where

$$A_{12}^{s_1}(s,t) = \frac{1}{\pi^2}\int_{s_0}^{s_1}\int_{t_1}^{\infty} ds'\,dt' \frac{\rho_{st}(s',t')}{(s'-s)(t'-t)}, \quad (4.8)$$

with a similar expression for $A_{12}^{t_1}(s, t)$; s_1 and t_1 are determined by the inequality[12]

$$\mathrm{Re}\,\alpha_j(x) < -\tfrac{1}{2}, \quad \text{for} \quad x > x_1, \quad (4.9)$$

where $x = s, t$. Now $\rho_{st}(s, t)$ is bounded in regions 1′ and 2′ of Fig. 1; furthermore, for s and t in region 2′, $\rho_{st}(s, t)$ vanishes faster than $x^{-\frac{1}{2}}$ for large $x(x = s$ or $t)$; it therefore follows that the first two integrals in (4.7) need no subtractions; we shall refer to them as "background integrals." A similar decomposition to (4.7) can be made for the amplitudes $A_{13}(s, u)$ and $A_{23}(t, u)$. In what follows we shall concentrate our attention on the contributions to $A(s, t, u)$ coming from strips 1 through 6 (see Fig. 1), since they will lead to Regge asymptotic behavior. We proceed as follows: to evaluate the contributions to the amplitude coming from strips 1 and 2, we compute the double spectral functions $\rho_{st}(s, t)$ and $\rho_{su}(s, u)$ from expression (4.2a), where $A^{\sigma}(s, z_s)$ is given by (4.4) with $x = s$. Similarly, to evaluate the contributions from strips 3 and 4, we compute the double spectral functions $\rho_{st}(s, t)$ and $\rho_{tu}(t, u)$ from expression (4.2b), where $A^{\eta}(t, z_t)$ is given by (4.4) with $x = t$. Finally, we obtain the contribution from strips 5 and 6, using expression (4.2c). It should be noticed that *either* $A^{\pm}(x, z_x)$ *or* $A^{\pm}(x, -z_x)$ contributes to the double spectral function in a given strip, but not both; this will become clearer in what follows. As an example we compute the contributions

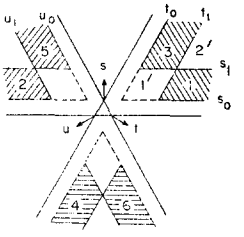

FIG. 1. The Mandelstam diagram showing strips 1 through 6 which give rise to Regge asymptotic behavior; the remaining double spectral regions contribute only to the background terms.

[10] For simplicity we shall omit throughout this paper any bound-state pole terms in the Mandelstam representation and in any other dispersion relation, for these terms do not contribute to the final answer. The bound states will appear as poles in the Legendre function of the second kind.

[11] The general spirit of the calculation is that of Refs. 3 and 5.

[12] With this definition of x_1 plus the assumption that $\beta_j(x) < x^{-\frac{1}{2}}$ for large x, our background terms will vanish faster than $y^{-\frac{1}{2}}$ for large y, where y stands for either variable of its argument.

to the full amplitude coming from strips 1 and 2 of Fig. 1:

$$A^s(s, t, u) = A^{s_1}_{12}(s, t) + A^{s_1}_{13}(s, u). \quad (4.10)$$

The double spectral functions $\rho_{st}(s, t)$ and $\rho_{su}(s, u)$ may be computed from expressions (4.2a) and (4.4), i.e., from

$$A(s, z_s) = -\frac{i}{4}\sum_\sigma \int_{-\infty-i\infty}^{-\infty+i\infty} dl(2l+1)\frac{a^\sigma(l, s)}{\pi\cos\pi l} \times [\tilde{Q}_{-l-1}(-z_s) + \xi_\sigma \tilde{Q}_{-l-1}(z_s)] + \frac{1}{2}\sum_j \frac{\beta_j(s)}{\cos\pi\alpha_j} \times \left[\tilde{Q}_{-\alpha_j-1}\left(-1-\frac{t}{2q_s^2}\right) + \xi_j \tilde{Q}_{-\alpha_j-1}\left(-1-\frac{u}{2q_s^2}\right)\right], \quad \alpha_j \equiv \alpha_j(s), \quad (4.11)$$

where we have written z_s explicitly in terms of s and t, and of s and u, using relation (4.1a); $\tilde{Q}_l(z)$ is defined by (3.4). Notice that the summation index j runs over *all* Regge trajectories, and $\xi_j = \pm 1$ depending on the signature of the jth trajectory. From (4.11) we see that $\rho_{st}(s, t)$ gets a contribution only from the terms involving $\tilde{Q}_{-p-1}(-z_s)$, $p = l, \alpha$, since $\tilde{Q}_{-p-1}(z_s)$ has no right-hand cut in t for $s > s_0$. Similarly, $\rho_{su}(s, u)$ gets a contribution only from the terms involving $\tilde{Q}_{-p-1}(z_s)$. It is sufficient to evaluate explicitly, say $A^{s_1}_{12}(s, t)$; the contributions from the remaining strips may then be obtained in a similar way. The first step consists in splitting $A^{s_1}_{12}(s, t)$ into the following integrals:

$$A^{s_1}_{12}(s, t) = \frac{1}{\pi^2}\int_{s_0}^{s_1}\int_{t_1}^{\infty} ds'\,dt' \frac{B^s_{st}(s', t')}{(s'-s)(t'-t)} - \frac{1}{\pi^2}\int_{s_0}^{s_1}\int_{t_0}^{t_1} ds'\,dt' \frac{R^s_{st}(s', t')}{(s'-s)(t'-t)} - \frac{1}{\pi^2}\int_{s_1}^{\infty}\int_{t_0}^{\infty} ds'\,dt' \frac{R^s_{st}(s', t')}{(s'-s)(t'-t)} + \sum_i R(\alpha_i(s); s, t), \quad (4.12)$$

where

$$\sum_i R(\alpha_i(s); s, t) = \frac{1}{\pi^2}\int_{s_0}^{\infty}\int_{t_0}^{\infty} ds'\,dt' \frac{R^s_{st}(s', t')}{(s'-s)(t'-t)}, \quad (4.13)$$

and where $B^s_{st}(s, t)$ and $R^s_{st}(s, t)$ denote the contributions to the double spectral function coming from the "background integral" and "Regge term" of (4.11), respectively. The reason for the notation in (4.13) will soon become apparent. If we assume that $\beta_j(s) < s^{-\frac{1}{2}}$ for $s \to \infty$, then it follows from the definition of s_1, Eq. (4.9), that the first three integrals of (4.12) need no subtractions; we therefore group them with the other "background terms." Expression (4.13) is the desired candidate which exhibits Regge asymptotic behavior and has only the right-hand threshold cuts in s and t. Now $R^s(s, t) = \frac{1}{2}\sum_j R_j(s, t)$ where $R_j(s, t)$ is given by (3.6); for $s > s_0$ only the first integral on the rhs of (3.6) has a right-hand cut in t; hence we obtain

$$\sum_j R(\alpha_j(s); s, t) = -\sum_j \frac{1}{2\pi i}\int_{s_0}^{\infty}\frac{ds'}{s'-s}\Delta_s\gamma_j(s')\frac{\tan\pi\alpha_j(s')}{2\pi} \times \int_{t_0}^{\infty}\frac{dt'}{t'-t}(q^2_{s'})^{\alpha_j(s')}Q_{-\alpha_j(s')-1}\left(1+\frac{t'}{2q^2_{s'}}\right). \quad (4.14)$$

Next consider the expression

$$\tilde{R}(\alpha_j(s); s, t) = -\gamma_j(s)\frac{\tan\pi\alpha_j}{2\pi} \times \int_{t_0}^{\infty}\frac{dt'}{t'-t}(q_s^2)^{\alpha_j(s)}Q_{-\alpha_j(s)-1}\left(1+\frac{t'}{2q_s^2}\right). \quad (4.15)$$

As we have pointed out before, the integrand of (4.15) has no discontinuity in s for the argument of the Legendre function between -1 and $-\infty$. Hence (4.15) defines an analytic function in the s plane cut from threshold to $+\infty$, and from $s_0 - t_0$ to $-\infty$. The discontinuity across the left-hand cut is

$$+\frac{i}{2}\gamma(s)(-q_s^2)^\alpha \tan\pi\alpha \int_{t_0}^{-4q_s^2} dt' \times [P_{-\alpha-1}(-1 - t'/2q_s^2)/t' - t],$$

with $\alpha \equiv \alpha_j(s)$. Thus (4.15) is seen to be the contribution of the right-hand cut in s to the dispersion relation at fixed t for the function $R(\alpha_j(s); s, t)$. Hence we obtain

$$R(\alpha_j(s); s, t) = -\beta_j(s)\frac{\tan\pi\alpha_j(s)}{2\pi}\int_{t_0}^{\infty}\frac{dt'}{t'-t}Q_{-\alpha_j(s)-1}\left(1+\frac{t'}{2q_s^2}\right) - \frac{1}{2}\int_{-\infty}^{s_0-t_0}\frac{ds'}{s'-s}\gamma_j(s')(-q^2_{s'})^{\alpha_j(s')}\frac{\tan\pi\alpha_j(s')}{2\pi} \times \int_{t_0}^{-4q^2_{s'}}\frac{dt'}{t'-t}P_{-\alpha_j(s')-1}\left(-1-\frac{t'}{2q^2_{s'}}\right), \quad (4.16)$$

where

$$\beta_j(s) = (q_s^2)^{\alpha_j(s)}\gamma_j(s).$$

The second term of (4.16) merely removes the left-hand cut in s of the first integral. The full contribution to $A^s(s, t, u)$, Eq. (4.10), which exhibits Regge behavior, is given by

$$\sum_j [R(\alpha_j(s); s, t) + \xi_j R(\alpha_j(s); s, u)].$$

We remind the reader that the first integral appearing on the rhs of (4.16) is to be taken in the ordinary sense if it converges and is determined otherwise by analytic continuation.

The method we have used to evaluate $A^{s_1}_{12}(s, t)$ may be applied, of course, to the remaining strips. Collecting the various background terms, which we did not explicitly evaluate, we find that we can bring them to the form

$$B_{12}(s, t) = \frac{1}{\pi^2}\int_{s_0}^{\infty}\int_{t_0}^{\infty} ds'\, dt' \frac{b_{st}(s', t')}{(s' - s)(t' - t)},$$

using a method due to Khuri.[3] Here $b_{st}(s, t)$ is given as follows:

$$b_{st}(s, t) = \frac{1}{(2i)^2}\int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty} d\mu \int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty} d\nu C(\nu, \mu) s^\nu t^\mu,$$

where $C(\nu, \mu)$ is defined by

$$B_{12}(s, t) = \sum_{\mu,\nu} C(\nu, \mu) s^\nu t^\mu,$$

for s, t in the Mandelstam triangle. Since in practice $C(\nu, \mu)$ cannot be obtained explicitly, we shall omit giving its expression in terms of integrals over the double spectral functions, and shall limit ourselves to a statement of the final expression for the amplitude[13]:

$$\begin{aligned} A(s, t, u) = {} & \frac{1}{\pi^2}\int_{s_0}^{\infty}\int_{t_0}^{\infty} ds'\, dt' \frac{b_{st}(s', t')}{(s' - s)(t' - t)} \\ & + \frac{1}{\pi^2}\int_{s_0}^{\infty}\int_{u_0}^{\infty} ds'\, du' \frac{b_{su}(s', u')}{(s' - s)(u' - u)} \\ & + \frac{1}{\pi^2}\int_{t_0}^{\infty}\int_{u_0}^{\infty} dt'\, du' \frac{b_{tu}(t', u')}{(t' - t)(u' - u)} \\ & + \sum_i [R(\alpha_i(s); s, t) + \xi_i R(\alpha_i(s); s, u)] \\ & + \sum_i [R(\alpha_i(t); t, s) + \xi_i R(\alpha_i(t); t, u)] \\ & + \sum_i [R(\alpha_i(u); u, s) + \xi_i R(\alpha_i(u); u, t)]. \end{aligned} \tag{4.17}$$

Here $R(\alpha_i(s); s, t)$ is given by (4.16), with similar expressions for the other five "Regge functions." The "background terms" vanish at least as fast as $x^{-\frac{1}{2}}$ for large $x(x = s, t, \text{or } u)$.

With the assumption that $\beta_i(x) \lesssim x^{-\frac{1}{2}}$ and that Re $\alpha_i(x) < -\frac{1}{2}$ for $x \to \infty$, one may readily verify that for large t and fixed s

$$A(s, t, u) \to \tfrac{1}{2}\sum_i [R_i(s, t) + \xi_i R_i(s, u)] + r(s, t, u), \tag{4.18}$$

where $R_i(s, t)$ is given by (3.6) and where $r(s, t, u) \sim t^N$, $N < -\frac{1}{2}$, [a similar relation to (3.6) holds for $R_i(s, u)$]. Furthermore, with the help of the relation

$$\Gamma(\tfrac{1}{2} + z)\Gamma(\tfrac{1}{2} - z)/\Gamma(z)\Gamma(1 - z) = \tan \pi z$$

one may verify that

$$R_i(s, t) \to -\pi\beta_i(s) P_{\alpha_i(s)}(-1 - t/2q_s^2)/\sin \pi\alpha_i(s)$$

for large t, if Re $\alpha_i(s) > -\frac{1}{2}$. We therefore find that $A(s, t, u)$ does indeed have the Regge asymptotic behavior given by the usual Sommerfeld–Watson transform. With the assumption of the Mandelstam reflection symmetry, there presumably exists a further cancellation between the background terms and Regge terms, so that the amplitude is always dominated at large t and any s by the sum in (4.18).

5. DISCUSSION OF THE RESULTS

Expression (4.17) is the desired representation for the invariant amplitude with no subtractions needed in the background integrals, and with *all* Regge poles displayed in an explicit crossing symmetric way. To the extent that we ignored the possibility of cuts in the angular momentum plane, it is an exact expression, valid for all s, t, and u, and with no restrictions on the location of the Regge poles. The three background integrals and the collection of six Regge terms each separately satisfies the Mandelstam representation; furthermore, our assumption that the residue $\beta(x)$ vanishes faster than $x^{-\frac{1}{2}}$ for large $x(x = s, t, u)$, guarantees the usual Regge-type asymptotic behavior of (4.17) in all three channel variables. From the practical standpoint our expression seems to suffer from a disease, for the individual Regge functions have poles at the half integers of $\alpha_i(s)$; as we have pointed out in Sec. 1, these poles are absent in the sum. What this means in practice is that we must include the necessary Regge poles lying in the left half angular momentum plane to remove these spurious singularities. We wish to point out that the above difficulty may often be avoided. For reasons of comparison we make the following substitution in the first integral of (4.16):

$$(q_s^2)^\alpha Q_{-\alpha-1}(1 + t/2q_s^2) = (-q_s^2)^\alpha Q_{-\alpha-1}(-1 - t/2q_s^2);$$

although we had found it necessary to use $Q_l(z)$ instead of $P_l(z)$ in order to arrive at (4.17), we now reintroduce $P_l(z)$ with the help of the relation

$$Q_{-l-1}(z) = -\pi \cot \pi l P_l(z) + Q_l(z).$$

A typical Regge term, say $R(\alpha_i(s); s, t)$, then takes the form

[13] By $\alpha_j(x)$ we mean the jth trajectory in the channel where x is the square of the c.m. energy. Each one of the summations extends over all Regge trajectories in a given channel.

$$R(\alpha_i(s); s, t) = \frac{\pi}{2}\gamma_i(s)(-q_s^2)^{\alpha_i}\frac{1}{\pi}\int_{t_0}^{\infty}\frac{dt'}{t'-t} \times P_{\alpha_i(s)}\left(-1-\frac{t'}{2q_s^2}\right) + R'(\alpha_i(s); s, t). \quad (5.1)$$

Except for the switch in the signs of q_s^2 and of the argument of the Legendre function (which was not necessary, but convenient) the integral in (5.1) is essentially the conventional Regge term; furthermore we notice that this integral with t_0 replaced by t_1 is identical to the Chew–Jones definition of the Regge term, Eq. (II.3) of Ref. 5.[14] The quantity $R'(\alpha_i(s); s, t)$, which now contains the undesirable half integral poles, plays the role of a background term as long as Re $\alpha_i(s) > -\frac{1}{2}$, ($R' < t^{-\frac{1}{2}}$ for large t); this is often the domain of interest. Formula (5.1) also shows why (4.17) is valid regardless of the location of the Regge poles; the presence of the term $R'(\alpha_i(s); s, t)$, which competes with the first integral for Re $\alpha_i(s) \leq -\frac{1}{2}$ (both terms behave like $t^{-\alpha-1}$ for large t), produces the necessary cancellation to ensure the correct asymptotic behavior for all s. If in a calculation one wishes to go beyond the region Re $\alpha_i(s) > -\frac{1}{2}$, then one will have to deal with the half integral poles. In general, these will be few. The explicit crossing symmetry of (4.17) allows us to keep an easy watch on the approximations being made in certain calculations. As an illustration we shall use expression (4.17) to derive the Chew–Jones formula for $A^{\pm}(s, t)$ in the strip approximation [Eqs. (III.7) and (III.9) of Ref. 5]. $A^{\pm}(s, t)$ had been defined by Eq. (3.1); if we denote by $A_B^{\pm}(s, t)$ and $A_R^{\pm}(s, t)$ the contributions to this amplitude coming from the background integrals and Regge terms of (4.17), respectively, then

$$A_B^{\pm}(s, t) = \frac{1}{\pi^2}\iint ds'\,dt'\,\frac{b_{st}^{\pm}(s', t')}{(s'-s)(t'-t)}, \quad (5.2)$$

where

$$b_{st}^{\pm}(s, t) = \begin{cases} b_{st}(s, t) \pm b_{su}(s, \mathbf{u}) & \text{for } s > s_0, \\ -b_{tu}(t, u) \mp b_{tu}(\mathbf{t}, \mathbf{u}) & \text{for } s < 0, \end{cases}$$

and where

$$s + \mathbf{t} + \mathbf{u} = 4m^2.$$

Here $\mathbf{u}$ and $\mathbf{t}$ are obtained from u and t, respectively, by letting $z_s \to -z_s$ in definition (4.1a); for the equal-mass case $\mathbf{u} = t$, and $\mathbf{t} = u$. Formula (5.2) is readily obtained by using the dispersion relations for $A_t(s, t)$ and $A_u(s, u)$—i.e., Eq. (3.2)—and the definition of $A^{\pm}(s, t)$. To obtain $A_R^{\pm}(s, t)$ we compute the contributions to the absorptive parts, $A_t(s, t)$ and $A_u(s, u)$, coming from the six Regge functions of (4.17); for $s > s_0$ we obtain

$$A_t(s, t) \to \sum_i R(\alpha_i(s); s, t) + \sum_i R_t(\alpha_i(t); t, s) + \sum_i \xi_i R_t(\alpha_i(t); t, u) + \sum_i \xi_i R_t(\alpha_i(u); u, t), \quad (5.3)$$

where u and t are related by $s + t + u = 4m^2$. The first two terms of (5.3), when substituted into (3.1), clearly yield

$$\sum_i R(\alpha_i(s); s, t) + \sum_i R(\alpha_i(t); t, s).$$

This follows from the analytic structure of $R(\alpha_i(x); x, y)$. The contribution of the third term in (5.3) to $A^{\pm}(s, t)$ may be rewritten in the following manner:

$$\sum_i \frac{1}{\pi}\int_{t_0}^{\infty}\frac{dt'}{t'-t}\xi_i R_t(\alpha_i(t'); t', u') = \sum_i \xi_i R(\alpha_i(t); t, u) - \sum_i \frac{1}{\pi}\int_{u_0}^{\infty}\frac{du'}{u'-u} \xi_i R_u(\alpha_i(t'); t', u'),$$

where $s + u' + t' = 4m^2$; we have made a change of variables in the last integral. Hence we obtain

$$\frac{1}{\pi}\int_{t_0}^{\infty} dt'\,\frac{A_t(s, t')}{t'-t} = \sum_i R(\alpha_i(s); s, t) + \sum_i [R(\alpha_i(t); t, s) + \xi_i R(\alpha_i(t); t, u)] + \sum_i \frac{1}{\pi}\int_{t_0}^{\infty}\frac{dt'}{t'-t}\xi_i R_t(\alpha_i(u'); u', t') - \sum_i \frac{1}{\pi}\int_{u_0}^{\infty}\frac{du'}{u'-u}\xi_i R_u(\alpha_i(t'); t', u'). \quad (5.4)$$

The second integral in (3.1) may be evaluated in a similar way. Hence $A^{\pm}(s, t)$ becomes

$$A^{\pm}(s, t) = A_B^{\pm}(s, t) + \sum_i [R(\alpha_i(s); s, t) \pm \xi_i R(\alpha_i(s); s, \mathbf{u})] + \sum_i [R(\alpha_i(t); t, s) + \xi_i R(\alpha_i(t); t, u)] \pm \sum_i [R(\alpha_i(\mathbf{u}); \mathbf{u}, s) + \xi_i R(\alpha_i(\mathbf{u}); \mathbf{u}, \mathbf{t})] \pm \sum_i \frac{1}{\pi}\int_{u_0}^{\infty} du'\left[\frac{1}{u'-\mathbf{u}} \mp \frac{1}{u'-u}\right]\xi_i R_u(\alpha_i(t'); t', u') + \sum_i \frac{1}{\pi}\int_{t_0}^{\infty} dt'\left[\frac{1}{t'-t} \mp \frac{1}{t'-\mathbf{t}}\right]\xi_i R_t(\alpha_i(u'); u', t'). \quad (5.5)$$

So far we have made no approximations. If we neglect

[14] Our reduced residue $\gamma_i(s)$ differs from their reduced residue by the factor $[2\alpha_i(s) + 1]$.

the background contribution to $A^{\pm}(s, t)$—i.e., the quantity $A_B^{\pm}(s, t)$—and if we make the substitution $u_0 \to u_1$ and $t_0 \to t_1$ in the limits of integration, then we obtain an approximate expression for $A^{\pm}(s, t)$ which is seen to be identical in form with the Chew–Jones formula, Eqs. (III.7) and (III.9) of Ref. 5; the two expressions differ only in the definition of the Regge functions. As we have pointed out before, Chew and Jones define $R(\alpha_i(s); s, t)$ to be equal to the integral appearing in (5.1) with t_0 replaced by t_1. In view of the previous discussion of this expression, we see that there is no essential difference between (5.5) and the Chew–Jones formula if we worry only about those trajectories which stay in the right half angular momentum plane; however, we point out once more, that at least in principle, our definition of the Regge function allows us to include the effects of *all* Regge poles; but until we have more knowledge about the region Re $\alpha < -\frac{1}{2}$, this is of purely academic interest.

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Correlation Functions and the Coexistence of Phases*

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We discuss the existence, continuity and other properties of the canonical and grand canonical many-particle correlation functions $n_s(\mathbf{r}_1, \cdots \mathbf{r}_s)$ in the thermodynamic limit of classical and quantum mechanical systems.

If the pressure of the system for fixed T is constant in the range of specific volume v_a to v_b, one expects physically to observe the coexistence of two separated phases. In terms of the correlation functions this is expressed by

$$n_s(v) = x_a(v_a/v)n_s(v_a) + x_b(v_b/v)n_s(v_b),$$

where x_a and x_b are the mole fractions of the phases so that $v = x_a v_a + x_b v_b$. With the aid of various lemmas on convex functions we prove that such a "separation of the phases" follows rigorously from statistical mechanics provided the correlation functions are "well defined" in an appropriate sense.

1. INTRODUCTION

RECENTLY, attention has been given to proving rigorously the existence of the canonical and grand canonical potentials (Helmholtz free energy and pressure, respectively, divided by k_BT) in the thermodynamic limit of an infinite system[1] under appropriate general conditions on the potentials of interaction, two-body[2] or many-body,[3] and on the shapes of the domains enclosing the system.[3,4] In this paper we take up the question of the definition, existence and properties of the many-particle correlation functions in classical and quantum mechanical systems in the thermodynamic limit. With a suitable definition of the correlation functions in a finite system, we prove that they approach limits in an infinite system provided the limiting correlation functions are "well defined" in the sense that they change infinitesimally for infinitesimal changes in the interaction potentials of the system. When the correlation functions are well defined, they are proved to be continuous functions of the temperature and density (or activity).

We then consider the situation where, at fixed temperature T, the pressure p is constant as a function of specific volume v in a range v_a to v_b, as observed when a liquid is in equilibrium with its vapor or a solid is in equilibrium with its liquid melt. In such circumstances we expect, on the grounds of physical observation, to find that the system separates into two or more macroscopic regions each filled with one or other of the two coexisting phases, either liquid and gas or solid and fluid. The proportions of the two phases, each with its characteristic number density and free-energy density, must be such as to give the observed over-all density and free energy.

How can this "separation of the phases" be expressed in theoretical terms? This question seems first to have been answered by the late Norbert Wiener who is quoted by Mayer and Montroll.[5] Wiener observed that, since the two separated phases should be of macroscopic extent, the s-particle correlation function $n_s(v)$ for the overall system at specific volume v should break into a linear combination of two correlation functions $n_s(v_a)$ and $n_s(v_b)$ characteristic of the two single phases. The coefficients of $n_s(v_a)$ and $n_s(v_b)$ should be determined simply by the probability of finding *one* particle in the respective phase. This follows from the assumption that the phases are of macroscopic extent so that a negligibly small proportion of particles will be near an interphase boundary. Thus if one particle is in phase A, say, any other particles at a finite distance from it are overwhelmingly likely to be in the *same* phase. In the absence of external forces, such as gravity, neither phase should preferentially occupy particular regions of space so that the probability of a particle being in a given phase is proportional to its volume. If N_a and N_b are the

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[1] By the thermodynamic limit in the canonical and grand canonical ensembles for a system in a domain Ω we understand the limit in which the volume $V(\Omega)$ approaches infinity at constant temperature while the specific volume v or activity z, respectively, approaches a finite limit. (See Refs. 2–4.)

[2] D. Ruelle, Helv. Phys. Acta **36**, 183, 789 (1963).

[3] M. E. Fisher, Arch. Ratl. Mech. Anal. **17**, 377 (1964).

[4] A similar analysis of the microcanonical ensemble for quantum mechanical systems has been given recently by R. B. Griffiths (to be published). Griffiths has also discussed spin systems [J. Math. Phys. **5**, 1215 (1964)].

[5] J. E. Mayer and E. W. Montroll, J. Chem. Phys. **9**, 2 (1941).

numbers of particles in the two phases we thus expect

$$n_s(v) = (N_a v_a/Nv)n_s(v_a) + (N_b v_b/Nv)n_s(v_b). \quad (1.1)$$

Alternatively, in terms of the mole fractions,

$$x_a = N_a/N = (v_b - v)/(v_b - v_a), \qquad x_b = N_b/N = (v - v_a)/(v_b - v_a), \quad (1.2)$$

we have $v = x_a v_a + x_b v_b$ and can write

$$n_s(v) = x_a(v_a/v)n_s(v_a) + x_b(v_b/v)n_s(v_b). \quad (1.3)$$

Conversely, if by calculation one finds that the correlation functions break into linear combinations of the form (1.3), one may infer that the system contains two separated phases with corresponding correlation functions $n_s(v_a)$ and $n_s(v_b)$. Such a situation was indeed discovered by Uhlenbeck, Hemmer, and Kac[6] when they investigated the correlation functions of a one-dimensional system of particles with hard cores and attractive pair potentials $\varphi(r) = -\alpha_0\gamma e^{-\gamma r}$. If the "Van der Waals limit", $\gamma \to 0$, is taken *after* the thermodynamic limit, this system exhibits a phase transition resembling condensation from gas to liquid. In the region of constant pressure the result (1.1) is found to hold (at least for $s = 2$ and 3).

It is natural to ask how far this relation between a flat (p, v) isotherm and the separation of coexisting phases should follow from the general theoretical principles of statistical mechanics. In this paper we answer this question by proving the following theorem: if, in the thermodynamic limit, the pressure is constant in a region v_a to v_b and the correlation functions are "well defined" in this region (in the sense mentioned above and made more precise in Sec. 4), then they decompose into a sum of two terms which, as in (1.3), can be associated with two separated phases of specific volumes v_a and v_b.

The mathematical techniques used to prove this theorem and the existence and continuity of the correlation functions are relatively straightforward. The correlation functions are defined with the aid of additional test functions (effectively as functional derivatives). The properties of convex functions and sequences of convex functions yield the existence proofs. A simple but evidently new theorem on functions, convex in two variables and linear in one of them, is used to prove the theorem on the separation of phases.

It should be mentioned that the existence of the limiting correlation functions for systems with two-body potentials in the grand canonical ensemble has been discussed by Ruelle,[7] Penrose,[7] and Ginibre,[8] but their results are restricted to activities and densities so low that the virial (and activity) expansions can be proved convergent. Evidently such results are insufficient for a discussion of any multiphase region.

2. EXISTENCE OF THE THERMODYNAMIC POTENTIALS

In this section we introduce the notation (which will follow Ref. 3) and state the established general theorems on the existence of the canonical and grand canonical thermodynamic potentials which will be needed to prove the existence of the correlation functions. We consider a system of N particles confined in a domain Ω of volume $V(\Omega)$ so that the specific volume is $v = V/N = 1/\rho$. The Hamiltonian $\mathcal{H}_N$ is the sum of the total kinetic energy T_N depending on the momenta $\mathbf{p}_i$, and the total potential energy U_N depending on the particle coordinates $\mathbf{r}_i$, on one or more external parameters ζ, η, $\cdots$ (and possibly on internal coordinates which we will, however, ignore for simplicity). The potential energy may be expressed in terms of translationally invariant many-body potentials $U^{(l)}(\mathbf{r}_i \cdots \mathbf{r}_l)$ each bounded below, as

$$U_N(\mathbf{r}_1 \cdots \mathbf{r}_N) = \sum_{(ij)} U^{(2)}(\mathbf{r}_i, \mathbf{r}_j) + \sum_{(ijk)} U^{(3)}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \cdots, \quad (2.1)$$

where the sums run over all pairs, triples etc., and there is *no restriction* on the order l of the many-body-potentials.

The classical canonical partition function is

$$Z(\beta, N, \Omega) = \frac{h^{-\nu N}}{N!} \int \cdots \int d\mathbf{p}_1 \cdots d\mathbf{p}_N \times \int_\Omega \cdots \int_\Omega d\mathbf{r}_1 \cdots d\mathbf{r}_N \exp(-\beta \mathcal{H}_N), \quad (2.2)$$

where h is Planck's constant, ν is the dimensionality of the system and $\beta = 1/k_B T$. The quantum mechanical partition function is defined by the appropriate trace depending on the statistics of the particles.[3] The canonical thermodynamic potential for the finite system is defined by

$$f(\beta, N, \Omega) = -F_N/Nk_BT = (1/N) \ln Z(\beta, N, \Omega), \quad (2.3)$$

where F_N is the total Helmholtz free energy.

[6] G. E. Uhlenbeck, P. C. Hemmer and M. Kac, J. Math. Phys. 4, 229 (1963).

[7] D. Ruelle, Ann. Phys. (N.Y.) 25, 109 (1963); Rev. Mod. Phys. 36, 580 (1964); J. Math. Phys. 6, 201 (1964); O. Penrose, J. Math. Phys. 4, 1312, 1488 (1963).

[8] J. Ginibre, J. Math. Phys. 6, 238, 252, 1432 (1965).

If z is the activity the grand canonical partition function is

$$\Xi(\beta, z, \Omega) = 1 + \sum_{N=1} (\Lambda^{\nu} z)^N Z(\beta, N, \Omega), \tag{2.4}$$

where

$$\Lambda = (h^2/2\pi m k_B T)^{\frac{1}{2}} \tag{2.5}$$

in which m is the particle mass. The corresponding grand canonical thermodynamic potential is defined by

$$\pi(\beta, z, \Omega) = \beta\bar{p} = [1/V(\Omega)] \ln \Xi(\beta, z, \Omega) \tag{2.6}$$

where $\bar{p}$ is the (grand canonical) pressure.

To obtain the thermodynamic limit we introduce a sequence Ω_k of domains with $V(\Omega_k) \to \infty$ as $k \to \infty$ and consider the limiting thermodynamic potentials

$$f(\zeta, \beta, v) = \lim_{k\to\infty} f(\zeta, \beta, N, \Omega_k) \tag{2.7}$$

and

$$\pi(\zeta, \beta, z) = \lim_{k\to\infty} \pi(\zeta, \beta, z, \Omega_k), \tag{2.8}$$

where we have indicated explicitly the dependence on the external parameter ζ. The limiting canonical pressure is defined by

$$p = p(v) = (\partial f/\partial v)_{\beta,\zeta}. \tag{2.9}$$

The grand canonical density is

$$\bar{\rho} = 1/\bar{v}(z) = z(\partial\pi/\partial z)_{\beta,\zeta}, \tag{2.10}$$

while the grand canonical Helmholtz free energy is given by

$$\bar{f}(\zeta, \beta, z) = -\bar{F}/k_B T = \bar{v}\pi - \ln(\Lambda^{\nu} z). \tag{2.11}$$

If the canonical and grand canonical results are consistent we must have

$$f(\zeta, \beta, v) \equiv \bar{f}(\zeta, \beta, z) \quad \text{for} \quad v = \bar{v}(z). \tag{2.12}$$

If this is valid, one may easily verify by partial differentiation, using (2.10) and (2.11), that when $v = \bar{v}(z)$

$$(\partial f/\partial\zeta)_{\beta,v} \equiv (\partial\pi/\partial\zeta)_{\beta,z}, \tag{2.13}$$

provided the derivatives with respect to the external parameter ζ exist.

Sufficient conditions for the existence and uniqueness of the limits (2.7) and (2.8) and for the identity (2.13) may be stated as follows.[3]

Firstly, for the potentials:

A *Stability* For some fixed positive w_A and all N

$$U_N(\mathbf{r}_1 \cdots \mathbf{r}_N) \geq -N w_A; \tag{2.14}$$

B *Tempering* If, for fixed R_0, $|\mathbf{r}_i - \mathbf{r}'_j| \geq R \geq R_0$ for all $i = 1, 2, \cdots, N$ and $j = 1, 2, \cdots, N'$ and if w_B and ϵ are fixed and positive, the mutual potential energy defined by

$$\Phi_{N,N'}(\mathbf{r}_1 \cdots \mathbf{r}_N; \mathbf{r}'_1 \cdots \mathbf{r}'_{N'}) = U_{N+N'}(\mathbf{r}_1 \cdots \mathbf{r}_N; \mathbf{r}'_1 \cdots \mathbf{r}'_{N'}) - U_N(\mathbf{r}_1 \cdots \mathbf{r}_N) - U_{N'}(\mathbf{r}'_1 \cdots \mathbf{r}'_{N'}), \tag{2.15}$$

satisfies

$$\Phi_{N,N'} \leq NN' w_B/R^{\nu+\epsilon} \tag{2.16}$$

for all N and N' if $(N + N')/R^{\nu+\epsilon}$ is sufficiently small.

Secondly, for the domains:

C The domains Ω_k are bounded and connected and $\sigma(\alpha; \Omega_k)$, the fraction of the volume within a distance $h = \alpha V_k^{1/\nu}$ of the boundary of Ω_k (internal to Ω_k if $\alpha > 0$ but external if $\alpha < 0$) vanishes as $\alpha \to 0$;

D* For the sequence of domains Ω_k there is a fixed α' and a function $\sigma_0(\alpha) \to 0$ as $|\alpha| \to 0$ such that for $\alpha \leq \alpha'$

$$\sigma(\alpha, \Omega_k) \leq \sigma_0(\alpha). \tag{2.17}$$

The detailed significance of these conditions is discussed in Ref. 3 (where alternative conditions are also given). It will suffice here to note (a) that conditions **A** and **B** will be satisfied if, for example, the pair potential $U^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \varphi(\mathbf{r}_1 - \mathbf{r}_2)$ has an infinite hard core of positive radius and $|\varphi(\mathbf{r})|$ decays when $r \to \infty$ as fast as $1/r^{\nu+\epsilon}$ ($\epsilon > 0$), while the many-body potentials $U^{(l)}$ are bounded everywhere and vanish identically for large enough separations of their arguments; and (b) that any sequence of domains Ω_k obtained by successive isotropic expansions of some domain Ω_0 will satisfy **C** and **D***.[9]

The existence theorems[3] show that $f(\beta, v)$ and $\pi(\beta, z)$ are convex functions of β and of v and $\ln z$, respectively. It follows from the convexity that the derivatives with respect to v and $\ln z$, namely $p(\beta, v)$ and $\bar{\rho}(\beta, z)$, are monotonic and exist everywhere except for a denumerable number of values of v or z where they may exhibit simple jump discontinui-

[9] If the pair potential does not have a hard core but satisfies instead the stability condition $\varphi(\mathbf{r}) \geq C/r^{\nu+\epsilon}$ as $r \to 0$, the total potential will satisfy **A** and **B** for positive three- and more-body potentials but may not do so if these are negative unless $\varphi(\mathbf{r})$ diverges more strongly. Indeed if $\varphi(\mathbf{r})$ is finite at $\mathbf{r} = 0$ one can prove that **A** cannot be satisfied if some of the many-body potentials are negative in certain regions (U_N will diverge to $-\infty$ as N^l). In such a case the corresponding l-particle ($l \geq 3$) correlation functions cannot be "well defined," in the sense explained below. I am indebted to D. Ruelle for observations on this point.

ties.[10] The same holds for the derivatives with respect to β.

3. DEFINITION OF THE CORRELATION FUNCTIONS

The s-particle correlation (or distribution) function $n_s(\mathbf{r}_1 \cdots \mathbf{r}_s; \beta, N, \Omega)$ of a classical system is defined[11] so that $n_s d\mathbf{r}_1 \cdots d\mathbf{r}_s$ is the probability of finding *any* s particles in $d\mathbf{r}_1 \cdots d\mathbf{r}_s$, irrespective of the positions of the remaining particles (or the momenta of any of the particles). Thus in the canonical ensemble

$$n_s(\mathbf{r}_1, \cdots, \mathbf{r}_s; \beta, N, \Omega) = \frac{\Lambda^{-\nu N}}{(N-s)!} \int_\Omega \cdots \int_\Omega d\mathbf{r}_{s+1} \cdots d\mathbf{r}_N \times \exp(-\beta U_N)/Z(\beta, N, \Omega), \tag{3.1}$$

where the factor $\Lambda^{-\nu N}$ comes from integrating over the N momenta. Correspondingly, in the grand canonical ensemble

$$\bar{n}_s(\mathbf{r}_1 \cdots \mathbf{r}_s; \beta, z, \Omega) = \sum_{N=s}^{\infty} \frac{1}{(N-s)!} \int_\Omega \cdots \int_\Omega d\mathbf{r}_{s+1} \cdots d\mathbf{r}_N \, z^N \exp(-\beta U_N)/\Xi(\beta, z, \Omega) \tag{3.2}$$

$$= \sum_{N=s}^{\infty} n_s(\mathbf{r}_1 \cdots \mathbf{r}_s; \beta, N, \Omega)(\Lambda^\nu z)^N Z(\beta, N, \Omega)/\Xi(\beta, z, \Omega). \tag{3.3}$$

It is usually stated that, in the limit of a large system, "the correlation functions should depend only on the separations between the particles," that is, on $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$, $\mathbf{r}_{13} = \mathbf{r}_3 - \mathbf{r}_1$, $\cdots$ $\mathbf{r}_{1s} = \mathbf{r}_s - \mathbf{r}_1$. Indeed if, as is often supposed for theoretical convenience, the system is contained in a torus (or, equivalently, *periodic* boundary conditions are imposed), this will be true even in a finite system. On the other hand, in general, the correlation functions must depend on $\mathbf{r}_1$ as well as on $\mathbf{r}_{12}$ to $\mathbf{r}_{1s}$. Thus, trivially, if $\mathbf{r}_1$ is outside Ω we must always have $n_s \equiv 0$ and, more generally, the correlation functions for positions near the boundary of the system will differ from those when all particles are far from the boundary. It is evident that the influence of the boundary should persist even as the volume of the domain becomes infinite so that if an origin is taken in the wall of Ω_k, the limiting correlation functions will *not* in general be independent of $\mathbf{r}_1$ even when $k \to \infty$. (This conclusion can be checked by explicit calculation.[12]) It might be thought that if the chosen origin becomes infinitely far from the walls as $k \to \infty$, n_s would then become independent of $\mathbf{r}_1$ in the limit. This does, in fact, happen in the low-density region where the virial expansion converges,[7] but it is by no means clear that it should be true at all densities. Thus in a crystalline state one expects "long-range order" to appear so that the effects of a boundary might be felt even infinitely far away. [Note that as $V(\Omega_k) \to \infty$ various orders of infinity might be relevant.]

From the foregoing discussion we see that a precise statement of the general conditions under which $n_s(\mathbf{r}_1 \cdots \mathbf{r}_s)$ approaches a limit depending only on $\mathbf{r}_{12} \cdots \mathbf{r}_{1s}$ might be rather complicated. Rather than attempt such a program, which, as we have seen, would essentially represent a study of "surface" rather than bulk effects, we redefine the correlation functions of interest by averaging over $\mathbf{r}_1$. Thus we introduce modified correlation functions by

$$n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, N, \Omega) = \frac{1}{V(\Omega)} \int_\Omega d\mathbf{r}_1 \, n_s(\mathbf{r}_1, \mathbf{r}_1 + \mathbf{r}_{12}, \cdots, \mathbf{r}_1 + \mathbf{r}_{1s}; \beta, N, \Omega). \tag{3.4}$$

By definition $n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s})$ is independent of $\mathbf{r}_1$ even in a finite system. Notice that if toroidal boundary conditions are used n_s' is simply equal to $n_s(\mathbf{r}_1, \mathbf{r}_1 + \mathbf{r}_{12}, \cdots, \mathbf{r}_1 + \mathbf{r}_{1s})$. Furthermore we always have $n_1' = N/V = \rho$. By a formula precisely analogous to (3.4) we similarly define modified grand canonical correlation functions $\bar{n}_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, z, \Omega)$.

To obtain a theoretically more useful expression for the correlation functions, we introduce a set of bounded, piecewise continuous $(s-1)$-variable test functions $\gamma_s(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s})$ which vanish identically outside a bounded region. (With no loss of generality, they may be taken as the characteristic functions of a region.) With the aid of the correlation functions we may define a linear functional on the γ_s by

[10] See, for example, G. H. Hardy, J. E. Littlewood, and G. Polya, *Inequalities* (Cambridge University Press, New York, 1952), 2nd ed.

[11] See, for example, G. E. Uhlenbeck and G. W. Ford, *Studies in Statistical Mechanics I*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland Publishing Company, Amsterdam, 1962), Part B.

[12] See, for example, M. E. Fisher and J. Stephenson, Phys. Rev. **132**, 1411 (1963), where the effects of the boundary on singlet and pair correlation functions in a lattice filled with hard "dimers" are derived.

$$M_s\{\gamma_s; \beta, N, \Omega\}$$
$$= \int \cdots \int d\mathbf{r}_{12} \cdots d\mathbf{r}_{1s} n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, N, \Omega)$$
$$\times \gamma_s(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}), \tag{3.5}$$

where the integrals may be extended over all space. From the definitions (3.1) and (3.4) and the stability condition (2.14) we readily obtain a bound on $n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, N, \Omega)$. Thus $M_s\{\gamma_s; \beta, N, \Omega\}$ is a bounded linear functional and, as such, knowledge of its value for a sufficiently large class of γ_s defines $n_s'(\beta, N, \Omega)$ uniquely.[13] From a physical viewpoint we may note that if γ_s is chosen as the characteristic function of a small $(s-1)$-dimensional domain centred at $\mathbf{R}_{12} \cdots \mathbf{R}_{1s}$ and of volume $\delta\tau\{\gamma_s\} = d\mathbf{R}_{12} d\mathbf{R}_{13} \cdots d\mathbf{R}_{15}$, the functional

$$m_s(\mathbf{R}_{12}, \cdots, \mathbf{R}_{1s}; \beta, N, \Omega)$$
$$= M_s\{\gamma_s; \beta, N, \Omega\}/\delta\tau\{\gamma_s\} \tag{3.6}$$

is a "coarse-grained" correlation function which for most practical purposes is essentially equivalent to the original "fine-grained" correlation function $n_s'(\mathbf{R}_{12}, \cdots, \mathbf{R}_{1s}; \beta, N, \Omega)$. With these points in mind we now restrict attention to the *correlation functionals* $M_s\{\gamma_s; \beta, N, \Omega\}$ and to the similarly defined grand canonical correlation functionals $\bar{M}_s\{\gamma_s; \beta, z, \Omega\}$.

From the test function $\gamma_s(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s})$ an additional many-body potential may be defined by

$$-\beta U_\gamma^{(s)}(\mathbf{r}_1, \mathbf{r}_1 + \mathbf{r}_{12}, \cdots, \mathbf{r}_1 + \mathbf{r}_{1s})$$
$$= \eta \sum_{(i)} \gamma_s(\mathbf{r}_{i(1)i(2)} \cdots \mathbf{r}_{i(1)i(s)}), \tag{3.7}$$

where the sum runs over the $s!$ permutations of the subscripts $i(j)(j = 1, 2, \cdots, s)$ and η is a parameter. By adding the appropriate $N!/s!(N-s)!$ terms in $U_\gamma^{(s)}$ to the total potential energy U_N we obtain an extended Hamiltonian of the form

$$-\beta\mathcal{H}_N(\eta) = -\beta\mathcal{H}_N + \eta\mathcal{G}_N \tag{3.8}$$

and corresponding partition functions and thermodynamic potentials.

Note that, at least for small enough η, the extended Hamiltonian will in general still satisfy the conditions **A** and **B** as required for the existence of the thermodynamic limit. It is now easily verified from the definitions that

$$M_s\{\gamma_s; \beta, N, \Omega\}$$
$$= [1/V(\Omega)](\partial/\partial\eta) \ln Z(\eta, \beta, N, \Omega)\,|_{\eta=0}$$
$$= v^{-1}(\partial/\partial\eta) f(\eta, \beta, N, \Omega)\,|_{\eta=0}, \tag{3.9}$$

and similarly,

$$\bar{M}_s\{\gamma_s; \beta, z, \Omega\} = (\partial/\partial\eta)\pi(\eta, \beta, z, \Omega)\,|_{\eta=0}, \tag{3.10}$$

where the functional dependence of the right-hand sides on γ_s is understood. These expressions for the correlation functionals as derivatives of the thermodynamic potentials provide the most direct method of investigating the limiting behavior.

We could, of course, rewrite (3.9) and (3.10) formally as expressions for the correlation functions themselves in terms of first functional derivatives with respect to γ_s of $f\{\gamma_s\}$ and $\pi\{\gamma_s\}$. The representation of the correlation functions as functional derivatives is very useful for formal developments but it may be pointed out that the usual procedure which introduces inhomogeneous external fields $\gamma_1(\mathbf{r})$ and represents n_s or $\bar{n}_s$ by s-fold *repeated* functional derivatives[14] is unsatisfactory for rigorous work. The reason lies in the difficulty of discussing the behavior of second- and higher-order derivatives of the thermodynamic potentials and in establishing the existence of the thermodynamic limit in the presence of inhomogeneous external fields.

Although the derivation of the expressions (3.9) and (3.10) for the correlation functionals was carried through only for classical systems they may equally be used, together with (3.5) and the corresponding expression for $\bar{M}_s$, to define the quantum mechanical correlation functions.[15]

4. EXISTENCE OF THE LIMITING CORRELATION FUNCTIONS

From the general theorems stated in Sec. 2, the limits

$$\lim_{k\to\infty} f(\eta, \beta, N, \Omega_k) = f(\eta, \beta, v) \tag{4.1}$$

and

$$\lim_{k\to\infty} \pi(\eta, \beta, z, \Omega_k) = \pi(\eta, \beta, z) \tag{4.2}$$

exist provided the conditions **A**, **B**, **C**, and **D*** are satisfied with the Hamiltonian $\mathcal{H}_N(\eta)$. Before we can use these limits to define the limiting correlation functions by differentiating with respect to η we must establish the differentiability of $f(\eta)$ and $\pi(\eta)$.

Consider firstly a classical system and write the

[13] See, for example, F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Fredrick Ungar Publishing Company, New York, 1955), p. 61 *et seq.*

[14] See, for example, N. N. Bogoliubov, *Studies in Statistical Mechanics I*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland Publishing Company, 1962), Part A; and J. L. Lebowitz and J. K. Percus, J. Math. Phys. **4**, 116 (1963).

[15] If one starts from the usual quantum mechanical definitions in terms of the diagonal elements of the reduced density matrices it is only necessary to recall that $(\partial/\partial\eta)$ $\mathrm{Tr}\{\exp(A + \eta B)\} = \mathrm{Tr}\{B \exp(A + \eta B)\}$ even when A and B do not commute.

Boltzmann factor as

$$\exp(-\beta\mathcal{H}_N + \eta\mathcal{G}_N) = \exp(-\tfrac{1}{2}\beta\mathcal{H}_N + \tfrac{1}{2}\eta_1\mathcal{G}_N) \times \exp(-\tfrac{1}{2}\beta\mathcal{H}_N + \tfrac{1}{2}\eta_2\mathcal{G}_N), \quad (4.3)$$

where $\frac{1}{2}(\eta_1 + \eta_2) = \eta$. On applying Schwarz's inequality[10] to the partition function and taking logarithms we then find

$$f(\tfrac{1}{2}\eta_1 + \tfrac{1}{2}\eta_2; \beta, N, \Omega) \leq \tfrac{1}{2}f(\eta_1, \beta, N, \Omega) + \tfrac{1}{2}f(\eta_2, \beta, N, \Omega). \quad (4.4)$$

Consequently, $f(\eta, \beta, N, \Omega)$ is a *convex function* of η. It follows that the limiting thermodynamic potential $f(\eta, \beta, v)$ is also convex in η at fixed v and β. [Recall that the general theorems establish that $f(\eta, \beta, v)$ is also convex (or rather concave) in v and convex in β at fixed η.]

For a quantum mechanical system the same results follow from

Lemma I. If $A + \eta B$ is a self-adjoint operator with a discrete spectrum bounded above, then $F(\eta) = \ln \mathrm{Tr}\,\{e^{A+\eta B}\}$ is a convex function.

For completeness, this lemma, which follows easily from Peierls' theorem,[16] is demonstrated in Appendix A.

The grand canonical partition function is an absolutely convergent sum of canonical partition functions.[17] The following lemma, proved in Appendix A, thus enables one to conclude from the convexity of the canonical potential $f(\eta, \beta, N, \Omega)$ that the grand canonical potential $\pi(\eta, \beta, z, \Omega)$ is also convex.

Lemma II. If $f_t(\eta) = \ln q_t(\eta)$ $(t = 1, 2, 3, \cdots)$ is a set of convex functions and $Q(\eta) = \sum_t q_t(\eta)$ then $F(\eta) = \ln Q(\eta)$ is also convex.

The convexity of $\pi(\eta, \beta, z, \Omega)$ implies the convexity of the limit $\pi(\eta, \beta, z)$ (which is also convex in β and $\ln z$).

We have thus proved that $f(\eta, \beta, v)$ and $\pi(\eta, \beta, z)$ are convex in η. From this it follows[10] that both functions are continuous in η and differentiable everywhere except, possibly, at a denumerable number of points η_h where the derivative can exhibit a jump discontinuity. We may thus *define* the *correlation functions in the thermodynamic limit* by

$$M_s\{\gamma; \beta, v\} = v^{-1}(\partial/\partial\eta)f(\eta, \beta, v)\,|_{\eta=0} \quad (4.5)$$

and

$$\bar{M}_s\{\gamma; \beta, z\} = (\partial/\partial\eta)\pi(\eta, \beta, z)\,|_{\eta=0}. \quad (4.6)$$

These definitions can fail only if $\eta = 0$ is a point of discontinuity of the derivatives, that is if the derivatives from the left ($\eta < 0$) and the right ($\eta > 0$) are different. When the derivatives in (4.5) and (4.6) exist (that is the left and right derivatives agree) we will say the correlation functions are *well defined.*

For the moment we postpone a discussion of the circumstances in which the correlation functions in the thermodynamic limit might not be well defined and consider the limiting behavior of the correlation functionals of a finite system [Eqs. (3.9) and (3.10)]. For this purpose we require the following simple lemma which is proved in Appendix A.

Lemma III. Given a sequence of convex functions $f_k(\eta)$ which converge to a limit $f(\eta)$ as $k \to \infty$ the left and right derivatives satisfy

$$\frac{d^-f}{d\eta} \leq \liminf_{k\to\infty} \frac{d^-f_k}{d\eta} \leq \limsup_{k\to\infty} \frac{d^+f_k}{d\eta} \leq \frac{d^+f}{d\eta}. \quad (4.7)$$

If the functions $f_k(\eta)$ are differentiable at η_0 and if the limit $f(\eta)$ is also differentiable at η_0 it follows, as an immediate corollary of this lemma, that the derivatives at η_0 approach the derivative of the limit. (This corollary has been derived independently by Griffiths.[4])

Applying this result to the functions $f(\eta, \beta, v, \Omega_k)$ and $\pi(\eta, \beta, z, \Omega_k)$ for any suitable sequence of domains Ω_k, we see that the correlation functionals $M_s\{\gamma; \beta, N; \Omega_k\}$ and $\bar{M}_s\{\gamma; \beta, z; \Omega_k\}$ of the finite system must approach the correlation functionals in the thermodynamic limit whenever these latter are well defined. (If the limiting correlations are *not* well defined the limits, if any, of the finite system functionals will be bounded by the right and left derivatives of the limiting thermodynamic potentials; see the further discussion below.)

When the correlation functions are well defined in both the canonical and grand canonical ensembles it follows from the identity (2.13) between the ensembles that

$$M_s\{\gamma; \beta, \bar{v}(z)\} \equiv \bar{M}_s\{\gamma; \beta, z\}. \quad (4.8)$$

In other words the canonical and grand canonical correlation functions at the same density and temperature are identical.

Consider now the question of when the limiting correlation functions will be well defined. Since the points of discontinuity η_h of the derivative of a convex function are denumerable, there is a point of con-

[16] R. Peierls, Phys. Rev. 54, 918 (1938). See also Ref. 3 and K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963), p. 220.

[17] This may fail for large enough z in a Bose system with insufficiently strong repulsions between the particles, but such values of z are essentially without physical significance (see the discussion in Ref. 3).

tinuity in the neighborhood of any η_k. It follows that *the correlation functions can always be made well defined by adding infinitesimal terms to the interaction potentials* (for example terms proportional to $\mathcal{G}_N$). Conversely we see that the correlation functionals will always be well defined unless the system is in some "hypercritical" state in which infinitesimal changes of the potentials (at fixed β and v or fixed β and z) result in *finite* changes in the correlation functions.[18] Such hypercritical states may evidently occur at normal first-order phase transition points. Thus in the *grand* canonical ensemble the activity z_t and inverse temperature β_t at which a condensation transition, say, takes place will be points of discontinuity of the density $\bar{p}(\beta, z)$ and of the internal energy $\bar{U}(\beta, z)$. An infinitesimal change in the interactions could (and, in general, would) drive the system into either the denser or the lighter phase with consequent finite changes in the correlation functions.[19] The analogous situation in the canonical ensemble would arise if the pressure or energy were discontinuous functions of specific volume or temperature. Although such discontinuities have not been proved impossible in general[20] they have apparently never been observed experimentally. (As a function of v and β the energy and pressure are, of course, continuous through a condensation process.)

At a hypercritical point where the correlation functions fail to be well defined the finite system functionals $M_s\{\Omega_k\}$ and $\bar{M}_s\{\Omega_k\}$ do not necessarily approach limits as $k \to \infty$. Whether a limit is approached and what its value will be (within the bounds following from Lemma III) will evidently depend on the finer details of the potentials and of the precise way the thermodynamic limit is taken. The task of specifying such details generally would seem to be rather difficult but, at the same time, of relatively little physical interest [One might, nevertheless, attempt to prove more restricted conjectures such as: if $\bar{p}(\beta, z)$ is discontinuous at (β_t, z_t) but $\bar{p}_k = \bar{p}(\beta_t, z_t, \Omega_k)$ approaches a limit $1/v^*$ then $\lim_{k\to\infty} \bar{M}_s\{\gamma; \beta_t, z_t; \Omega_k\} = M_s\{\gamma, \beta_t, v^*\}$ provided the canonical functional is itself well defined at $v = v^*$.]

The fact that points of discontinuity of the derivatives of the thermodynamic potentials will generally be points where the correlation functions are not well defined suggests the converse question, namely, will the correlation functions themselves be continuous when they *are* well defined? This is answered by the following lemma which follows easily from Lemma III as shown in Appendix A.

Lemma IV. If $f(\eta, y)$ is convex in η and continuous in y for small η and $y_a \leq y \leq y_b$ then if the derivative $m(y) = (\partial f/\partial\eta)_{\eta=0}$ exists it is continuous for $y_a \leq y \leq y_b$.

To apply this result we need only recall that the convexity of the limiting potentials $f(\eta, \beta, v)$ and $\pi(\eta, \beta, z)$ in β and v or $\ln z$, implies their continuity in the same variables. If the correlations are well defined, so that $(\partial f/\partial\eta)_{\eta=0}$ or $(\partial\pi/\partial\eta)_{\eta=0}$ exist, for some interval of β or v, or z, we may thus conclude that the functionals $M_s\{\gamma; \beta, v\}$ and $\bar{M}_s\{\gamma; \beta, z\}$ will be continuous in β or v or z, respectively, in the same interval.

It may be remarked that the same lemma implies, for example, that if the pressure $p(v_0, \beta)$ exists at $v = v_0$ for some range of β [that is $p(v, \beta)$ is *not* discontinuous in v at v_0 for fixed β] then $p(v_0, \beta)$ is continuous for β in the same range. Similarly if the canonical and grand canonical energies $U(\beta, v)$ and $\bar{U}(\beta, z)$ exist at $\beta = \beta_0$ for a range of v or of z then $U(\beta_0, v)$ and $\bar{U}(\beta_0, z)$ will be continuous in v or z, respectively.

To summarize our results so far we have defined (a) the correlation functionals with the aid of a set of test functions γ_s [Eq. (3.5)], (b) an extended Hamiltonian $\mathcal{H}_N(\eta)$ in terms of the test functions [Eqs. (3.7) and (3.8)] and, hence, (c) corresponding canonical and grand canonical limiting thermodynamic potentials $f(\eta, \beta, v)$ and $\pi(\eta, \beta, z)$. We have then proved:

Theorem A. Under conditions **A**, **B**, **C**, and **D***, the correlation functionals satisfy

$$\lim_{k\to\infty} M_s\{\gamma; \beta, N; \Omega_k\} = M_s\{\gamma; \beta, v\} = v^{-1}(\partial/\partial\eta) f(\eta, \beta, v)\,|_{\eta=0} \qquad (4.9)$$

and

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[18] We use the adjective "hypercritical" in contradistinction to "critical" since in normal usage a critical point is one at which certain double derivatives of the thermodynamic potentials become continuously infinite (e.g., the compressibility at the gas–liquid critical point or the specific heat at a lambda transition) but their integrals remain *continuous*. In this sense the usual first-order transition points (e. g., an ideal ferromagnet below its Curie point in zero magnet field) are examples of hypercritical points.

[19] Notice that for a system with pair interactions only, the energy $\bar{U}(\beta, z)$ is equal to a correlation functional evaluated with a $\gamma_2(\mathbf{r})$ proportional to the pair potential $\varphi(\mathbf{r})$. A change in η is then precisely equivalent to a change in β.

[20] Note, however, that Ruelle (Ref. 2) *has* proved that the pressure is continuous in v for a classical system of particles interacting through pair potentials which are bounded *above* (in addition to satisfying conditions **A** and **B**). It seems probable that the pressure should remain continuous under much weaker restrictions.

$$\lim_{k\to\infty} \bar{M}_s\{\gamma;\beta,z;\Omega_k\} = \bar{M}_s\{\gamma;\beta,z\}$$
$$= (\partial/\partial\eta)\pi(\eta,\beta,z)\,|_{\eta=0}, \qquad (4.10)$$

provided the derivatives with respect to η exist in which case the correlation functions in the limit are said to be well defined. When the correlations are well defined, M_s and $\bar{M}_s$ are continuous functions of β and of v or z, respectively, and, furthermore $M_s \equiv \bar{M}_s$ if $v = \bar{v}(z)$. (If the η derivatives do not exist at $\eta = 0$ for some β and v or z the functionals for $k \to \infty$ are bounded by the right and left derivatives.)

5. SEPARATION OF PHASES

In this section we consider only the canonical ensemble at constant temperature and investigate the limiting correlation functions when the pressure $p(v)$ is constant in a range of density. [A precisely analogous discussion could be given for the grand canonical ensemble in the situation, alluded to before, where the density $\bar{\rho}(z)$ is constant in a range z_a to z_b so that the pressure increases discontinuously with density.[20]]

If the pressure is constant in the region v_a to v_b the canonical thermodynamic potential for $\eta = 0$ must vary linearly with v, that is

$$f(0,v) = a + pv, \qquad (v_a \le v \le v_b). \qquad (5.1)$$

By defining

$$x_a = (v_b - v)/(v_b - v_a),\ x_b = (v - v_a)/(v_b - v_a) \qquad (5.2)$$

so that $x_a + x_b = 1$ and

$$v = x_a v_a + x_b v_b, \qquad (5.3)$$

one can, quite generally, rewrite (5.1) as

$$f(0,v) = x_a f_a + x_b f_b, \qquad (5.4)$$

where $f_a = f(0,v_a)$ and $f_b = f(0,v_b)$. As indicated in the introduction one may then interpret x_a and x_b as the mole fractions of two separate phases of specific volumes v_a and v_b and free energies corresponding to f_a and f_b.

As shown in the previous section the correlation functionals are given by

$$m(v) = vM_s\{\gamma;\beta,v\} = (\partial/\partial\eta)f(\eta,v)\,|_{\eta=0}. \qquad (5.5)$$

If we assume the correlation functions are well defined in the interval $v_a \le v \le v_b$, the derivative $\partial f/\partial\eta$ at $\eta = 0$ will, by definition, exist in the same region. In order to draw a conclusion from this assumption and the linearity (5.1) we prove a fundamental lemma concerning the linearity of the derivative of a convex function $f(\eta, y)$.

Lemma V. Suppose $f(\eta, y)$ is convex (or concave) in y for all small enough η and that the derivative $m(y) = (\partial f/\partial\eta)_{\eta=0}$ exists. Then, if $f(0, y) = a + by$ for fixed a and b and $y_a \le y \le y_b$, one can write $m(y) = c + dy$ for $y_a \le y \le y_b$, where c and d are fixed.

Proof. We will make the hypothesis that $m(y)$ is not linear in y and then use the existence of the derivative at $\eta = 0$ to show that $f(\eta, y)$ cannot be convex (or concave) for both positive and negative values of η.

If $m(y)$ is not linear we can find y_1, y_2 and y_3 such that

$$K = \frac{m_3 - m_2}{y_3 - y_2} - \frac{m_2 - m_1}{y_2 - y_1}, \qquad (5.6)$$

where $m_i = m(y_i)(j = 1, 2, 3)$, does not vanish. The vanishing of K for all sets y_i would imply the linearity of $m(y)$. Because the derivative with respect to η exists at $\eta = 0$ we have

$$f_i(\eta) = f(\eta, y_i) = f_i(0) + \eta m_i[1 + e_i(\eta)], \qquad (5.7)$$

where for given $\epsilon > 0$, there is a $\delta = \delta(\epsilon) > 0$ such that $|e_i(\eta)| < \epsilon$ for $|\eta| < \delta$. The convexity of $f(\eta, y)$ is tested by

$$C(\eta) = \frac{f_3(\eta) - f_2(\eta)}{y_3 - y_2} - \frac{f_2(\eta) - f_1(\eta)}{y_2 - y_1}, \qquad (5.8)$$

which will vanish only if the three points $[y_i, f_i(\eta)]$ are colinear. On substituting with (5.7), using the linearity of $f(0, y)$ which implies $C(0) \equiv 0$, and the definition (5.6), we obtain

$$C(\eta) = \eta[K + L(\eta)], \qquad (5.9)$$

where

$$L(\eta) = \frac{m_3 e_3(\eta) - m_2 e_2(\eta)}{y_3 - y_2} - \frac{m_2 e_2(\eta) - m_1 e_1(\eta)}{y_2 - y_1}. \qquad (5.10)$$

For $|\eta| < \delta$ we have

$$|L(\eta)| \le \epsilon\left[\frac{|m_3| + |m_2|}{|y_3 - y_2|} + \frac{|m_2| + |m_1|}{|y_2 - y_1|}\right]$$
$$\le 4\epsilon \max_i \{m(y_i)\}/\min_i \{|y_{i+1} - y_i|\}. \qquad (5.11)$$

Thus one can choose ϵ so small that $|L|/|K| < 1$. The relation (5.9) then shows that the sign of $C(\eta)$ for $|\eta| < \delta(\epsilon)$ is the same as that of ηK and hence changes as η changes sign. But this is impossible if $f(\eta, y)$ is convex (or concave) for all η in the neighborhood of zero. Hence the hypothesis is untenable and we conclude that $m(y)$ must be linear in the interval $y_a \le y \le y_b$. (Note that both end points of the in-

terval are included since either could have been chosen as one of the y_i.)

To apply this lemma we use the linearity of the limiting canonical potential $f(\eta, v)$ at $\eta = 0$ [Eq. (5.1)], the concavity of $f(\eta, v)$ in v for all small enough η and the assumption that the correlation functions are well defined [Eq. (3.5)]. We can then infer that $vM_s\{\gamma; \beta, v\}$ must be linear in v for $v_a \leq v \leq v_b$. Defining x_a and x_b by Eq. (5.2) we have thus established

Theorem B. If the pressure $p(\beta, v)$ at fixed β is constant for $v_a \leq v \leq v_b$ and the correlation functions are well defined in the same interval, the correlation functionals may be written

$$M_s\{\gamma; \beta, v\} = x_a(v_a/v)M_s\{\gamma; \beta, v_a\} + x_b(v_b/v)M_s\{\gamma; \beta, v_b\}. \quad (5.12)$$

We can hence express the correlation function $n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, v)$ as a linear combination of the two correlation functions $n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, v_a)$ and $n_s'(\mathbf{r}_{12}, \cdots, \mathbf{r}_{1s}; \beta, v_b)$ in the form (1.3) anticipated by Wiener. We may interpret $n_s'(v_a)$ and $n_s'(v_b)$ as the correlation functions of the two separate phases. Indeed if the region in which the correlations are well defined extends beyond the interval (v_a, v_b) into the "single-phase" regions we may, by Theorem A which ensures the continuity of the correlation functions, define $n_s'(v_a)$ and $n_s'(v_b)$ as the limits of the single-phase correlation functions $n_s'(v)$ as v approaches v_a from below and v_b from above, respectively. This accords fully with the usual physical picture which assumes the two coexisting phases have the same nature and properties as the corresponding single phases just outside the two-phase region. We cannot at present, however, rule out completely the possibility that the correlation functions cease to be well defined just on the two-phase boundary and are not continuous across it.

Although this last possibility may seem highly improbable on physical grounds, the question of when one might expect the correlation functions to be well defined in a region of constant pressure should be discussed a little further. In a normal isothermal first-order phase change occurring away from any critical or triple point, an infinitesimal change in the interactions should merely alter infinitesimally the proportions of the two phases and the properties of each phase (as does an infinitesimal change in temperature[19]). In such typical circumstances we may confidently expect the correlation functions to be well defined. Suppose, on the other hand, that the constant pressure isotherm in question corresponds exactly to the gas–liquid critical temperature T_c of a system with a "flat-topped" coexistence curve so that for $T > T_c$ the pressure is strictly decreasing with v. (Such "flat-topped" coexistence curves have probably not been observed experimentally in equilibrium systems in negligible external fields but they can arise in certain theoretical models which nevertheless satisfy the conditions **A**, **B**, **C**, and **D***.[21]) Since a change of temperature is effectively equivalent to a change of the interactions[19] and since an infinitesimal change of temperature will send the system either completely into the "single-phase" region above T_c or down into the normal "two-phase" region below T_c with, probably, finite changes in the correlation properties in at least one case, it seems quite likely that the correlation functions would *not* be well defined on this isotherm. A similar situation might arise just *at* a pressure and temperature corresponding to a triple point.

The foregoing discussions show that we should not expect to find simple criteria which will specify completely the circumstances in which the correlation functions are well defined since that would be tantemount to a prescription for locating the position and nature of any phase transitions. It is known from examples that the presence of a phase transition depends sensitively on the detailed properties of the interactions. Further progress might be possible, however, in special regions following the results for low densities where the limiting correlation functions can be specified by their virial expansions.[7–9] Despite the possibility of singular isotherms on which the correlation functions may not always be well defined, Theorem B does nevertheless show us theoretically why the "separation of two coexisting phases" is the general rule.

In conclusion we mention that an outstanding problem in the theory of correlation functions concerns the rigorous derivation of the fluctuation relation for the compressibility in the thermodynamic limit, namely,

$$\frac{1}{\beta}\frac{\partial p}{\partial \rho} = 1 + \rho \int [v^2 n_2'(\mathbf{r}) - 1]\, d\mathbf{r}, \quad (5.13)$$

and, in case there are only pair interactions, of the related virial relation for the pressure.[11]

ACKNOWLEDGMENTS

The work described here was undertaken while the author was a guest at The Rockefeller Institute.

[21] M. E. Fisher, *The Theory of Condensation*, Lecture on the Centennial Conference on Phase Transformation, University of Kentucky, March, 1965, to be published in the Proceedings.

It is a pleasure to acknowledge the stimulation and advice received there from Professor Mark Kac and Professor G. E. Uhlenbeck. I am also grateful to Professor David Ruelle for a number of valuable comments on the manuscript.

APPENDIX A: PROOFS OF LEMMAS ON CONVEX FUNCTIONS

Throughout the appendix we take

$$\eta = \tfrac{1}{2}\eta_1 + \tfrac{1}{2}\eta_2. \tag{A1}$$

A function $F(\eta)$ is convex if

$$F(\eta) \leq \tfrac{1}{2}F(\eta_1) + \tfrac{1}{2}F(\eta_2). \tag{A2}$$

The most important properties of convex functions, their continuity and differentiability, are discussed in Ref. 10. For convenience of reference we restate the lemmas before proving them.

Lemma I. If $A + \eta B$ is a self-adjoint operator with a discrete spectrum bounded above then $F(\eta) = \ln \mathrm{Tr}\ \{e^{A+\eta B}\}$ is convex.

Proof. Let φ_n be the eigenfunctions of $A + \eta B$ and denote $(\varphi_n, C\varphi_n)$ by C_n. Then

$$\mathrm{Tr}\ \{e^{A+\eta B}\} = \sum_n \exp\,(A_n + \eta B_n)$$

$$= \sum_n \exp\,(\tfrac{1}{2}A_n + \tfrac{1}{2}\eta_1 B_n) \exp\,(\tfrac{1}{2}A_n + \tfrac{1}{2}\eta_2 B_n). \tag{A3}$$

By Cauchy's inequality therefore

$$\exp F(\eta) \leq [\sum_n \exp\,(A_n + \eta_1 B_n)]^{\frac{1}{2}} \times [\sum_n \exp\,(A_n + \eta_2 B_n)]^{\frac{1}{2}}. \tag{A4}$$

For any orthonormal set ψ_m Peierls' theorem[16] states

$$\sum_m \exp\,(C_m) \leq \mathrm{Tr}\ \{e^C\}. \tag{A5}$$

Applying this to (A4) and taking logarithms yields (A2) as required.

Lemma II. If $f_t(\eta) = \ln q_t(\eta)$ $(t = 1, 2, 3, \cdots)$ is a set of convex functions and $Q(\eta) = \sum_t q_t(\eta)$ then $F(\eta) = \ln Q(\eta)$ is also convex.

Proof. We have

$$Q(\eta_1)Q(\eta_2) - Q^2(\eta) = \sum_t [q_t(\eta_1)q_t(\eta_2) - q_t^2(\eta)] + \sum_{t<s} [q_t(\eta_1)q_s(\eta_2) + q_s(\eta_1)q_t(\eta_2) - 2q_t(\eta)q_s(\eta)]. \tag{A6}$$

By the convexity of $f_t(\eta)$

$$q_t(\eta) \leq q_t^{\frac{1}{2}}(\eta_1)q_t^{\frac{1}{2}}(\eta_2) \tag{A7}$$

so that the first sum in (A6) is positive and the general term of the second exceeds

$$q_t(\eta_1)q_s(\eta_2) - 2q_t^{\frac{1}{2}}(\eta_1)q_t^{\frac{1}{2}}(\eta_2)q_s^{\frac{1}{2}}(\eta_1)q_s^{\frac{1}{2}}(\eta_2) + q_s(\eta_1)q_t(\eta_2) = [q_t^{\frac{1}{2}}(\eta_1)q_s^{\frac{1}{2}}(\eta_2) - q_s^{\frac{1}{2}}(\eta_1)q_t^{\frac{1}{2}}(\eta_2)]^2 \geq 0. \tag{A8}$$

Thus

$$Q(\eta_1)Q(\eta_2) \geq Q^2(\eta) \tag{A9}$$

from which (A2) follows.

Lemma III. Given a sequence of convex functions $f_k(\eta)$ which converge to a limit $f(\eta)$ as $k \to \infty$, the left and right derivatives satisfy

$$\frac{d^-}{d\eta} f(\eta) \leq \liminf_{k\to\infty} \frac{d^-}{d\eta} f_k(\eta) \leq \limsup_{k\to\infty} \frac{d^+}{d\eta} f_k(\eta) \leq \frac{d^+}{d\eta} f(\eta). \tag{A10}$$

Proof. Since $f_k(\eta)$ and hence $f(\eta)$ are convex the left and right derivatives exist everywhere. Given η_0 choose $\delta > 0$ and $\epsilon > 0$. Then there is a k_0 such that for $k \geq k_0$

$$|f_k(\eta_0 + \delta) - f(\eta_0 + \delta)| \leq \epsilon, \quad |f_k(\eta_0) - f(\eta_0)| \leq \epsilon,$$

and

$$|f_k(\eta_0 - \delta) - f(\eta_0 - \delta)| \leq \epsilon. \tag{A11}$$

By the convexity of $f_k(\eta)$ at η_0 we have

$$(d^-/d\eta)f_k(\eta_0) \geq [f_k(\eta_0) - f_k(\eta_0 - \delta)]/\delta$$

and for $k \geq k_0$

$$\geq [f(\eta_0) + \epsilon - f(\eta_0 - \delta) + \epsilon]/\delta. \tag{A12}$$

Similarly

$$(d^+/d\eta)f_k(\eta_0) \leq [f(\eta_0 + \delta) - f(\eta_0)]/\delta - 2\epsilon/\delta. \tag{A13}$$

Let $k \to \infty$ and then let $\epsilon \to 0$ to obtain

$$\liminf_{k\to\infty} \frac{d^-}{d\eta} f(\eta_0) \geq [f(\eta_0) - f(\eta_0 - \delta)]/\delta \tag{A14}$$

and

$$\limsup_{k\to\infty} \frac{d^+}{d\eta} f_k(\eta_0) \leq [f(\eta_0 + \delta) - f(\eta_0)]/\delta. \tag{A15}$$

On letting $\delta \to 0$ the right-hand sides tend to $(d^-/d\eta)f(\eta_0)$ and $(d^+/d\eta)f(\eta_0)$, respectively, which yields (A10).

Lemma IV. If $f(\eta, y)$ is convex in η and continuous in y for small η and $y_a \leq y \leq y_b$ then if the derivative $m(y) = (\partial f/\partial \eta)_{\eta=0}$ exists it is continuous for $y_a \leq y \leq y_b$.

Proof. Choose any y_0 in (y_a, y_b). For any sequence y_k $(k = 1, 2, 3, \cdots)$ in (y_a, y_b) for which $y_k \to y_0$ as

$k \to \infty$, we have by continuity in y for small enough η, $f(\eta, y_k) \to f(\eta, y_0)$. Since the sequence of functions $f_k(\eta) = f(\eta, y_k)$ and their limit $f(\eta, y_0)$ are convex in η we may apply Lemma III to conclude

$$\frac{\partial^-}{\partial \eta} f(\eta, y_0) \leq \lim_{y \to y_0} \inf \frac{\partial^-}{\partial \eta} f(\eta, y)$$

$$\leq \lim_{y \to y_0} \sup \frac{\partial^+}{\partial \eta} f(\eta, y) \leq \frac{\partial^+}{\partial \eta} f(\eta, y_0). \quad \text{(A16)}$$

The existence of $m(y)$, the derivative at $\eta = 0$, yields immediately

$$\lim_{y \to y_0} m(y) = m(y_0), \quad \text{(A17)}$$

which implies the continuity of $m(y)$ at $y = y_0$. More generally (A16) shows that the right and left derivatives $m^+(y)$ and $m^-(y)$, say, are upper and lower semicontinuous, respectively.

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Alternative Formulations of Scattering in Model Field Theories

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(Received 4 January 1965)

A comparison is made between the expression for the boson–fermion scattering amplitude, in a model theory, obtained by renormalizing Feynman diagrams, and the one that originates from the dressed-particle picture. A proof is given of a surmise, previously verified to sixth order, that the two expressions for the transition amplitude are identical, although the former stems from a theory that leads to paradoxes from which the latter is exempt. The proof of the identity of the two representations is extended to transition amplitudes in which a weak interaction, considered to first order, is modified by a strong one considered to all orders. It is shown how the operations in the dressed-particle picture directly lead to iterations in terms of the physical mass and coupling constant, whereas the expressions obtained from the Feynman diagrams require renormalization before they have this form.

I. INTRODUCTION

THE theory of quantized boson fields interacting with fixed sources that have only a finite number of degrees of freedom (like spin and isospin, for example), has been extensively studied in the history of quantum field theory. Some of the early work on quantized fields was done with this type of theory.[1] About ten years ago extensive use was made of these model theories to represent actual low-energy pion–nucleon processes[2]; and these models have served and continue to serve as mathematical models for realistic field theories. It is in this last capacity that static model theories will be examined in this paper. They are well suited for this purpose because they strongly resemble fully relativistic field theories in those respects in which the latter exhibit their most challenging and interesting pathologies. In spite of these important similarities, the static model theories are nevertheless mathematically much simpler to understand than their fully relativistic counterparts, and questions which are still unresolved for the latter, can be understood in the case of the former. Scattering in the case of static model theories has been treated by a number of alternative methods. In the first place, the traditional approach to quantum field theory has been invoked[3]: In this procedure, a time-dependent scattering wavefunction is used to represent the combined target–projectile system. The incident wave (as well as

* Based upon a dissertation, submitted to the faculty of the Graduate School of Arts and Sciences of New York University, in partial fulfillment of the requirements for the degree of Doctor of Philosophy.

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[1] G. Wentzel, *Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1949).

[2] G. F. Chew and F. E. Low, Phys. Rev. **101**, 1570 (1956); M. H. Friedman, T. D. Lee, and R. Christian, Phys. Rev. **100**, 1494 (1955); A. Pais and R. Serber, Phys. Rev. **105**, 1636 (1959); **113**, 955 (1959).

[3] S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1961), Chapter 11.

$k \to \infty$, we have by continuity in y for small enough η, $f(\eta, y_k) \to f(\eta, y_0)$. Since the sequence of functions $f_k(\eta) = f(\eta, y_k)$ and their limit $f(\eta, y_0)$ are convex in η we may apply Lemma III to conclude

$$\frac{\partial^-}{\partial \eta} f(\eta, y_0) \leq \lim_{y \to y_0} \inf \frac{\partial^-}{\partial \eta} f(\eta, y)$$

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The existence of $m(y)$, the derivative at $\eta = 0$, yields immediately

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the asymptotic limit, as time $\rightarrow \infty$, of the scattered wave) is presumed to be an n-particle eigenfunction of the interaction-free part of the Hamiltonian, and a linear singular integral equation for the transition matrix is derived.[4] The latter is expanded into the Liouville–Neumann (or Born) series in a form which, for relativistic theories, would be manifestly covariant. The results of evaluating the individual terms of this series markedly resemble those that appear when fully relativistic field theories are treated: A set of Feynman rules can be constructed for static model theories and, higher-order terms in the series (the radiative corrections) exhibit divergent integrals in the case of point sources. These divergent integrals can be divided into various classes such as "fermion"[5] self-energy parts, vertex parts and wavefunction renormalization parts. The major difference between these theories and fully relativistic ones lies in the absence of boson self-energy parts in the case of the former, and therefore the absence of the renormalization constant Z_3 in static theories. Moreover in static model theories, in the place of Ward's identity of electrodynamics, the relation $d\Sigma(E)/dE = -\Lambda_i(E)$ holds, where $\Sigma(E)$ is the sum of all proper self-energy parts and $\Lambda_i(E)$ is the sum of all proper "internal" vertex parts. The latter differ from the regular vertex parts by having the contribution from each diagram differently weighted by some diagram-dependent number (usually an integer). These theories require coupling constant, fermion self-energy and fermion wavefunction renormalization; in the case of interactions for which the skeleton vertex parts are logarithmically divergent (such as the Lee model[6]; the Ruijgrok–Van Hove[7] model and the charge-symmetric scalar model) only finite integrals remain after renormalization, as is also the case in some relativistic theories such as quantum electrodynamics.

In response to criticisms that questioned the consistency of the renormalization program,[8] and that deplored its ineffectuality in anything other than power-series expansions, (in spite of its success in quantum electrodynamics) alternative treatments of the scattering process were devised.

The particular alternative approach to scattering in field theories, which we will here concentrate on, is based on a scattering theory due to Ekstein which, succeeds in eliminating the requirement that the incident wave (and the asymptotic limit, as $t \rightarrow \pm \infty$, of the scattered wave) be an eigenfunction of an interaction free Hamiltonian H_0, or in fact of any operator at all.[9] The importance of this theory lies in the fact that, in the first place, in freeing us from the need to force the incident and asymptotic wavefunctions to be eigenfunctions of H_0, it allows us to avoid an important paradox which has far reaching consequences. In the second place, the theory enables us to derive a set of integral equations for the scattering transition amplitudes (in this case, nonlinear singular integral equations) which, though quite likely poorer in content than the linear equations[10] obtained from the traditionally invoked, older scattering theory, still allows us to obtain an iterative expansion of the scattering transition amplitude. This iterative solution exhibits the surprising feature that the divergences previously discussed completely fail to appear in this case. This feature of the theory is discussed further in succeeding sections.

II. DYNAMICS OF STATIC MODEL FIELD THEORIES

The Hamiltonian for the typical static model theory is given by $H = \mathrm{H}_0 + \mathrm{H}_1$ where H_0 and H_1, the "free field" and interaction Hamiltonians, respectively, are given by

$$\mathrm{H}_0 = \sum_{\mathbf{k},\alpha} a^\dagger_{\mathbf{k},\alpha} a_{\mathbf{k},\alpha} \omega_k + M_0 n^\dagger n \tag{1a}$$

and

$$\mathrm{H}_1 = \sum_{\mathbf{k},\alpha} (V_{\mathbf{k},\alpha} a_{\mathbf{k},\alpha} + V^\dagger_{\mathbf{k},\alpha} a^\dagger_{\mathbf{k},\alpha}). \tag{1b}$$

The boson and fermion operators obey the commutation rules $\{n, n^\dagger\} = 1$ and $[a_{\mathbf{k},\alpha}, a^\dagger_{\mathbf{k},\beta}] = \delta_{\mathbf{k}\mathbf{k}}\delta_{\alpha,\beta}$, respectively. We will here use the charge-symmetric scalar theory as an illustrative example; in that case $V_{\mathbf{k},\alpha} = gu(k)\tau_\alpha(2\omega_k)^{-\frac{1}{2}}$ where g is the so-called "bare" coupling constant and τ_α is the isospin operator. The Hamiltonian H for this problem commutes with the total isospin operator so that no reference need be made to charge states in this problem. Hence the isospin indices can be suppressed hereafter.

If we restrict our investigation to that sector of the entire space characterized by having a nucleon

[4] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950); M. Gell-Mann and M. L. Goldberger, *ibid.* **91**, 398 (1953).

[5] We will refer to the static source as the "fermion" in this paper.

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[8] G. Kallen, Kgl. Danske Videnskab. Selskab Mat.-Fys. Medd. **27**, 12 (1953); Helv. Phys. Acta **25**, 417 (1952); L. Van Hove, Physica **18**, 901 (1952); R. Haag, Kgl. Danske Videnskab. Selskab Mat.-Fys. Medd. **29**, No. 12, (1955).

[9] H. Ekstein, Phys. Rev. **101**, 880 (1956).

[10] The nonlinear equations for the Lee Model allow for spurious solutions; for example: L. Castilleyo, R. H. Dalitz, and F. J. Dyson, Phys. Rev. **101**, 453 (1956).

occupation number 1, then the spectrum of H_0 consists of a discrete nucleon state of energy M_0, and a continuum of eigenstates from $M_0 + m$ (where m is the boson mass) to infinity. Similarly the total Hamiltonian H has a spectrum consisting of a discrete state of energy M and a continuum of eigenstates from $M + m$ to infinity.

It is possible to evaluate the discrete eigenfunction of H in closed form; if we define $|N\rangle$ by $(H - M)\,|N\rangle = 0$, then $|N\rangle$ can be shown to be given by[11]

$$|N\rangle = (Z_2)^{\frac{1}{2}}[1 + (M - \mathrm{H}_0 - R\mathrm{H}_1R)^{-1}R\mathrm{H}_1]\,|N), \quad (2)$$

where $|N)$ is the eigenstate $(H_0 - M_0)|N) = 0$ and R is the projection operator that eliminates the state in which there are no bosons. Since the lowest eigenvalue of the operator $\mathrm{H}_0 + R\mathrm{H}_1R$ is higher than M, the operator in the above expression is nonsingular. A second expression for $|N\rangle$ that we also will have recourse to is[12]

$$|N\rangle = \lim_{\eta\to 0}(Z_2)^{-\frac{1}{2}}[1 + (M - H \pm i\eta)^{-1}H_1]\,|N). \quad (3)$$

In this case, unlike that of states in the continuous spectrum, the direction from which η approaches zero is immaterial. [H_1 in Eq. (3) is given by $H_1 = \mathrm{H}_1 - \delta M$ and $H_0 = \mathrm{H}_0 + \delta M$, where $\delta M = M - M_0$.]

The scattering formalism that has traditionally been applied to field theory problems is one in which the exact time-dependent wavefunctions have been forced to approach eigenfunctions of the interaction-free Hamiltonian asymptotically as $t \to \pm\,\infty$. This has resulted in the definition of a time-dependent $\psi(t)$, composed of a narrow spectral packet of spectrally pure eigenstates $\psi(E)$ such that $\psi(t) = \Sigma_E f(E, E_0)\psi(E)\exp[-iEt]$ where $f(E, E_0)$ is a narrow packet function centered about E_0. $\psi(E)$ can be represented as the zero time eigenfunction $(H - E)\psi(E) = 0$, and is given by the integral equation[4]

$$\psi^{(\pm)}(E;\eta) = \varphi(E) + (E - H_0 \pm i\eta)^{-1}H_1\psi^{(\pm)}(E;\eta) \quad (4)$$

and $\psi^{(\pm)}(E) = \lim\,(\eta \to 0)\psi^{(\pm)}(E;\eta)$; here $(\pm)$ denotes outgoing for the $(+)$ and incoming for the $(-)$ case. The equation can be formally resolved as

$$\psi^{(\pm)}(E;\eta) = \varphi(E) + (E - H \pm i\eta)^{-1}H_1\varphi(E), \quad (5)$$

and the transition amplitude is given by the "T matrix," $T^{(+)}(\beta;\alpha) = \langle\varphi_{(\beta)}|H_1|\psi^{(+)}_{(\alpha)}\rangle$ or $T^{(-)}(\beta;\alpha) = \langle\psi^{(-)}(\beta)\,|H_1|\varphi(\alpha)\rangle$ which, two, are identical on the energy shell. It can be shown that $\psi^{(\pm)}(t)$ can be explicitly constructed by a transformation,[13]

$$\psi^{(\pm)}(t) = \pm\lim_{\eta\to 0}\eta\int_0^{\pm\infty} d\tau\, e^{-\eta|\tau|}e^{-iH(t-\tau)}\varphi(\tau). \quad (6)$$

Since this transformation is a weighted sum of unitary transformations,[14] we should not be surprised if it itself is nonunitary. In the case of static model field theories, it does in fact transpire that $\psi(t)$ and $\varphi(t)$ are not unitary transforms of each other, so that $\psi(E)$ and $\varphi(E)$ are not normalized the same way.

In the scattering theory of Ekstein[9] the time-dependent wavefunction $\Psi(t)$ is also written as a narrow packet of spectrally pure states

$$\Psi(t) = \Sigma_E f(E, E_0)\Psi(E)\exp[-iEt]$$

and $\Psi(E;\eta)$ is given by

$$\Psi^{(\pm)}(E;\eta) = \Phi(E) + (E - H \pm i\eta)^{-1}\chi(E).$$

In this case, however, $\Phi(E)$ is taken as the true asymptotic wavefunction, and is not required to be a solution of the equation $(H_0 - E)\Phi(E) = 0$. In field theories, $\Phi(E)$ will be taken as the product wavefunction of one-particle solutions, $\Phi(E) = U_1(\epsilon_1)U_2(\epsilon_2)\cdots U_n(\epsilon_n)$, where $(H - \epsilon_i)U_i = 0$ and $E = \Sigma_i\epsilon_i$. In static model theories, since the bare boson already is a solution of the exact Schrödinger equation, the asymptotic states will have the form $\Phi(\mathbf{k}_1, \cdots, \mathbf{k}_n) = a^\dagger_{\mathbf{k}(1)}\cdots a^\dagger_{\mathbf{k}(n)}|N\rangle$. Time-dependent packets of these states satisfy the time-dependent equation $(H - i\partial/\partial t)\Phi(t) = 0$ *only in the limit* $t \to \pm\,\infty$, but not in general.[15] The time-independent states $\chi(E)$ in this theory are given by $(H - E)\Phi(E) = \chi(E)$. Although $\chi(E)$ reduces to $H_1\Phi(E)$ for those cases in which the asymptotic states really do satisfy the equation $(H_0 - E)\Phi(E) = 0$, (as in potential scattering from short-range potentials), this is not in general the case in field theories. For the case of boson–fermion scattering in this particular model theory the equation $(H - M - \omega_k)a^\dagger_{\mathbf{k}}\,|N\rangle = V_{\mathbf{k}}\,|N\rangle$ holds; thus $\chi_{\mathbf{k}}$ differs from $H_1a^\dagger_{\mathbf{k}}\,|N\rangle$ by much more than the absence of the "dressing" of the fermion in the latter case.

The scattering transition amplitude in this formalism is given by

$$R^{(+)}(\beta;\alpha) = \langle\chi(\beta)\,|\,\Psi^{(+)}(\alpha)\rangle \quad (9a)$$

[11] G. C. Wick, Rev. Mod. Phys. **27**, 339 (1955).
[12] B. S. DeWitt, "The Operator Formalism of Quantum Perturbation Theory," Radiation Laboratory, University of California, Berkeley, California; UCRL Report 2884 (1955), Chapter 6.
[13] M. Gell-Mann and M. L. Goldberger, Ref. 4.
[14] B. S. DeWitt, Ref. 12, p. 45.
[15] G. C. Wick, Ref. 11; H. Ekstein, Nuovo Cimento **4**, 1017 (1956).

and

$$R^{(-)}(\beta;\alpha) = \langle \Psi^{(-)}(\beta) \mid \chi(\alpha)\rangle. \tag{9b}$$

$R^{(+)}$ and $R^{(-)}$ again are identical on the energy shell, and the S matrix is given by

$$S(\beta;\alpha) = \delta_{\alpha,\beta} - 2\pi i\delta(E_\alpha - E_\beta)R(\beta;\alpha),$$

so that the R matrix plays the kinematic role that the T matrix has in the older theory.

The first question that must be answered in an attempt to understand the relation between the two alternate forms of scattering theory, is whether the wavefunctions in the "adiabatically switched" scattering theory are correct.

Criteria have been established[16] for deciding when the "adiabatic switching" Hamiltonian may legitimately replace a constant Hamiltonian and asymptotic packets of eigenstates of the interaction-free Hamiltonian. These are that the continuous parts of the spectrum of H and H_0 must overlap and that the T matrix itself must exist and have a left- and right-hand derivative on the energy shell. Since M and M_0 are not identical, the first of these conditions is not satisfied for the case of H_0 and H in Eqs. (1a) and (1b). This difficulty is however easily removed by rewriting H as

$$H = H_0 + H_1, \tag{10}$$

where

$$H_0 = \Sigma_{\mathbf{k},\alpha} a^\dagger_{\mathbf{k},\alpha} a_{k,\alpha}\omega_k + Mn^\dagger n \tag{10a}$$

and

$$H_1 = \Sigma_{\mathbf{k},\alpha}(V_{\mathbf{k},\alpha}a_{\mathbf{k},\alpha} + V^\dagger_{\mathbf{k},\alpha}a^\dagger_{\mathbf{k},\alpha}) - \delta M n^\dagger n \tag{10b}$$

and taking H_0 as the interaction-free Hamiltonian. The inclusion of the so-called self-energy correction term in H_0 and H_1 does not, however, eliminate the problem of asymptotic approach. Van Hove[17] has pointed out that, even when the self-energy corrections are included, packets of the eigenstates $\varphi(\mathbf{k}_1, \cdots, \mathbf{k}_n)$ of H_0 are not the asymptotic forms of $\psi(t)$. We will here present a simplified and somewhat modified version of Van Hove's argument:

All of the time-dependent wavefunctions can be written

$$\xi^{(\pm)}(t) = \xi_1(t) + \xi_2^{(\pm)}(t), \tag{11}$$

where

$$\xi_1(t) = \Sigma_E f(E, E_0)u(E)e^{-iEt} \tag{11a}$$

and

$$\xi_2^{(\pm)}(t) = \Sigma_E f(E, E_0)(E - H \pm i\eta)^{-1}v(E)e^{-iEt}, \tag{11b}$$

where $u(E)$ is the representation of the ostensible asymptotic state and $v(E)$ is given by $(H - E)u(E) = v(E)$. It is part of the kinematic framework of all of the scattering theories here discussed that $\lim (t \to \mp\infty)\xi_2^{(\pm)}(t) = 0$; this follows either from the externally applied "adiabatic switching" or from some simple theorems in complex analysis and assumptions about the integrability of transition matrix elements off the energy shell.[18] It is immediately apparent that $\langle \xi(t) \mid \xi(t)\rangle$ must remain a constant, in particular $\langle \xi(t) \mid \xi(t)\rangle = \langle \xi_1(t) \mid \xi_1(t)\rangle$ at all times, therefore also at $t = 0$. Hence the two inner products $\langle \varphi(E) \mid \varphi(E)\rangle$ and $\langle \psi(E) \mid \psi(E)\rangle$ must be identical; but this is not the case for static model field theories. These latter are among a class of theories that have so called "persistent effects." The transition amplitudes (even with self-energy corrections included) have the form

$$T(\mathbf{q};\mathbf{p}) = D\delta_{\mathbf{q},\mathbf{p}} + [T(\mathbf{q};\mathbf{p})]' \tag{12a}$$

or, more generally if

$$T(\mathbf{q};\mathbf{p} : \eta) = \langle \varphi(\mathbf{q}) \mid H_1 \mid \psi^{(+)}(\mathbf{p};\eta)\rangle$$

with

$$T(\mathbf{q};\mathbf{p}) = \lim (\eta \to 0)T(\mathbf{q};\mathbf{p} : \eta),$$

then

$$T(\mathbf{q};\mathbf{p} : \eta) = D(\eta)\delta_{\mathbf{q},\mathbf{p}} + [T(\mathbf{q};\mathbf{p} : \eta)]'. \tag{12b}$$

$[T(\mathbf{q};\mathbf{p} : \eta)]'$ is chosen so that $[T(\mathbf{p};\mathbf{p} : \eta]' = 0$. $D(\eta)$ is called the diagonal, $[T(\mathbf{p};\mathbf{p} : \eta)]'$ the off-diagonal part of $T(\mathbf{p};\mathbf{p} : \eta)$. When the self-energy correction is not included in the Hamiltonian, then in all but the most trivial instances,[19] the T matrix has diagonal elements (namely, the self-energy graphs). When the self-energy corrections are included, however, so that H_1 is the interaction Hamiltonian, the diagonal element D disappears, precisely because the self-energy correction subtracts all the contributions from the self-energy graphs. Let us define the inner product

$$\lambda(\mathbf{q};\mathbf{p}) = \langle \psi^{(+)}(\mathbf{q}) \mid \psi^{(+)}(\mathbf{p})\rangle$$
$$= \lim_{\epsilon\to 0}\lim_{\eta\to 0}\langle \psi^{(+)}(\mathbf{q};\epsilon) \mid \psi^{(+)}(\mathbf{p};\eta)\rangle, \tag{13}$$

which can be written

$$\lambda(\mathbf{q};\mathbf{p}) = \lim_{\epsilon\to 0}\lim_{\eta\to 0}\{(N \mid a_{\mathbf{q}} \mid \psi^{(+)}(\mathbf{p};\eta)\rangle$$
$$+\tfrac{1}{2}(N \mid a_{\mathbf{q}}H_1(E_q - H - i\epsilon)^{-1} \mid \psi^{(+)}(\mathbf{p};\eta)\rangle\}. \tag{13a}$$

[16] H. E. Moses, Nuovo Cimento 1, 103 (1955).
[17] L. Van Hove, Physica 21, 901 (1955).
[18] H. E. Moses, Ref. 16.
[19] As, for example, in N-θ scattering in the Lee Model.

From substituting for $a_q^\dagger |N\rangle$ from Eq. (5), we have that

$$(N| a_q |\psi^{(+)}(\mathbf{p};\eta)\rangle = \delta_{q,p} + \lim_{\eta\to 0} \frac{T(\mathbf{q};\mathbf{p}:\eta)}{\omega_p - \omega_q + i\eta}. \quad (14)$$

In evaluating the second term on the right-hand side of Eq. (13a), we must be careful to remember that $(H - M - \omega_p)\psi^{(+)}(\mathbf{p};\eta) \neq 0$ until after the limit $\eta \to 0$ has been reached. Therefore, if we let $\eta \to 0$ first, we have

$$\lim_{\epsilon\to 0} (N| a_q H_1 (E_q - H - i\epsilon)^{-1} |\psi^{(+)}(\mathbf{p})\rangle$$
$$= \lim_{\epsilon\to 0} (N| a_q H_1 |\psi^{(+)}(\mathbf{p})\rangle [\omega_q - \omega_p - i\epsilon]^{-1}$$
$$= \lim_{\epsilon\to 0} \frac{T^{(+)}(\mathbf{q};\mathbf{p})}{\omega_q - \omega_p - i\epsilon}. \quad (15)$$

It is easy to verify, by direct calculation that reversing the order in which the two limits are taken leaves the above result unchanged. We have, therefore, that

$$\lambda(\mathbf{q};\mathbf{p}) = \delta_{q,p}\left[1 + \lim_{\eta\to 0}\left(\frac{D(\eta) - D}{\omega_p - \omega_q + i\eta}\right)\right]$$
$$+ \lim_{\eta\to 0}\left[\frac{[T^{(+)}(\mathbf{q};\mathbf{p}:\eta)]' - [T^{(+)}(\mathbf{q};\mathbf{p})]'}{\omega_p - \omega_q - i\eta}\right]. \quad (16)$$

Since we are only concerned with the case in which $q = p$, and since $[T^{(+)}(\mathbf{p};\mathbf{p}:\eta)]' = 0$, we have that

$$\lambda(\mathbf{p};\mathbf{p}) = 1 + \lim_{\eta\to 0} \frac{D(\eta)}{i\eta}. \quad (16a)$$

The diagonal part $D(\eta)$ can be shown to be given by[20]

$$D(\eta) = i\eta(Z_2 - 1) + O(\eta^2) \quad (17)$$

and we obtain that $\lambda(\mathbf{p};\mathbf{p}) = Z_2$; therefore, the properly normalized eigenstate $\bar{\psi}(\mathbf{p})$ must be written

$$\bar{\psi}^{(\pm)}(\mathbf{p};\eta) = (Z_2)^{-\frac{1}{2}}[1$$
$$+ (M + \omega_p - H \pm i\eta)^{-1} H_1] a_p^\dagger |N\rangle, \quad (18)$$

and, since according to Eq. (2) $(Z_2)^{\frac{1}{2}} = (N|N\rangle$, we have $Z_2 < 1$. Hence $a_p^\dagger |N\rangle$ cannot be the asymptotic state for $\psi^{(+)}(\mathbf{p})$ even when the Hamiltonian already includes the self-energy correction.

III. TRANSITION AMPLITUDES IN DIFFERENT REPRESENTATIONS

A. T and R Equations

For both the T and the R matrices, integral equations can be simply derived by substituting Eqs. (4) and (7), respectively, into the expressions for T and R, and then inserting the unit operator expressed as $\mathbb{1} = \varphi_n\rangle\langle\varphi_n$ in the case of T, and $\mathbb{1} = \Psi_n\rangle\langle\Psi_n$ in the case of R. As already pointed out, this procedure, in the case of the T matrix, is the starting point of the usual Dyson–Ward method in quantum field theory, in which infinities are removed by renormalization.

In the case of the R equations, this procedure results in a set of equations, the first one of which is (the isospin indices α, β refer to bosons of momenta $\mathbf{p}$ and $\mathbf{q}$, respectively)

$$\underline{R}^{(+)}(\mathbf{q};\mathbf{p}) = -\frac{(g_p)^2 u(q)u(p)}{2\omega_q^{\frac{1}{2}}\omega_p^{\frac{1}{2}}}(\tau_\beta\tau_\alpha - \tau_\alpha\tau_\beta)$$
$$- \sum_{\mathbf{k}}\left[\frac{R^{(+)}(\mathbf{q};\mathbf{k})R^{(+)*}(\mathbf{p};\mathbf{k})}{\omega_k - \omega_q - i\eta}\right.$$
$$\left. + \frac{R^{(+)}(\mathbf{p};\mathbf{k})R^{(+)*}(\mathbf{q};\mathbf{k})}{\omega_k + \omega_q}\right]$$
$$- \sum_{n=2}^{\infty}\left[\frac{R^{(+)}(\mathbf{q};\mathbf{k}(1),\cdots\mathbf{k}(n))R^{(+)*}(\mathbf{p};\mathbf{k}(1),\cdots\mathbf{k}(n))}{\omega_{k(1)} + \cdots\omega_{k(n)} - \omega_q - i\eta}\right.$$
$$\left. + \frac{R^{(+)}(\mathbf{p};\mathbf{k}(1),\cdots\mathbf{k}(n))R^{(+)*}(\mathbf{q};\mathbf{k}(1),\cdots\mathbf{k}(n))}{\omega_{k(1)} + \cdots\omega_{k(n)} + \omega_q}\right]. \quad (19)$$

Here $R^{(+)}(\mathbf{p};\mathbf{k}(1),\cdots\mathbf{k}(n))$ with $n > 1$ refers to inelastic production processes, and g_p is the "dressed" or renormalized coupling constant. The complete set of these equations is easily generated and the resulting equations are readily recognized as the Chew–Low equations.

An earlier form of these equations were obtained by Low[21] in a derivation that took, as its point of departure, the S matrix in the conventional formulation of field theory. Since it is an S-matrix element that is treated in this work, the T-matrix element that is expanded is restricted to the energy shell, though the integral equation that is derived involves similar T-matrix elements off the energy shell. It is to be noted in this connection that the T and R matrices are not simply related off the energy shell; it will be apparent that, because of the difference between the behavior of the T and R matrix elements off the energy shell, the T-matrix, in its spectral representation, is not directly iterable in terms of dressed particle parameters as is the R-matrix.

It was shown by one of us[22] that when the integral equations (19) are iterative the following results are obtained: (1) the iterative integrals are all finite and involve "dressed" particle parameters only; (2)

[20] B. S. DeWitt, Ref. 12, Chap. 10.

[21] F. E. Low, Phys. Rev. 97, 1392 (1955).

[22] K. Haller, Phys. Rev. 120, 1045 (1960).

up to sixth order, all iterated terms agree with the results of renormalizing the matrix elements corresponding to the appropriate Feynman diagram; (3) wavefunction renormalization diagrams never appear when a diagrammatic analysis is made of the iteration series, though all other types of diagrams can be located in these expressions.

When judged from the point of view of the very different behavior of the asymptotic states in the two scattering theories and from the inconsistencies in the application of the "adiabatic switching" formalism to this problem, the identity of these two results is quite remarkable. It is no less of interest that the fact that the R-matrix theory is free of any unphysical parameters, and along with them of divergent integrals, stems from the use of the proper asymptotic states. In the succeeding portions of this paper, we provide a general proof of this identity, which was previously demonstrated up to sixth order. We also examine the origin of the connection between the appearance of infinities and the use of improper representations of the asymptotic states.

B. Identity of the Exact Wavefunction in the Bare-Particle and Dressed-Particle Representations

It is possible to demonstrate that the properly normalized Gell-Mann–Goldberger wavefunction,[23] $\psi^{(\pm)}(\mathbf{p})$, and the Ekstein wavefunction, $\Psi(\mathbf{p})$, are identical for the one-fermion, n-boson case. It was previously demonstrated that $(Z_2)^{-\frac{1}{2}}$ is the proper normalization for $\psi^{(\pm)}(\mathbf{p})$.

The normalized GG wavefunction for the one-boson case is given by Eq. (18). Use of the identity[22]

$$(E - H \pm i\eta)^{-1}a_p^\dagger = a_p^\dagger(E - H - \omega_p \pm i\eta)^{-1} + (E - H \pm i\eta)^{-1}V_p(E - H - \omega_p \pm i\eta)^{-1} \quad (20)$$

leads to

$$\psi^{(\pm)}(\mathbf{p}) = [a_p^\dagger + (M + \omega_p - H \pm i\eta)^{-1}V_p] \times \{(Z_2)^{-\frac{1}{2}}[1 + (M - H \pm i\eta)^{-1}H_1]\,|N\rangle\}, \quad (21)$$

which, upon identification of the curly-bracketted term as the physical fermion $|N\rangle$ (Eq. 3) leads to the result

$$\psi^{(\pm)}(\mathbf{p}) = \Psi^{(\pm)}(\mathbf{p}). \quad (22)$$

A straightforward generalization of this argument in the appendix extends this proof to the n-particle case.

The identity of these two wavefunctions at zero time stands in marked contrast to the asymptotic behavior of the GG wavefunction $\psi(t)$ and the Ekstein wavefunction $\Psi(t)$ in the limit $t \to \pm\infty$. It must be recalled in this connection, that neither in the Ekstein nor the adiabatic switching theory are the asymptotic states calculated from the dynamics of the theory; instead, as in the so-called "axiomatic" treatments of field theory,[24] the asymptotic behavior of wavefunctions is postulated. The situation can be quickly summarized by remarking that

$$[\xi_1(0)]_{G\text{-}G} + [\xi_2^{(\pm)}(0)]_{G\text{-}G} = [\xi_1(0)]_E + [\xi_2^{(\pm)}(0)]_E,$$

but

$$[\xi_1(0)]_{G\text{-}G} \neq [\xi_1(0)]_E \quad \text{and} \quad [\xi_2^{(\pm)}(0)]_{G\text{-}G} \neq [\xi_2^{(\pm)}(0)]_E;$$

it is therefore not the wavefunction $\psi(\mathbf{p})$ that is wrong, but rather the naïve surmise, $\lim [t \to \pm\infty]$ $[\xi_2^{(\pm)}(t)]_{G\text{-}G} = 0$, that is in error. It is, of course, only $\xi^{(\pm)}(0)$ itself that appears in the transition amplitude (in either theory).

C. Identity of Normalized Transition Amplitudes on the Energy Shell

The T-matrix element for the fermion–boson scattering process

$$\text{fermion} + (\text{boson})_p \to \text{fermion} + (\text{boson})_q$$

is given by

$$T^{(+)}(\mathbf{q};\mathbf{p}) = \langle\varphi_{(q)}\,|H_1|\,\psi^{(+)}(\mathbf{p})\rangle. \quad (23)$$

If we define a "normalized transition amplitude", $\bar{T}(\mathbf{q};\mathbf{p}) = (Z_2)^{-1}T(\mathbf{q};\mathbf{p})$, then we can show that, on the energy shell $\bar{T}(\mathbf{q};\mathbf{p}) = R(\mathbf{q};\mathbf{p})$.

If we make use of the identity proven in the previous section, we can write

$$\bar{T}^{(+)}(\mathbf{q};\mathbf{p}) = (Z_2)^{-\frac{1}{2}}[(N|\,a_qH_1a_p^\dagger\,|N\rangle + (N|\,a_qH_1(M + \omega_p - H - i\eta)^{-1}V_p\,|N\rangle]. \quad (24)$$

We have that

$$(N|\,a_qH_1a_p^\dagger\,|N\rangle = \delta_{q,p}(N|\,H_1\,|N\rangle + (N|\,V_p(H - M + \omega_p)^{-1}V_q^\dagger\,|N\rangle$$

and

$$(N|\,a_qH_1(M + \omega_p - H - i\eta)^{-1}V_p\,|N\rangle = (N|\,V_q^\dagger(M + \omega_p - H - i\eta)^{-1}V_p\,|N\rangle + (N|\,H_1a_q(M + \omega_p - H - i\eta)^{-1}V_p\,|N\rangle.$$

[23] We will henceforth abbreviate Gell-Mann–Goldberger as GG.

[24] See, for example, H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo Cimento 1, 1425 (1955); 2, 425 (1955); and 6, 319 (1957).

Applying Eq. (21) we have that

$$(N|\, H_1 a_q(M + \omega_p - H - i\eta)^{-1} V_p \,|N\rangle$$
$$= -(N|\, H_1(M + \omega_p - \omega_q - H - i\eta)^{-1}$$
$$\times V_p(H + \omega_q - M)^{-1} V_q^\dagger \,|N\rangle$$
$$- (N|\, H_1(M + \omega_p - \omega_q - H - i\eta)^{-1}$$
$$\times V_q^\dagger(H - \omega_p - M - i\eta)^{-1} V_p \,|N\rangle.$$

Therefore, the normalized T-matrix element is given by

$$\bar{T}^{(+)}(\mathbf{q};\mathbf{p}) = (Z_2)^{-\frac{1}{2}}$$
$$\times [(N|\, \{1 + H_1(M + \omega_p - \omega_q - H - i\eta)^{-1}\}$$
$$\times \{V_q^\dagger[M + \omega_p - H - i\eta]^{-1} V_p$$
$$+ V_p[M + H + \omega_q]^{-1} V_q^\dagger\} \,|N\rangle]. \qquad (25)$$

Comparing with Eq. (3) we observe that for $\omega_q = \omega_p$

$$\bar{T}^{(+)}(\mathbf{q},\mathbf{p}) = \{\langle N|\, V_q^\dagger[M + \omega_p - H - i\eta]^{-1} V_p \,|N\rangle$$
$$- \langle N|\, V_p[M + H + \omega_q]^{-1} V_q^\dagger \,|N\rangle\}, \qquad (26)$$

and, therefore, $\bar{T}^{(+)}(\mathbf{q};\mathbf{p}) = R^{(+)}(\mathbf{q};\mathbf{p})$. Moreover, the expansion parameter of $R(\mathbf{q};\mathbf{p})$ is $g_\rho = g\langle N'|\, \tau_\alpha \,|N\rangle/(N'|\, \tau_\alpha \,|N)$, the physical coupling constant, and the latter is given by $g_\rho = g(Z_2/Z_1)$ and is identical to the renormalized coupling constant.[25] The iterative series expansion of $R(\mathbf{q};\mathbf{p})$ and the renormalized series for $\bar{T}(\mathbf{q};\mathbf{p})$ therefore are shown to be expansions of the same quantity in terms of identical parameters, and must be equal within their radius of convergence. It is noteworthy that the appearance of $\bar{T}(\mathbf{q};\mathbf{p})$ instead of $T(\mathbf{q};\mathbf{p})$ in these formulas accounts for the absence of wavefunction renormalization graphs in the expansion of $R(\mathbf{q};\mathbf{p})$.

In the adiabatic switching theory, after the expressions corresponding to their respective Feynman diagrams are renormalized, there is an over-all factor of $(Z_2)^{-1}$ that appears in $T(\mathbf{q};\mathbf{p})$, multiplied by an expression that consists of "renormalized" quantities only. This factor of $(Z_2)^{-1}$ is accounted for by wavefunction renormalization and $(Z_2)^{\frac{1}{2}}$ is associated with each of the external fermion lines, though, properly speaking, on external self-energy correction should provide a factor of Z_2 for each external line.[26] This is the only feature of the traditional renormalization program in which the normalization of anything is changed, and which can not be described as a rearrangement of terms in a series that represents the same quantity. We see here that the additional factor $(Z_2)^{-1}$ can be taken out at the start, that its appearance in $T(\mathbf{q};\mathbf{p})$ stems in part from an erroneous normalization of the GG wavefunction and in part from a misidentification of the asymptotic scattering state; and, that it is $\bar{T}(\mathbf{q};\mathbf{p})$ and *not* $T(\mathbf{q};\mathbf{p})$ that is identical to $R(\mathbf{q};\mathbf{p})$ on the energy shell.[27]

Equation (25) also shows us how $\bar{T}(\mathbf{q};\mathbf{p})$ differs from $R(\mathbf{q};\mathbf{p})$ off the energy shell: When ω_p and ω_q are not identical, the wavefunction $(Z_2)^{-\frac{1}{2}}[1 + (M + \omega_p - \omega_q - H - i\eta)^{-1} H_1] \,|N)$ is not identifiable either as an eigenstate or an asymptotic state in the Ekstein theory; even if one were to insert $\mathbb{1} = \Psi_n\rangle\langle\Psi_n$ into the right-hand side of Eq. (25) with $\omega_p \neq \omega_q$, the resulting integral equations could not be iterated exclusively in terms of physical coupling constants, and infinite integrals would continue to appear. It is only when all the states that appear in matrix elements are eigenfunctions of H or products of eigenfunctions of H that the absence of bare coupling constants and infinite integrals in the theory can be guaranteed.

If one is satisfied to abandon the study of the T-matrix element off the energy shell a quite simple proof of the identity $\bar{T}(\mathbf{q};\mathbf{p}) = R(\mathbf{q};\mathbf{p})$ can be given. If α, β denote two n-boson states, then

$$(Z_2)^{-1}\langle\psi_\beta^{(-)} \mid \psi_\alpha^{(+)}\rangle = \delta_{\alpha,\beta} - 2\pi i\delta(E_\alpha - E_\beta)\bar{T}(\beta;\alpha)$$

and

$$\langle\Psi_\beta^{(-)} \mid \Psi_\alpha^{(-)}\rangle = \delta_{\alpha,\beta} - 2\pi i\delta(E_\alpha - E_\beta)R(\beta;\alpha);$$

then the identity of $\bar{T}(\beta;\alpha)$ and $R(\beta;\alpha)$ on the energy shell follows from Eq. (23).

D. The Mixed Representations for T and R

Although, as was pointed out in the previous section, there is no spectral representation for the T matrix in which the iteration primitively proceeds in terms of the dressed-particle parameters, there is a so-called "mixed" representation, in which the T and R matrices appear jointly, and in which all other inhomogeneous terms are given in terms of

[25] G. F. Chew, Phys. Rev. **93**, 341 (1954); G. C. Wick, Ref. 11.

[26] B. S. DeWitt, Ref. 12, Chap. 10, especially Eqs. (10.86)–(10.94).

[27] It has, sometimes, mistakenly been supposed that it is $T(\mathbf{q};\mathbf{p})$ and not $\bar{T}(\mathbf{q};\mathbf{p})$ that is identical to $R(\mathbf{q};\mathbf{p})$ [see for example, N. Fukuda and S. Kovacs, Phys. Rev. **104**, 1784, (1956)]. This surmise was based upon the belief that the Møller scattering operator can be used as a "dressing" operator to convert normalized bare to normalized physical particle eigenstates, and that this operator is unitary at least where there are no bound states. As has been pointed out (see for example, B. S. DeWitt, Ref. 12, Chap. 5, especially p. 45 and 48), this belief is in error by an important normalization constant, which just accounts for the difference between the $\bar{T}$ and the T operators.

dressed-particle parameters. This representation is obtained by making the substitution indicated in Eq. (23) both in Eq. (9a) and in the equation for the T matrix. The resulting equations are

$$R^{(+)}(\mathbf{q};\mathbf{p}) = (Z_2)^{-\frac{1}{2}}[\langle\chi(\mathbf{q}) \mid \varphi(\mathbf{p})\rangle + \langle\chi(\mathbf{q})\mid (\omega_p - H + i\eta)^{-1}H_1 \mid\varphi(\mathbf{p})\rangle \tag{27a}$$

and

$$\bar{T}^{(+)}(\mathbf{q};\mathbf{p}) = (Z_2)^{-\frac{1}{2}}[\langle\varphi(\mathbf{q})\mid H_1 \mid\Phi(\mathbf{p})\rangle + \langle\varphi(\mathbf{q})\mid H_1(\omega_p - H + i\eta)^{-1} \mid\chi(\mathbf{p})\rangle]. \tag{27b}$$

When the cloture relation is inserted into these equations, then, with the help of the previously cited identities we obtain

$$\bar{T}^{(+)}(\mathbf{q};\mathbf{p}) = R^{(+)*}(\mathbf{p};\mathbf{q}) - g_\rho \frac{(\omega_p - \omega_q)(N\mid a_\mathbf{q}\mid N)u(p)\tau_\alpha}{(Z_2)^{\frac{1}{2}}\omega_p^{\frac{1}{2}}\sqrt{2}}$$
$$+ (\omega_p - \omega_q)\sum_n \frac{\bar{T}^{(+)}(\mathbf{q};\mathbf{k}(1),\cdots\mathbf{k}(n))R^{(+)*}(\mathbf{p};\mathbf{k}(1),\cdots\mathbf{k}(n))}{(\omega_p - \omega_{k(1)} - \cdots - \omega_{k(n)} + i\eta)(\omega_q - \omega_{k(1)} + \cdots - \omega_{k(n)} - i\eta)}. \tag{28}$$

It remains now only to evaluate the expression $(Z_2)^{-\frac{1}{2}}(N\mid a_a \mid N\rangle$. From Eq. (2) we have that

$$(Z_2)^{-\frac{1}{2}}(N\mid a_\mathbf{q}\mid N\rangle = (N\mid (M - \omega_q - H)^{-1}V_\mathbf{q}^\dagger \mid N) + (N\mid (M - \omega_q - H)^{-1}$$
$$\times V_\mathbf{q}^\dagger(M - H_0 - RH_1R)^{-1}RH_1 \mid N). \tag{29}$$

Diagrammatic representation of the series expansion of these terms shows that

$$(Z_2)^{-\frac{1}{2}}(N\mid a_\mathbf{q}\mid N\rangle = [gu(q)\tau_\beta/(2\omega_q)^{-\frac{1}{2}}S(-\omega_q)\Gamma^e(0;-\omega_q), \tag{30}$$

where $S(E)$ is the self-energy part and $\Gamma^e(E, E')$ the external vertex part.[25] Substituting the renormalized, finite expressions

$$[\Gamma^e(E,E')]_r = Z_1\Gamma^e(E,E'),$$
$$[S(E)]_r = (Z_2)^{-1}S(E),$$

and

$$g_\rho = Z_2(Z_1)^{-1}g,$$

we obtain

$$\bar{T}^{(+)}(\mathbf{q};\mathbf{p}) = R^{(+)*}(\mathbf{p};\mathbf{q}) + g_\rho^2\frac{u(q)u(p)\tau_\beta\tau_\alpha}{2(\omega_q\omega_p)^{\frac{1}{2}}}(\omega_p - \omega_q)[S(-\omega_q)]_r[\Gamma^e(0,-\omega_p)]_r$$
$$- (\omega_p - \omega_q)\sum_n \frac{\bar{T}^{(+)}(\mathbf{q};\mathbf{k}(1),\cdots\mathbf{k}(n))R^{(+)*}(\mathbf{p};\mathbf{k}(1),\cdots\mathbf{k}(n))}{(\omega_p - \omega_{k(1)} - \cdots - \omega_{k(n)} + i\eta)(\omega_q - \omega_{k(1)} - \cdots - \omega_{k(n)} + i\eta)}. \tag{31}$$

This equation can be directly iterated for $\bar{T}$ in terms of R, if we assume the series for $R(\mathbf{p};\mathbf{q})$ known from the iteration of Eq. (19). Thus we get, for example,

$$[\bar{T}^{(+)}(\mathbf{q};\mathbf{p})]^{(2)} = \frac{g_\rho^2u(q)u(p)}{2(\omega_p\omega_q)^{\frac{1}{2}}}\left(\frac{\tau_\beta\tau_\alpha}{\omega_p} - \frac{\tau_\alpha\tau_\beta}{\omega_q}\right) \tag{32a}$$

and

$$[\bar{T}^{(+)}(\mathbf{q};\mathbf{p})]^{(4)} = \frac{g_\rho^4u(q)u(p)}{(2\pi^2)2(\omega_p\omega_q)^{\frac{1}{2}}}\int_0^\infty \frac{u^2(k)k^2\,dk}{\omega_k^3(\omega_q + \omega_k)(\omega_p - \omega_k + i\eta)(\omega_p - \omega_q - \omega_k + i\eta)}$$
$$\times [\tau_\beta\tau_\alpha F(\omega_q;\omega_p;\omega_k) - \tau_\alpha\tau_\beta F(\omega_p;\omega_q;\omega_k)], \tag{32b}$$

where

$$F(\omega_q;\omega_p;\omega_k) = (\omega_p)^{-1}[4\omega_p^2\omega_q - 4\omega_p\omega_q^2 + 2\omega_q^2\omega_k + 5\omega_p^2\omega_k + 2\omega_q\omega_k^2 - 6\omega_p\omega_k^2 - 9\omega_p\omega_q\omega_k].$$

It is immediately apparent from these expressions that to these orders, although the $\bar{T}$ and the R matrices agree on the energy shell, they differ everywhere off the energy shell.

IV. BOSON BREMSSTRAHLUNG AND OTHER RADIATIVE PROCESSES

In view of the result that the T and R matrices are identical on the energy shell but differ everywhere else, it is of interest to study the case of such inelastic processes, as, for example, boson bremstrahlung

$$\pi_\kappa + N \rightarrow \pi_p + \gamma_q + N.$$

In this case, a Hamiltonian H_{em} provides a two-meson–photon vertex, and each of the two mesons interact with the static fermion. The latter interaction is typically much stronger than the former. H_{em} is given by

$$H_{em} = e \sum_{\mathbf{q},\varepsilon(\mathbf{q})=1,2} [\mathcal{K}_{\mathbf{q},\varepsilon(\mathbf{q})}\alpha_{\mathbf{q},\varepsilon(\mathbf{q})} + \mathcal{K}^{\dagger}_{\mathbf{q},\varepsilon(\mathbf{q})}\alpha^{\dagger}_{\mathbf{q},\varepsilon(\mathbf{q})}] \quad (33)$$

with

$$\mathcal{K}_{\mathbf{q},\varepsilon(\mathbf{q})} = 2i \sum_{\mathbf{k}} \frac{\boldsymbol{\epsilon}(\mathbf{q})\cdot\mathbf{k}}{(8q\omega_k\omega_{|\mathbf{q}-\mathbf{k}|})^{\frac{1}{2}}} [a^{\dagger}_{\mathbf{k},1}a^{\dagger}_{\mathbf{q}-\mathbf{k},2} + a^{\dagger}_{\mathbf{k},1}a_{\mathbf{k}-\mathbf{q},2} + a_{-\mathbf{k},1}a^{\dagger}_{\mathbf{q}-\mathbf{k},2} + a_{-\mathbf{k},1}a_{\mathbf{k}-\mathbf{q},2}],$$

where $\alpha_{\mathbf{q},\varepsilon(\mathbf{q})}$, $\alpha^{\dagger}_{\mathbf{q},\varepsilon(\mathbf{q})}$ are the photon operators, and $\boldsymbol{\varepsilon}(\mathbf{q})$ is the photon polarization vector.

A typical diagram in such a process is one in which a meson of momentum $\boldsymbol{\kappa}$ is absorbed, a meson of momentum $(\mathbf{p}+\mathbf{q})$ is scattered, and subsequently dissociates into a meson of momentum $\mathbf{p}$ and a photon of momentum $\mathbf{q}$. Since on the energy shell for this reaction we have $\omega_\kappa = \omega_p + q$, we might expect the matrix element for this process to depend on the R matrix, $R^{(-)}(\kappa, \mathbf{p}+\mathbf{q})$, where the energy $\omega_\kappa \neq \omega_{|\mathbf{p}+\mathbf{q}|}$. We might therefore be led to think that for this case the choice of the asymptotic states $\varphi(\mathbf{p})$ and $\varphi(\mathbf{q})$ of Eq. (4) might not be as benign an inconsistency as it was shown to be in the previous sections for the case of purely mesonic processes.

The fact however is, that although the matrix element $\mathfrak{M}(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q})$ for meson bremsstrahlung is dependent upon off-the-energy-shell R-matrix elements, there is nevertheless still agreement between calculations carried out with the correct meson–fermion asymptotic states, and with those states shown by Van Hove to lead to an inconsistent theory. This result is not, in fact limited to the bremsstrahlung process, nor even to any very particular form of the Hamiltonian; we will, however, use this process as an illustrative example which will be seen to be easily generalizable.

Let us define the Hamiltonian

$$H_T = H + H_\gamma + H_{em}, \quad (34)$$

where

$$H_\gamma = \sum_{\mathbf{k},\varepsilon(\mathbf{k})} \alpha^{\dagger}_{\mathbf{k},\varepsilon}\alpha_{\mathbf{k},\varepsilon}k.$$

Then let us define $\tilde{\chi}(\boldsymbol{\kappa})$ and $\tilde{\chi}(\mathbf{p}, \mathbf{q})$ for the asymptotic states $a^{\dagger}_{\kappa}|N\rangle$ and $\alpha^{\dagger}_{\mathbf{q}}a^{\dagger}_{\mathbf{p}}|N\rangle$, respectively, as

$$\tilde{\chi}(\boldsymbol{\kappa}) = (H_T - \omega_\kappa - M)a^{\dagger}_{\kappa}|N\rangle \quad (35)$$

$$\tilde{\chi}(\mathbf{p}, \mathbf{q}) = (H_T - \omega_p - q - M)\alpha^{\dagger}_{\mathbf{q}}a^{\dagger}_{\mathbf{p}}|N\rangle.$$

These equations lead to

$$\tilde{\chi}(\boldsymbol{\kappa}) = V_\kappa|N\rangle + H_{em}a^{\dagger}_{\kappa}|N\rangle \quad (36)$$

and

$$\tilde{\chi}(\mathbf{p}, \mathbf{q}) = V_p\alpha^{\dagger}_{\mathbf{q}}|N\rangle + H_{em}a^{\dagger}_{p}\alpha^{\dagger}_{\mathbf{q}}|N\rangle.$$

We can now write the bremsstrahlung transition amplitude

$$\mathfrak{M}(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = \langle\tilde{\Psi}^{(-)}(\mathbf{p}, \mathbf{q})|\tilde{\chi}(\boldsymbol{\kappa})\rangle \quad (37)$$

with

$$\tilde{\Psi}^{(-)}(\mathbf{p}, \mathbf{q}) = a^{\dagger}_{p}\alpha^{\dagger}_{\mathbf{q}}|N\rangle + (M + \omega_p + q - H_T - i\eta)^{-1}\tilde{\chi}(\mathbf{p}, \mathbf{q}). \quad (37a)$$

If we eliminate all terms higher than first order in H_{em}, and if we make use of $\alpha_{\mathbf{q}}(C - H_\gamma)^{-1} = (C - q - H_\gamma)^{-1}\alpha_{\mathbf{q}}$, then we can write

$$\begin{aligned}\mathfrak{M}^1(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) &= \langle N|\, a_p\alpha_{\mathbf{q}}H_{em}a^{\dagger}_{\kappa}|N\rangle \\ &+ \langle N|\, V^{\dagger}_{p}(M + \omega_p - H + i\eta)^{-1}\alpha_{\mathbf{q}}H_{em} \\ &\times (M + \omega_\kappa - H + i\eta)^{-1}V_\kappa|N\rangle \\ &+ \langle N|\, a_p\alpha_{\mathbf{q}}H_{em}(M + \omega_\kappa - H + i\eta)^{-1}V_\kappa|N\rangle \\ &+ \langle N|\, V^{\dagger}_{p}(M + \omega_p - H + i\eta)^{-1}\alpha_{\mathbf{q}}H_{em}a^{\dagger}_{\kappa}|N\rangle, \end{aligned} \quad (38)$$

where the energy denominators operate to the left when to the left of $\alpha_{\mathbf{q}}$, and to the right when to the right of $\alpha_{\mathbf{q}}$. The first and fourth term on the right-hand side can be combined to form

$$M^1_A(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = \langle\Psi^{(-)}(\mathbf{p})|\, \alpha_{\mathbf{q}}H_{em}a^{\dagger}_{\kappa}|N\rangle$$

and the second and third terms form

$$\mathfrak{M}^1_B(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = \langle\Psi^{(-)}(\mathbf{p})|\, \alpha_{\mathbf{q}}H_{em}(M + \omega_k - H + i\eta)^{-1}V_\kappa|N\rangle,$$

so that we have

$$\mathfrak{M}^1(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = \langle\Psi^{(-)}(\mathbf{p})|\, \alpha_{\mathbf{q}}H_{em}|\Psi^{(+)}(\boldsymbol{\kappa})\rangle. \quad (39)$$

This can be rewritten as

$$\mathfrak{M}^1(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = \langle\Psi^{(-)}(\mathbf{p})|\, \mathcal{K}^{\dagger}_{\mathbf{q}}|\Psi^{(+)}(\boldsymbol{\kappa})\rangle. \quad (40)$$

Equation (23) allows us to rewrite Eq. (40) using GG wavefunctions

$$\mathfrak{M}^1(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = (Z_2)^{-1}\langle\psi^{(-)}(\mathbf{p})|\, \mathcal{K}^{\dagger}_{\mathbf{q}}|\psi^{(+)}(\boldsymbol{\kappa})\rangle \quad (41)$$

and, it can easily be shown[28] that this is equivalent to the first-order term, in H_{em}, of

$$\mathfrak{M}_{G\text{-}G}(\boldsymbol{\kappa}; \mathbf{p}, \mathbf{q}) = (Z_2)^{-1} \times \langle\varphi(\mathbf{p}, \mathbf{q})|\, (H_1 + H_{em})|\xi^{(+)}(\boldsymbol{\kappa})\rangle \quad (42)$$

[28] M. L. Goldberger and K. M. Watson, *Collision Theory*, (John Wiley & Sons, Inc., New York, 1964), Sec. 5.4.

where $\zeta^{(+)}(\kappa)$ is given by

$$\zeta^{(+)}(\kappa) = \varphi(\kappa) + (M + \omega_\kappa - H_0 - H_\gamma + i\eta)^{-1} \times (H_1 + H_{\rm em})\zeta^{(+)}(\kappa). \quad (43)$$

Equation (43) is the starting point of the traditional field-theoretic approach to this problem, which terminates in the Feynman diagrammatic analysis and rules, and the Dyson–Ward renormalization program, with the exception that as in the scattering problem, the wavefunction renormalization is included in the formulation used in this paper.

We see from the aforegoing that the equality of the Ekstein and the properly normalized GG wavefunctions is sufficient to allow us to substitute the improper "bare-particle" asymptotic states for the correct ones, even in the case of a "weak interaction" that is modified by a strong one, considered to all orders. In spite of this substitution we are led to correct, though unrenormalized, results by the iterative expansion of the resulting transition amplitude.

If we wish to examine the meson bremsstrahlung process to lowest order in e and g_ρ^2, we observe that Eq. (40) can be written

$$\mathfrak{M}^1(\kappa; \mathbf{p}, \mathbf{q}) = \sum_{\kappa,n} \frac{2ie\boldsymbol{\varepsilon}(\mathbf{q})\cdot\mathbf{k}}{(8q\omega_k\omega_{|\mathbf{q}-\mathbf{k}|})^{\frac{1}{2}}} \times \langle\Psi^{(-)}(\mathbf{p})|\,(a_{\mathbf{k},1} + a^\dagger_{-\mathbf{k},1})\,|\Psi_n\rangle \times \langle\Psi_n|\,(a_{\mathbf{q}-\mathbf{k},2} + a^\dagger_{\mathbf{k}-\mathbf{q},2})\,|\Psi^{(+)}(\kappa)\rangle, \quad (40a)$$

where Σn indicates a summation over a complete set of eigenstates of H. If we want $\mathfrak{M}^1(\kappa; \mathbf{p}, \mathbf{q})$ to order g_ρ^2 only, it is easy to see that for $\omega_\kappa = \omega_p + q$ only the dressed-nucleon state contributes to the summation. Thus, using some well-known identities, we have to this order

$$[\mathfrak{M}^1(\kappa; \mathbf{p}, \mathbf{q})]_{(2)} = 2ie \times \left[\frac{2\omega_{|\mathbf{q}+\mathbf{p}|}}{(\omega^2_{|\mathbf{q}+\mathbf{p}|} - \omega^2_\kappa)} R^{(+)}(\mathbf{q}+\mathbf{p}; \kappa) \frac{\boldsymbol{\varepsilon}(\mathbf{q})\cdot\mathbf{p}}{(8q\omega_{|\mathbf{q}+\mathbf{p}|}\omega_p)^{\frac{1}{2}}} - \frac{2\omega_{|\mathbf{q}-\kappa|}}{(\omega_p^2 - \omega^2_{|\mathbf{q}-\kappa|})} R^{(-)}(\mathbf{p}; \kappa - \mathbf{q}) \frac{\boldsymbol{\varepsilon}(\mathbf{q})\cdot\kappa}{(8q\omega_{|\mathbf{q}-\kappa|}\omega_\kappa)^{\frac{1}{2}}}\right]. \quad (40b)$$

If we write the R matrices to second order, in the "physical" coupling constant g_ρ, we have

$$[\mathfrak{M}^1(\kappa; \mathbf{p}, \mathbf{q})]_{(2)} = -2ieg_\rho^2\Bigg\{\frac{\boldsymbol{\varepsilon}(\mathbf{q})\cdot\kappa u(q)u(\mathbf{q}-\kappa)}{(8q\omega_\kappa)^{\frac{1}{2}}\omega_p^{\frac{1}{2}}} \times \left[\frac{(\tau_2\tau_\alpha\delta_{\nu,1} - \tau_1\tau_\alpha\delta_{\nu,2}) + (\tau_\alpha\tau_1\delta_{\nu,2} - \tau_\alpha\tau_2\delta_{\nu,1})}{p_\mu p_\mu - (q-\kappa)_\mu(q-\kappa)_\mu}\right] - \frac{\boldsymbol{\varepsilon}(\mathbf{q})\cdot\mathbf{p}u(\mathbf{q}+\mathbf{p})u(\kappa)}{(8q\omega_p)^{\frac{1}{2}}\omega_\kappa^{\frac{1}{2}}} \times \left[\frac{(\tau_1\tau_\nu - \tau_\nu\tau_1)\delta_{\alpha,2} - (\tau_2\tau_\nu - \tau_\nu\tau_2)\delta_{\alpha,1}}{\kappa_\mu\kappa_\mu - (q+p)_\mu(q+p)_\mu}\right]\Bigg\}; \quad (40c)$$

here, α, ν refer to isospin indices of bosons of momenta p and κ, respectively. $k_\mu k_\mu$ is the four-dimensional inner product taken on the mass shell. Equation (40b) demonstrates explicitly the appearance of off-the-energy-shell matrix elements of $R^{(-)}$ and $R^{(+)}$. If we evaluate the transition amplitude for this process by adding the expressions for the Feynman diagrams in Fig. 1, we see that we obtain the same expression as in Eq. (40c).

It is, however, equally clear that this process provides us with an important example of the difference between the R matrix and the T matrix for the elastic scattering process. If we had incorrectly believed that T and R were the same everywhere, on and off the energy shell, and if we had used the T-matrix elements from Eq. (32a) in Eq. (40b), then we would have obtained the wrong expression for $\mathfrak{M}^1(\kappa; \mathbf{p}, \mathbf{q})$.

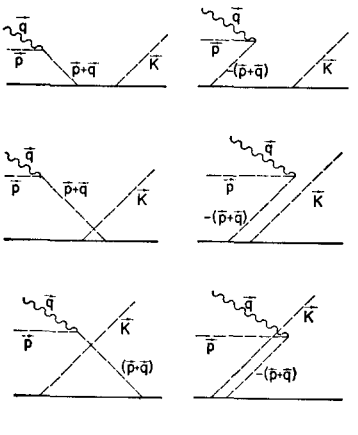

FIG. 1. Feyman diagrams for boson bremsstrahlung in the charge-symmetric scalar static-source theory. The diagrams include all process in the lowest order of the electric charge and the second order of the boson–fermion coupling constant; however, processes in which the boson–photon vertex is located on the incident boson line are not shown. The solid line represents the fermion, the dashed line the boson, and the wavy line the photon.

APPENDIX: EQUALITY OF THE PROPERLY NORMALIZED GELL-MANN–GOLDBERGER STATE WITH THE EKSTEIN STATE, FOR n MESONS

We first condense our notation so that scattering eigenstates with one nucleon, and r mesons of momenta $\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_r$, and isotopic spin indices $\alpha_1, \alpha_{(2)} \cdots, \alpha_r$, are denoted by $|\psi_r^{(\pm)}\rangle$ for the Gell-Mann–Goldberger states, and by $|\Psi_r^{(\pm)}\rangle$ for the Ekstein state. We will define a_i to mean the operator $a_{\mathbf{p}(i),\alpha(i)}$. The energy E_r is defined as

$$E_r = M + \omega_{p(1)} + \cdots + \omega_{p(r)}. \quad (A1)$$

The proof of equality is inductive and begins with the demonstration in Sec. III B, of the equality of the normalized GG state, with the Ekstein state, for one meson. We then compare the GG state with r mesons, to that with $(r+1)$ mesons, and simultaneously compare the Ekstein state with r mesons

to that with $(r+1)$ mesons. These states are given explicitly in our condensed notation by

$$\bar{\psi}_r^{(\pm)} = (Z_2)^{-\frac{1}{2}}(r!)^{-\frac{1}{2}} \times [1 + (E_r - H \pm i\eta)^{-1}H_1]\Pi_{i=1,r}a_i^\dagger |N) \quad \text{(A2a)}$$

$$\Psi_r^{(\pm)} = (r!)^{-\frac{1}{2}} \times [1 + (E_r - H \pm i\eta)^{-1}(H - E_r)]\Pi_{i=1,r}a_i^\dagger |N\rangle \quad \text{(A2b)}$$

and corresponding equations for $\bar{\psi}_{r+1}^{(\pm)}$, $\Psi_{r+1}^{(\pm)}$.

In the case of these latter, we commute the meson operator $a_{r+1}^\dagger$ through to the left of the operators $(E_{r+1} - H \pm i\eta)^{-1}H_1$, $(E_{r+1} - H \pm i\eta)^{-1}(E_{r+1} - H)$, by using the commutation properties of $a^\dagger$ with H and with $(E - H)^{-1}$, and the identity Eq. (21). By regrouping terms in the results and by comparing these results with Eqs. (A2a) and (A2b), we obtain identical recursion relations between $\bar{\psi}_{r+1}^{(\pm)}$ and $\bar{\psi}_r^{(\pm)}$, and between $\Psi_{r+1}^{(\pm)}$ and $\Psi_r^{(\pm)}$. These relations are

$$\begin{Bmatrix} \bar{\psi}_{r+1}^{(\pm)} \\ \Psi_{r+1}^{(\pm)} \end{Bmatrix} = \frac{1}{(r+1)^{\frac{1}{2}}}\left[a_{r+1}^\dagger \begin{Bmatrix} \bar{\psi}_r^{(\pm)} \\ \Psi_r^{(\pm)} \end{Bmatrix} + \frac{1}{E_{r+1} - H \pm i\eta} V_{r+1} \begin{Bmatrix} \bar{\psi}_r^{(\pm)} \\ \Psi_r^{(\pm)} \end{Bmatrix}\right]. \quad \text{(A3)}$$

Now suppose it has been proven that, for all integers up to some integer n,

$$\bar{\psi}_r^{(\pm)} = \Psi_r^{(\pm)}. \quad \text{(A4)}$$

Then the identical recursion relations (A3) assure us that

$$\bar{\psi}_{r+1}^{(\pm)} = \Psi_{r+1}^{(\pm)}.$$

Since Eq. (A4) has already been proven directly for $r = 1$, the theorem of complete induction then asserts the truth of Eq. (A4) for all integers r.

Higher-Dimensional Periodic Systems

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This short note describes a technique which is useful for solving higher-dimensional periodic systems in which a large amount of homogeneity and symmetry is absent.

THIS note describes a technique which is useful for solving higher dimensional periodic systems, such as harmonic lattices, diffusion in a lattice, etc., in which various boundary conditions destroy much of the symmetry which usually allows tractable analytic solutions. The technique yields more analytically useful solutions than the usual normal mode series expansions.

Let a higher-dimensional periodic system be described by the following difference–differential equations:

$$\mathbf{F}[w(d/dt)D,\ g_1(\Delta r_1)D,\ \cdots,\ g_n(\Delta r_n)D] = 0, \qquad \Delta r_i f(r_i) = f(r_i + 1) - f(r_i). \tag{1}$$

w and g_i are the time differential and difference operators of their respective arguments, $D = D(t, r_i)$ is the solution, and $\mathbf{F}$ is some functional relation among its arguments.

Now consider the partial differential equations

$$\mathbf{F}\left[w\left(\frac{\partial}{\partial t}\right)P,\ h_1\left(\frac{\partial}{\partial x_1}\right)P,\ \cdots,\ h_n\left(\frac{\partial}{\partial x_n}\right)P\right] = 0. \tag{2}$$

$\mathbf{F}$ and w have the same functional form as in Eq. (1), and the h_i are new differential operators of their arguments. The general solution, $P = P(t, x_i)$, will possess arbitrary functional properties in much the same way that the general solution of an ordinary differential equation possesses arbitrary constants of integration.[1] If we let these arbitrary functional properties depend on the indices r_i in such a way that the following transformation equations hold

$$g_i(\Delta r_i)P(t, x_i, r_i) = h_i(\partial/\partial x_i)P(t, x_i, r_i), \quad i = 1, 2, \cdots, n. \tag{3}$$

then it is clear that P, considered as a function of t, r_i, is a solution of the original difference–differential equations, Eq. (1). The x_i become arbitrary parameters, and we assign them any particular values which simplify the form of the solution.

Notice that if h_i and g_i had had the same functional form, then we would have merely been replacing the differences by partial derivatives. The partial differential equations thus formed would be subject to all the unsymmetric boundary conditions of the original problem, and it would be quite difficult to construct general integrals. This is the method used by Bateman[2] and Pinney[3]. The usefulness of the method presented here lies in the fact that by properly choosing the functional form of h_i the resulting partial differential equations are as simple as possible. Well-known general integrals may then be obtained from standard references,[4] and the unsymmetric boundary conditions are relegated to the transformation equations which, as can be seen from Eq. (3), are just one-dimensional difference–differential equations. These equations are then readily solved by transform methods.

As an application of this technique, let us examine the correlation function in a harmonic lattice as studied by Mazur and Montroll[5]. In order to avoid a confusing rash of multiple indices, we limit our example to two dimensions. The results apply in any dimension. Consider a two-dimensional rectangular lattice of mass m particles interacting harmonically with their nearest neighbors. A particle is specified by the two discrete variables (r_1, r_2). The dimensions in the r_1 and r_2 directions are $2N_1$

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[1] The simple equation $y'' + y = 0$ possesses two complete solutions, $y = C\cos(t + d)$, and $y = A\sin t + B\cos t$. There exists an analytic relation between the constants A, B, C, d. However, there is no apparant analytic relation between the functional properties of two different general integrals of a partial differential equation. This is discussed in E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, Cambridge, England, 1940), p. 390.

[2] H. Bateman, Bull. Am. Math. Soc. 49, 494 (1943).

[3] Edmund Pinney, *Ordinary Difference–Differential Equations* (University of California Press, Berkeley, California, 1958), Chap. VIII.

[4] General integrals such as those of Helmholtz, Kirchoff, Weber, Poincaré, Poisson, etc., may be found in any text on partial differential equations, e.g., I. N. Sneddon, *Elements of Partial Differential Equations* (McGraw-Hill, New York, 1957).

[5] P. Mazur and E. Montroll, J. Math. Phys. 1, 70 (1960). we follow the notation of this article.

and $2N_2$, respectively, and the corresponding spring constants are γ_1 and γ_2. The border particles in the r_1 direction, i.e., $(\pm N_1, r_2)$, are fixed while the corresponding particles in the r_2 direction are free. The correlation function is $\rho(t, r_1, r_2)$, and the difference–differential equations describing it are

$$
\begin{aligned}
&(md^2/dt^2)\rho(t, r_1, r_2) = [\gamma_1\Delta^2 r_1 + \gamma_2\Delta^2 r_2]\rho(t, r_1, r_2),\\
&\quad -N_1 + 1 < r_1 < N_1 - 1, \qquad -N_2 < r_2 < N_2,\\
&(md^2/dt^2)\rho(t, r_1, N_2) = \gamma_1\Delta^2 r_1\rho(t, r_1, N_2)\\
&\qquad + \gamma_2[\rho(t, r_1, N_2 - 1) - \rho(t, r_1, N_2)],\\
&\qquad\qquad -N_1 + 1 < r_1 < N_1 - 1,\\
&(md^2/dt^2)\rho(t, N_1 - 1, r_2) = \gamma_1[\rho(t, N_1 - 2, r_2)\\
&\quad - 2\rho(t, N_1 - 1, r_2)] + \gamma_2\Delta^2 r_2\rho(t, N_1 - 1, r_2),\\
&\qquad\qquad -N_2 < r_2 < N_2, \qquad (4)\\
&(md^2/dt^2)\rho(t, N_1 - 1, N_2)\\
&\quad = \gamma_1[\rho(t, N_1 - 2, N_2) - 2\rho(t, N_1 - 1, N_2)]\\
&\quad + \gamma_2[\rho(t, N_1 - 1, N_2 - 1) - \rho(t, N_1 - 1, N_2)],\\
&\qquad \Delta^2 r_i f(r_i) = f(r_i + 1) + f(r_i - 1) - 2f(r_i),
\end{aligned}
$$

$\rho(0, 0, 0) = 1$, with all other initial values zero.

Since N_1, N_2 are finite, a discrete frequency spectrum is a natural result of this system. Now let ρ be a function of the fictitious variables x_1, x_2 in such a way that the following transformation equations hold:

$$
\begin{aligned}
&\frac{\partial^2}{\partial x_1^2}\rho(r_i, x_1, x_2)\\
&\quad = \frac{\gamma_1}{m}\begin{cases}\Delta^2 r_1\rho(r_1, r_2, x_i), & -N_1 + 1 < r_1 < N_1 - 1\\ \rho(N_1 - 2, r_2, x_i) - 2\rho(N_1 - 1, r_2, x_i),\end{cases}\\
&\frac{\partial^2}{\partial x_2^2}\rho(r_i, x_1, x_2)\\
&\quad = \frac{\gamma_2}{m}\begin{cases}\Delta^2 r_2\rho(r_1, r_2, x_i), & -N_2 < r_2 < N_2\\ \rho(r_1, N_2 - 1, x_i) - \rho(r_1, N_2, x_i).\end{cases} \qquad (5)
\end{aligned}
$$

Using these transformation equations in Eq. (4), we obtain as the analog of Eq. (2)

$$\frac{\partial^2}{\partial t^2}\rho(t, x_1, x_2) = \left[\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right]\rho(t, x_1, x_2). \qquad (6)$$

This is just the scalar wave equation. A convenient general solution is given by the Poisson integral

$$\rho(t, x_i) = (\partial/\partial t)[M_1(t, x_i)] + M_2(t, x_i). \qquad (7)$$

In this equation M_i is a mean value over the unit sphere, i.e.,

$$
\begin{aligned}
M_i(t, x_i) = \frac{t}{4\pi}\int_0^{\pi}\int_0^{2\pi} f_i(x_1 + t\sin\theta\sin\phi,\\
x_2 + t\sin\theta\cos\phi)\sin\theta\, d\theta\, d\phi. \qquad (8)
\end{aligned}
$$

Except for the initial conditions

$$
\begin{aligned}
f_1(x_1, x_2) = \rho(0, x_1, x_2), \quad f_2(x_1, x_2) = (\partial/\partial t)\\
\times \rho(t, x_1, x_2)|_{t=0}, \qquad (9)
\end{aligned}
$$

the f_i are completely arbitrary functions and may be assigned the indices (r_1, r_2). The initial conditions on ρ allow us to set f_2 identically equal to zero. Assuming a separation of variables of the form[6]

$$f_1(r_1, r_2, x_1, x_2) = T_1(r_1, x_1)T_2(r_2, x_2), \qquad (10)$$

we obtain for the transformation equations, Eq. (5),

$$
\begin{aligned}
&\frac{\partial^2}{\partial x_1^2}T_1(r_1, x_1)\\
&\quad = \frac{\gamma_1}{m}\begin{cases}\Delta^2 r_1 T_1(r_1, x_1), & -N_1 + 1 < r_1 < N_1 - 1\\ T_1(N_1 - 2, x_1) - 2T_1(N_1 - 1, x_1),\end{cases} \qquad (11)\\
&\frac{\partial^2}{\partial x_2^2}T_2(r_2, x_2)\\
&\quad = \frac{\gamma_2}{m}\begin{cases}\Delta^2 r_2 T_2(r_2, x_2), & -N_2 < r_2 < N_2\\ T_2(N_2 - 1, x_2) - T_2(N_2, x_2).\end{cases}
\end{aligned}
$$

These one-dimensional equations may be readily solved by the use of a double Laplace, Laurent–Cauchy transform. Since the details are unrelated to this note and are documented elsewhere, we merely state the results,[7] i.e.,

$$
\begin{aligned}
T_1(r_1, x_1) &= \sum_{p=-\infty}^{\infty}(-)^k J[2(r_1 + 2N_1 p), \omega_1 x_1],\\
T_2(r_2, x_2) &= \sum_{q=-\infty}^{\infty} J[2(r_2 + (2N_2 + 1)q), \omega_2 x_2], \qquad (12)
\end{aligned}
$$

where $\omega_i = 2(\gamma_i/m)^{\frac{1}{2}}$, and $J[n, x]$ is the ordinary Bessel function of the first kind.

---

[6] Notice that although the transformation equations are one dimensional, they may be coupled so that the separation of variables will not always work.

[7] The Laurent–Cauchy transform, $F(s)$, of a discrete function, $f(n)$, $n = 0, 1, \cdots$, is defined to be $F(s) = \sum f(n)s^{-n}$. By very elementary manipulations with geometric series, it is possible to derive a table of transform pairs from which the above results may be obtained. The usefulness of the transform lies in its very efficient "bookkeeping" of the discrete variable indices. Truncated and polyatomic lattices, lattices with defects and impurities, higher nearest-neighbor interactions, etc., can all be handled with great ease in a straightforward, operational manner. A reference article for this transform is Y. H. Ku and A. A. Wolf, Proc. IRE 48, 923 (1960). For applications to various physical problems see C. Chambers and E. Kinzer, University of Alabama Research Institute Report No. 9 (1964).

Assembling these results into the Poisson integral, setting the fictitious x_i equal to zero, and doing the ϕ integration, we obtain the final solution

$$\rho(t, r_1, r_2) = \frac{1}{2}\frac{\partial}{\partial t}\Bigg[t \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} (-)^p \times \int_0^{\pi} J^2[(r_1 + 2N_1 p), \tfrac{1}{2}\omega_1 t \sin\theta] \times J[2(r_2 + (2N_2 + 1)q), \omega_2 t \cos\theta] \sin\theta \, d\theta \Bigg]. \quad (13)$$

Letting $N_1, N_2 \to \infty$, and $r_1 = r_2 = 0$, and expanding ρ in a power series in t, we have the result which Mazur and Montroll[8] obtained by normal mode series expansion,

$$\rho(t) = \sum_{n=0}^{\infty} \frac{(-)^n t^{2n}}{(2n)!} \mu_{2n}, \quad (14)$$

$$\mu_{2n} = \frac{1}{m^n} \sum_{l=0}^{n} \frac{(\gamma_1)^{n-l}(\gamma_2)^l (n)!\,(2(n-l))!\,(2l)!}{[(n-l)!\,(l)!]^3}.$$

[8] P. Mazur and E. Montroll, J. Math. Phys. **1**, 70 (1960), Eq. (5.9).

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Rotationally-Symmetric Model Field Theories

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A class of highly symmetric ,nonrelativistic, Euclidean invariant, model scalar field theories are examined assuming the existence of field and momentum operators that satisfy the canonical commutation relations (CCR). The high degree of symmetry that we assume permits explicit determination of every relevant CCR representation. These consist of a two-parameter family of unitarily inequivalent representations, some of which are irreducible while the others are reducible. It is demonstrated that only those models that are analogs of the free field can be encompassed within the irreducible representations. Hence every model with interaction—including an analog of the relativistic $\lambda\varphi^4$ theory—requires a reducible CCR representation. For the reducible representations, we determine every relevant Hamiltonian operator possessing the required high degree of symmetry. These Hamiltonians, as well as the generators of space translations, cannot be expressed (solely) as functions of the field and momentum operators, which is characteristic of any system with a unique ground state and reducible CCR representation. Nevertheless, it is demonstrated that these Hamiltonians, as well as the generators of space translations, fulfill the "weak correspondence principle," in which the expectation value of a quantum generator, such as the Hamiltonian operator, in a suitably labeled overcomplete family of states is identified with the associated classical generator, such as the classical Hamiltonian. Our principal results depend on the existence and make extensive use of the countably infinite number of degrees of freedom existing in a field theory. Entirely analogous results apply to related models defined in a finite spacial volume since they still have an infinite number of degrees of freedom.

I. INTRODUCTION AND FORMULATION; SUMMARY OF PRINCIPAL RESULTS

IN order to study the quantum properties of infinitely many degrees of freedom in the absence of the kinematic complications inherent in relativistic quantum field theory, we have studied a family of nonrelativistic, model quantum field theories possessing a high degree of symmetry.[1] The nature of this special symmetry is most easily and intuitively exhibited in the form of the allowed classical Hamiltonians, which serve as our heuristic starting point. If we adopt the notation

$$\varphi_{c1}(\mathbf{x}) = g(\mathbf{x}), \qquad \pi_{c1}(\mathbf{x}) = f(\mathbf{x})$$

for the classical scalar field and momentum, respectively, g and f being real-valued square-integrable functions in $L^2(R_3)$, $\mathbf{x}$ a point in Euclidean 3-space R_3, then the allowed classical Hamiltonians

[1] A preliminary report on this work appeared in J. R. Klauder, Bull. Am. Phys. Soc. **9**, 85 (1964); **10**, 484 (1965). While the present paper is self-contained, it draws on many of the ideas and mathematical methods developed in the series on Continuous-Representation Theory (CRT) by the author [J. Math. Phys. **4**, 1055, 1058 (1963); **5**, 177 (1964), referred to hereafter as CRT I, II, and III, respectively] and in collaboration with J. McKenna [J. Math. Phys. **5**, 878 (1964); **6**, 68 (1965), referred to hereafter as CRT IV and V, respectively]. It is important to note a change in the present paper of the phase convention for the Weyl operators brought about by the special nature of the present examples.

Assembling these results into the Poisson integral, setting the fictitious x_i equal to zero, and doing the ϕ integration, we obtain the final solution

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are of the general form

$$H(f, g) = \tfrac{1}{2}[(f, f) + m_0^2(g, g) + V_0\{(g, g)\}], \qquad (1)$$

where $m_0 > 0$, (f, f) denotes the real inner product on $L^2(R_3)$, i.e.,

$$(f, g) \equiv \int_{R_3} f(\mathbf{x})g(\mathbf{x})\, d^3x, \qquad (2)$$

and where $V_0\{x\}$, if it does not vanish identically, is a polynomial of degree exceeding one,

$$V_0\{x\} = \sum_{n=2}^{N} v_n x^n; \quad 2 \leq N < \infty, \qquad (3)$$

positive in a sense to be made precise, but which includes the important examples where each $v_n \geq 0$. This class of Hamiltonians includes

$$H_{m_0}(f, g) = \tfrac{1}{2}[(f, f) + m_0^2(g, g)], \qquad (4)$$

an analog of the relativistic free fields, and

$$H_{m_0,\lambda}(f, g) = \tfrac{1}{2}[(f, f) + m_0^2(g, g) + \lambda(g, g)^2], \qquad (5)$$

a variant of the so-called "$\lambda\varphi^4$-theory".[2] Our models differ from relativistic models in the absence of the (gradient)^2 terms in the free part and in the nonlocal nature of the interaction term.

It should be clear that our class of Hamiltonians is invariant under the group $O(R, \infty)$ of real orthogonal rotations of $L^2(R_3)$ onto itself. For it follows from (1) that for all $T \in O(R, \infty)$ [i.e., $(Tf, Tf) = (f, f)$ for all f and T^{-1} exists], we have

$$H(Tf, Tg) = H(f, g). \qquad (6)$$

These models represent infinite-dimensional analogs of familiar models in particle mechanics that possess three-dimensional rotational symmetry. For this reason we refer to the model fields discussed in this paper as *rotationally symmetric*, or simply as RS models. While such models are not Lorentz invariant, they are Euclidean invariant, since the transformations

$$(T\{\mathbf{a}, \mathbf{R}\}f)(\mathbf{x}) \equiv f(\mathbf{R}^{-1}(\mathbf{x} - \mathbf{a})), \qquad (7)$$

where $\mathbf{a}$ is a three vector and $\mathbf{R}$ is an orthogonal 3×3 matrix, form a subgroup of $O(R, \infty)$. We note further that our class of RS-model Hamiltonians are *time-reversal invariant* since $H(-f, g) = H(f, g)$.

In this paper we examine the quantum theory for the foregoing models. A conventional perturbation approach to these models—such as for that defined by (5)—is not straightforward in view of divergences that arise. A suitable cutoff serves to make the theory finite but only at the expense of the full symmetry of $O(R, \infty)$ (and it is not *a priori* clear that all results derived from cutoff theories necessarily converge to results of a no cutoff theory since orders of taking limits are being interchanged). Instead, we approach our model problems *directly* under what we feel to be three reasonable assumptions. First and foremost is the assumption of (smeared-in-space) field and momentum operators that obey the canonical commutation relations. This assumption is reasonable when we recall that even a divergent perturbation series, by itself, does not prohibit the field operators from fulfilling canonical commutation relations (CCR), as is examplified by perturbation in mass of a free field,[3] and by other cases.[4] Our two remaining assumptions—invariance, cyclicity, and uniqueness of the ground state, and invariance and spectral properties of the Hamiltonian—are very close in spirit to axioms of relativistic field theory,[5] apart, of course, from incorporating the high degree of symmetry inherent in our models. Let us spell out our assumptions explicitly and indicate their important consequences in this section, before proving these results in Secs. II and III.

Fundamental Assumptions

In terms of an abstract, separable[6] Hilbert space $\mathfrak{H}$ with inner product (Ψ, Φ), linear in the second variable, and positive definite norm $||\Psi|| \equiv (\Psi, \Psi)^{\frac{1}{2}}$, our fundamental assumptions take the following form:

(i) *Representation of the Canonical Commutation Relations*:

There exist two Abelian groups of unitary operators $W[f]$ and $V[g]$, $f, g \in L^2(R_3)$ and real, such that $V[0] = W[0] = I$, the identity operator. In terms of the *Weyl operators*

$$U[f, g] \equiv \exp\{i\tfrac{1}{2}(f, g)\}\, V[g]W[f], \qquad (8a)$$

[2] The $\lambda\varphi^4$ theory is discussed, e.g., by A. Salam, Phys. Rev. **82**, 217 (1951); J. C. Ward, *ibid.* **84**, 897 (1951); P. T. Matthews and A. Salam, *ibid.* **90**, 690 (1953); T. T. Wu, *ibid.* **125**, 1436 (1962); K. Symanzik (to be published).

[3] R. Haag, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **29**, 12 (1955).

[4] K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1953); L. van Hove, Physica **18**, 145 (1952); I. E. Segal, *Mathematical Problems of Relativistic Physics* (American Mathematical Society, Providence, Rhode Island, 1963). See also A. S. Wightman and S. S. Schweber, Phys. Rev. **98**, 812 (1955); H. Araki and E. J. Woods, J. Math. Phys. **4**, 637 (1963).

[5] An especially readable account is that of R. F. Streater and A. S. Wightman, *PCT, Spin & Statistics, and All That*, (W. A. Benjamin, Inc., New York, 1964).

[6] See R. F. Streater and A. S. Wightman Ref. 5, p. 86, for arguments in favor of separable Hilbert spaces for quantum field theory.

we require that

$$U[f, g]U[f_1, g_1] = \exp\{i\tfrac{1}{2}[(f, g_1) - (g, f_1)]\}U[f + f_1, g + g_1], \quad (8b)$$

which is the Weyl form of the CCR. The operators $W[cf]$ and $V[cg]$, c real, are weakly continuous in c for all c and for all real f and $g \in L^2(R_3)$. This weak continuity guarantees the existence of self-adjoint smeared field operators $\varphi(f)$ and momentum $\pi(g)$ such that

$$U[f, g] = \exp[i\tfrac{1}{2}(f, g)] \exp[-i\pi(g)] \exp[i\varphi(f)]. \quad (9)$$

With suitable domain conditions, it is these operators that fulfill the Heisenberg form of the CCR, $[\varphi(f), \pi(g)] = i(f, g)I$. [Our use of smearing functions f and g identical to the classical fields of Eq. (1) is deliberate, as will become apparent shortly.]

(ii) *Cyclicity of the Representation, and Invariance and Uniqueness of a Cyclic Vector (the Ground State)*:

There exists a vector Φ_0—a cyclic vector—such that finite linear combinations of vectors of the form

$$\Phi[f, g] \equiv U[f, g]\Phi_0, \quad (10)$$

$f, g \in L^2(R_3)$, are *dense* in the Hilbert space $\mathfrak{H}$. We call the set $\mathfrak{S} \equiv \{\Phi[f, g]\}$ an overcomplete family of states (OFS). The vector Φ_0 is invariant,

$$U[T]\Phi_0 = \Phi_0, \quad (11)$$

under all the unitary transformations $U[T]$, $T \in O(R, \infty)$, each essentially being defined by

$$U[T]U[f, g]\Phi_0 \equiv U[Tf, Tg]\Phi_0, \quad (12)$$

and extended to all of $\mathfrak{H}$ by linearity and continuity. As a consequence, Φ_0 is invariant under the transformations $U[T\{\mathbf{a}, \mathbf{R}\}]$ corresponding to the Euclidean group. There exists an antiunitary time-reversal operator $\mathfrak{I}$ defined by continuity from

$$\mathfrak{I}\sum_{i=1}^{M} c_i\Phi[f_i, g_i] \equiv \sum_{i=1}^{M} c_i^*\Phi[-f_i, g_i],$$

under which Φ_0 is invariant, $\mathfrak{I}\Phi_0 = \Phi_0$. Apart from a phase factor, there is to be only *one* normalized vector $\Phi_0 \in \mathfrak{H}$, $||\Phi_0|| = 1$, satisfying these invariance conditions.

(iii) *Spectral and Invariance Properties of Hamiltonian Operator*:

The time evolution is governed by a weakly continuous, one-parameter unitary group, $U(t) = \exp(-i\mathfrak{H}t)$, whose self-adjoint generator $\mathfrak{H}$, the Hamiltonian, has a nonnegative spectrum. The Hamiltonian—more precisely, $U(t)$ for all t—commutes with the unitary operators $U[T]$,

$$U[T]\mathfrak{H} = \mathfrak{H}U[T], \quad (13)$$

for all $T \in O(R, \infty)$. Under suitable domain conditions we require that

$$[\varphi(f), \mathfrak{H}] = i\pi(f). \quad (14)$$

The equation $\mathfrak{H}\Phi_0 = 0$ has a unique normalizable solution, the ground state Φ_0, which is thus the cyclic vector of condition (ii).

Free-Field Analogs

The foregoing assumptions are fully satisfied in the RS analog of the usual free fields, whose classical Hamiltonians are given in (4). If Φ_0 denotes the ground state of the relevant harmonic-oscillator-type Hamiltonian operator, then it is readily shown that

$$(\Phi_0, U[f, g]\Phi_0) = \exp\{-\tfrac{1}{4}[m_0^{-1}(f, f) + m_0(g, g)]\}. \quad (15)$$

Under the assumption of cyclicity, all relevant properties (i.e., up to unitary equivalence) of the representation of $U[f, g]$ can be deduced from the function[7]

$$\mathfrak{K}(\tilde{f}, \tilde{g}; f, g) = (\Phi[\tilde{f}, \tilde{g}], \Phi[f, g]) = \exp\{-i\tfrac{1}{2}[(\tilde{f}, g) - (\tilde{g}, f)]\}(\Phi_0, U[f - \tilde{f}, g - \tilde{g}]\Phi_0), \quad (16)$$

which we call the *reproducing kernel*.[1] In particular the methods developed in CRT V (and discussed here also in Sec. II) demonstrate that for each m_0 value, the associated representation of the field operators are each irreducible and unitarily inequivalent to one another. This inequivalence of representations for the RS free-field models is in direct analogy to a corresponding inequivalence of representations for relativistic free fields for different m_0 values, which is well known.[3]

General Aspects of the Operator Representations

The functional form (15) for the reproducing kernel characterizes one class of CCR representations consistent with assumptions (i) and (ii). In Sec. II we solve completely the representation problem posed by conditions (i) and (ii), and it is one of the central results of this paper that *every CCR representation satisfying our assumptions has a kernel*

[7] M. A. Naimark, *Normed Rings*, (P. Noordhoff, Groningen, The Netherlands, 1959), p. 242. We note that only under exceptional conditions could a noncyclic CCR representation have a unique invariant ground state.

of the form

$$(\Phi_0, U[f, g]\Phi_0) \equiv \mathcal{K}_{m,\xi}(0, 0; f, g)$$
$$= \exp\{-\tfrac{1}{4}[\xi m^{-1}(f, f) + m(g, g)]\}, \qquad (17)$$

where

$$m > 0, \qquad \xi \geq 1. \qquad (18)$$

The functional form of (17) is an almost immediate consequence under the assumption of the cluster decomposition property;[8] in essence our explicit proof in Sec. II justifies that assumption for the RS models in spite of their nonlocal interactions.

The most extraordinary fact about Eq. (17) is the appearance of only *two* free parameters, m and ξ. We show in Sec. II that each (m, ξ) pair labels a unitarily inequivalent representation of the CCR. However, if the RS model Hamiltonians of Eq. (1) are to fit this into scheme at all, then the *two* parameters m and ξ must accomodate all suitable polynomial potentials $V_0\{x\}$, which in turn depend on *any finite number* of parameters. Thus it is manifestly impossible for each distinct RS classical Hamiltonian (1) to be associated with its own "personal" representation (up to unitary equivalence) of the field operators, in marked contrast to the situation for the subset of free-field RS Hamiltonians in (4).

Of the two parameters, the value of m corresponds essentially to a choice of units and cannot profoundly influence the analysis. That leaves only ξ to carry the burden of incorporating the RS model Hamiltonians. Although each (m, ξ) pair labels *inequivalent* representations, only the special cases $(m, 1)$ correspond to *irreducible* representations of the field operators in the sence that the only bounded operators $\mathcal{B}$ that satisfy

$$\mathcal{B}U[f, g] = U[f, g]\mathcal{B} \qquad (19)$$

for all $f, g \in L^2(R_3)$ are multiples of the identity. In the irreducible case we prove that the *only* RS models that can be incorporated are the free fields in (4) where $m_0 = m$. All other RS models, if they exist, require $\xi > 1$, for which the representation $U[f, g]$ is *reducible*. That is, the operators $\mathcal{B}$ that satisfy (19) include other operators than just multiples of the identity. This makes possible the existence of operators that cannot be constructed (solely) as functions of the field and momentum operators. For $\mathcal{C}$ to be such an operator it sufficies that Φ_0 be a nondegenerate eigenvector of $\mathcal{C}$. {The argument due to Araki[9] is as follows: If $\mathcal{C}$ is a function of the φ and π (precisely: if $\mathcal{C}$ is obtainable as a weak operator limit of finite sums of the Weyl operators), and $\mathcal{B}$ satisfies Eq. (19), then $\mathcal{C}\mathcal{B} = \mathcal{B}\mathcal{C}$. But then $\mathcal{C}(\mathcal{B}\Phi_0) = \mathcal{B}(\mathcal{C}\Phi_0) = c(\mathcal{B}\Phi_0) \Rightarrow \mathcal{B}\Phi_0 = b\Phi_0$, c and b scalars, since Φ_0 is a nondegenerate eigenvector of $\mathcal{C}$. However $\mathcal{B}U[f, g]\Phi_0 = U[f, g]\mathcal{B}\Phi_0 = bU[f, g]\Phi_0$ which implies $\mathcal{B} = bI$ contrary to the assumption of reducibility.} But this is just the property possessed by $\mathcal{H}$ from (iii) and by $\mathcal{P}$, the three infinitesimal generators of space translations, from (ii). Hence, in the reducible case ($\xi > 1$), *neither* $\mathcal{H}$ *nor* $\mathcal{P}$ can be expressed solely as functions of the field and momentum operators.

Anticipating the form of the solution in the reducible case, let us at this point reformulate our basic classical Hamiltonian (1) by introducing a *common coupling constant* $\zeta^2 \geq 0$ (which depends on ξ in a manner to be specified) so as to facilitate "turning on and off" the interaction V_0. We now replace (1) by

$$H(f, g) = H_{\nu_0}(f, g)$$
$$= \tfrac{1}{2}[(f, f) + m_0^2(g, g) + V_0\{\zeta^2(g, g)\}], \qquad (20)$$

where V_0 is still a polynomial as in (3).

Weak Correspondence Principle

Assume for the moment that $\mathcal{H}$ *were* a function of the field and momentum operators, as is in fact the case when $\xi = 1$. To secure reasonable quantum operators it is necessary[10] to introduce a *normal ordering* in transcribing, for example, a classical Hamiltonian $H(f, g)$ into a quantum operator $\mathcal{H}$. However under a normal ordering the relation

$$H(f, g) = (\Phi[f, g], \mathcal{H}\Phi[f, g]) \qquad (21)$$

holds, which we call the *weak correspondence principle*, or simply the WCP. The truth of (21) follows from considering weak operator limits of the normal-order generating functional

$$:e^{-i\pi(k)}e^{i\varphi(j)}: \equiv U[j, k]/(\Phi_0, U[j, k]\Phi_0),$$

$j(\mathbf{x}), k(\mathbf{x}) \in L^2(R_3)$ and sufficiently small in norm, which in view of (8) fulfills

$$(\Phi[f, g], :e^{-i\pi(k)}e^{i\varphi(j)}: \Phi[f, g]) = e^{-i(f,k)+i(g,j)}.$$

It is clear that our use of smearing functions f and

[8] R. Haag, Phys. Rev. **112**, 669 (1958); D. Ruelle, Helv. Phys. Acta **35**, 34 (1962); H. Araki, Ann. Phys. (N. Y.) **11**, 260 (1960).

[9] H. Araki, thesis, Princeton University (1960) (unpublished).

[10] See, e.g., N. N. Boguliubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields*, (Interscience Publishers, Inc., New York, 1959), translated by G. M. Volkoff.

g identical to the classical fields f and g has been in anticipation of Eq. (21) and the WCP.[11]

Now consider the case at hand, the reducible case ($\xi > 1$) for which $\mathcal{P}$ and $\mathcal{H}$ are *not* expressible as functions of the field and momentum. Let us consider $\mathcal{P}$ first. Clearly $\mathcal{P}$ exists since our representations admit continuous unitary representations of the translation group $U[T\{\mathbf{a}, 1\}] = \exp(i\mathbf{a}\cdot\mathcal{P})$. It is straightforward to calculate the matrix elements of $\mathcal{P}$ from (7) and (12), which read

$$(\Phi[\tilde{f}, \tilde{g}], \mathcal{P}\Phi[f, g]) = \tfrac{1}{2}[(\tilde{f}, \nabla g) - (\tilde{g}, \nabla f) + i\xi m^{-1}(\tilde{f}, \nabla f) + im(\tilde{g}, \nabla g)]\, \mathcal{K}_{m,\xi}(\tilde{f}, \tilde{g}; f, g), \tag{22}$$

for suitable f and g. In no sense can it be thought that

$$\mathcal{P} = \int \pi(\mathbf{x})\nabla\varphi(\mathbf{x})\, d^3x, \tag{23}$$

no matter how carefully the right side of (23) is defined.[12] In short, the conventional correspondence principle [i.e., $\varphi_{cl}(\mathbf{x}) = g(\mathbf{x}) \to \varphi(\mathbf{x})$, etc. plus usual counter terms] is inapplicable here. Nevertheless, we note from (22) that

$$(\Phi[f, g], \mathcal{P}[f, g]) = (f, \nabla g) \tag{24}$$

so that $\mathcal{P}$ *does* satisfy the WCP since $(f, \nabla g)$ is the classical generator of spacial translations.

Let us now turn our attention to $\mathcal{H}$ when $\xi \geq 1$. The principal result proved in Sec. III is that for fixed m and ξ *all Hamiltonians satisfying assumption* (iii) *have matrix elements of the form*

$$(\Phi[\tilde{f}, \tilde{g}], \mathcal{H}_V\Phi[f, g]) = \tfrac{1}{2}[(\tilde{f} + im\tilde{g}, f - img) + V\{\zeta^2(\tilde{g}, g)\}]\mathcal{K}_{m,\xi}(\tilde{f}, \tilde{g}; f, g), \tag{25}$$

where the inner product involving f and g is still real and where

$$\zeta^2 = 1 - \xi^{-1} < 1, \tag{26a}$$

$$V\{x\} = v_1 x + V_0\{x\}, \qquad v_1 > 0. \tag{26b}$$

The real function $V_0\{x\}$ can be rather general although we confine our detailed proof in Sec. III to polynomials $V_0\{x\}$ of the form of (3).

The diagonal elements of (25) may be expressed as

$$(\Phi[f, g], \mathcal{H}_V\Phi[f, g]) = \tfrac{1}{2}[(f, f) + m^2(g, g) + V\{\zeta^2(g, g)\}] = \tfrac{1}{2}[(f, f) + m_0^2(g, g) + V_0\{\zeta^2(g, g)\}],$$

where we have set

$$m_0^2 = m^2 + v_1\zeta^2 \geq m^2. \tag{27}$$

Through this identification we have ensured that the diagonal elements of (25) equal $H_{V_0}(f, g)$ in (20). Moreover in the limit $\zeta^2 = 0$, $m_0 = m$, $\mathcal{K}_{m,\xi} = \mathcal{K}_{m,1} = \mathcal{K}_m$ the free-field kernel, and the only possible diagonal elements of (25) are those of $H_m(f, g)$ in (4). Thus each Hamiltonian $\mathcal{H}_V$ has acceptable behavior regarding vanishing of the coupling constant. Merely by counting powers of the field operators we find it emminently reasonable to regard $H_{V_0}(f, g)$ as the classical Hamiltonian associated with $\mathcal{H}_V$. Thus *the Hamiltonians for the RS models satisfy the WCP*, Eq. (21), in spite of the fact that $\mathcal{H}_V$ is not expressible as a function of the φ and π.

It is important to emphasize for the RS models that $H_{V_0}(f, g)$ does *not* determine $\mathcal{H}_V$ uniquely because it does not determine either the mass parameter m or the common coupling constant ζ^2. [*Remark*: However, $\mathcal{H}_V$ *is* uniquely determined by the diagonal elements $H_{V_0}(f, g)$ and by the kernel $\mathcal{K}_{m,\xi}$, from which m and ζ^2 may be found. For irreducible CCR representations for finitely many degrees of freedom, the degree to which the diagonal elements and the kernel determine the Hamiltonian operator is discussed in CRT III, Sec. 2.] Instead these two parameters must be treated phenomenologically. Curious as the indeterminacy of m and ζ^2 in these models may seem, it nevertheless has its "purpose". It can be shown that the indeterminacy of ζ^2 leads to the independence of the kernel $\mathcal{K}_{m,\xi}$ on the entire set of coefficients $\{v_n\}$. In turn, this independence of $\{v_n\}$ can be shown to be necessary *just for the Heisenberg equations of motion to exist.*

As an additional consequence we note that the independence on $\{v_n\}$ implies the existence of a kind of perturbation theory. This perturbation theory is not one in which the common coupling constant ζ^2 is increased from zero to some finite value [such a perturbation theory is manifestly impossible since for each (m, ξ) value the CCR representations are unitarily inequivalent]. Rather the perturbation is with respect to a free parameter, one on which the CCR representation does *not* depend. In the RS analog of the $\lambda\varphi^4$ theory, where from (20) $\lambda =$

[11] This relation between quantum and classical mechanics for particle problems was advocated in J. R. Klauder, Helv. Phys. Acta. 35, 333 (1962). A fuller discussion appears in CRT II and CRT III.

[12] It is instructive to formally calculate "matrix elements" in the OFS of the right side of (23) based on the reducible CCR representation not only to see the difference with (22) but to learn in fact that there is no operator with such "matrix elements."

$v_2\zeta^4$, v_2 is such a free parameter.[13] We note further that even the Hamiltonian matrix elements are not analytic in the coupling constant at the origin. For the RS analog of the $\lambda\varphi^4$ theory, $\lambda = v_2\zeta^4$ while the kernel depends on ζ^2; at best the matrix elements in this case can be considered analytic in $\lambda^{\frac{1}{2}}$.[14]

Lastly, although we have designed our models to exhibit Euclidean invariance, we choose our proofs so as to make no explicit use of this fact, nor even that the classical fields $f(\mathbf{x})$ and $g(\mathbf{x})$ are defined over all of space. If we drop Euclidean invariance, then similar remarks remain true for other classical-field domains as well if we but reinterpret the scalar product (f, g) and the space $L^2(R_3)$ as characterizing any other separable, infinite-dimensional, real Hilbert space. In particular, entirely analogous results hold for a system in a "box" of finite volume Ω, where the classical fields f and g are restricted to be real valued elements of $L^2(\Omega)$ and where the inner product (f, g) is given by (2) integrated over the finite domain Ω.

While the RS models discussed here surely have no direct physical relevance, they clearly suggest the possibility that interacting relativistic field theories may possess similar features, especially the feature of reducible CCR representations for which the weak correspondence principle may prove of value.

II. PROOF OF GENERAL FORM FOR ROTATIONALLY-SYMMETRIC REPRODUCING KERNELS

Our aim here is to derive the functional form in (17) on the basis of our assumptions (i) and (ii). We first begin by establishing the

Functional Form and Continuity of the Reproducing Kernel

In view of the invariance of the ground state under the unitary transformation $U[T]$ of (12), it follows that

$$(\Phi_0, U[f, g]\Phi_0) = (\Phi_0, U[Tf, Tg]\Phi_0) \tag{28}$$

for all $T \in O(R, \infty)$, and thus that (28) is a function of the scalar invariants under $O(R, \infty)$, which are only three in number:

$$X \equiv (f, f), \tag{29a}$$

$$Y \equiv (f, g), \tag{29b}$$

$$Z \equiv (g, g). \tag{29c}$$

As f and g range over $L^2(R_3)$, the variables X, Y, and Z take on values in the range

$$X \geq 0, \quad Z \geq 0, \quad -(XZ)^{\frac{1}{2}} \leq Y \leq (XZ)^{\frac{1}{2}}. \tag{30}$$

We call this domain the *physical domain* for these scalar variables, and it is straightforward to show that it is a convex set. To exhibit the special functional dependence, let us introduce the notation

$$\mathcal{K}\{(f, f), (f, g), (g, g)\} \equiv (\Phi_0, U[f, g]\Phi_0). \tag{31}$$

In order to ensure the existence of self-adjoint smeared field and momentum operators, we have assumed a minimum degree of continuity, in particular that both

$$(\Lambda, V[cf]\Psi), \qquad (\Lambda, W[cf]\Psi)$$

are everywhere continuous in c for all $\Lambda, \Psi \in \mathfrak{H}$ and $f \in L^2(R_3)$. This weak continuity of the unitary operators implies strong continuity;[15] i.e., that both

$$||(V[cf] - 1)\Psi||, \qquad ||(W[cf] - 1)\Psi||$$

are continuous in c for all $f \in L^2(R_3)$ and $\Psi \in \mathfrak{H}$. It is a straightforward deduction (by the use of triangle and Schwartz's inequalities) from this property,[16] that Eq. (31) is jointly continuous in the four real parameters p_1, p_2, q_1, q_2, where

$$f(\mathbf{x}) = p_1u_1(\mathbf{x}) + p_2u_2(\mathbf{x}),$$

$$g(\mathbf{x}) = q_1u_1(\mathbf{x}) + q_2u_2(\mathbf{x}),$$

and where for convenience we choose the u_i arbitrary save for $(u_i, u_j) = \delta_{ij}$, $i, j = 1, 2$. That is, it follows from the minimum continuity assumed that the function

$$\mathcal{K}\{p_1^2 + p_2^2, p_1q_1 + p_2q_2, q_1^2 + q_2^2\} \tag{32}$$

is jointly continuous for all real values of the four indicated variables. Since the domain of the arguments in (32) clearly coincides with the physical domian of X, Y, and Z, it follows that $\mathcal{K}\{X, Y, Z\}$ is continuous within the physical domain. Furthermore, the scalar product variables X, Y, and Z are, in turn, readily shown to be continuous functions[17] of the fields f and g in the $L^2 \times L^2$ metric

$$d(f_1, g_1; f_2, g_2) = ||f_1 - f_2|| + ||g_1 - g_2||, \tag{33}$$

[13] We intend to examine the perturbation property of our models in greater length in a separate study of the solutions of our dynamical equations for the RS analog of the $\lambda\varphi^4$ theory.

[14] Compare, e.g., E. R. Caianello, A. Campolattaro, and M. Marino (to be published), who argue that the relativistic $\lambda\varphi^4$ theory is analytic in $\lambda^{-\frac{1}{2}}$ and not in λ.

[15] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Fredrick Ungar Publishing Company, New York, 1955), p. 380.

[16] See, e.g., CRT IV, Lemma 3.2, or the proof by J. Lew, thesis, Princeton University (1960) (unpublished) which is quoted in CRT V, Sec. 2D.

[17] F. Riesz and B. Sz.-Nagy, Ref. 16, p. 199.

where $||f||^2 \equiv (f, f)$. Since continuous functions of continuous functions are themselves continuous, we have established

Lemma 2.1. Every reproducing kernel satisfying assumptions (i) and (ii) has the functional form

$$(\Phi_0, U[f, g]\Phi_0) = \mathcal{K}\{(f, f), (f, g), (g, g)\} \quad (34)$$

and is everywhere jointly continuous in $f(\mathbf{x})$ and $g(\mathbf{x})$ in the metric (33).

A general CCR representation exhibits the property

$$(\Phi_0, U[f, g]\Phi_0)^* = (U[f, g]\Phi_0, \Phi_0)$$
$$= (\Phi_0, U[f, g]^{-1}\Phi_0) = (\Phi_0, U[-f, -g]\Phi_0)$$

while time-reversal invariance of Φ_0 leads to

$$(\Phi_0, U[f, g]\Phi_0)^* = (\mathfrak{I}U[f, g]\Phi_0, \mathfrak{I}\Phi_0)^*$$
$$= (U[-f, g]\Phi_0, \Phi_0)^* = (\Phi_0, U[-f, g]\Phi_0).$$

Applying these conditions to the form of $\mathcal{K}$ in Lemma 2.1, we obtain

Lemma 2.2. Every reproducing kernel satisfying assumptions (i) and (ii) fulfills, in the notation of (29), the conditions

$$\mathcal{K}^*\{X, Y, Z\} = \mathcal{K}\{X, Y, Z\} = \mathcal{K}\{X, -Y, Z\}, \quad (35)$$

i.e., $\mathcal{K}$ is real and it is even in the variable $Y = (f, g)$.

Explicit Forms for the Reproducing Kernel

The derivation of an explicit functional form for the reproducing kernel conveniently proceeds by an elementary use of the "tag test" introduced in CRT V. Consider the Weyl commutation relation in the form

$$U[f_k, g_k]U[f, g] = \exp\{i[(f_k, g) - (g_k, f)]\}$$
$$\times U[f, g]U[f_k, g_k].$$

Suppose f_k, g_k, $k = 1, 2, \cdots$ form a pair-sequence such that two conditions hold: (1) f_k, g_k both converge weakly to zero in $L^2(R_3)$, i.e., for all $f, g \in L^2(R_3)$, $(f_k, g) \to 0$ and $(g_k, f) \to 0$ as $k \to \infty$; (2) $U[f_k, g_k]$ converges weakly to a bounded operator A, i.e., for all $\Lambda, \Psi \in \mathfrak{H}$,

$$(\Lambda, U[f_k, g_k]\Psi) \to (\Lambda, A\Psi) \quad \text{as} \quad k \to \infty.$$

Clearly A depends on the chosen sequence $\{f_k, g_k\}$. Under the preceding two conditions, we find the important commutation property,

$$AU[f, g] = U[f, g]A, \quad (36)$$

for all $f, g \in L^2(R_3)$. The norm of A satisfies $||A|| \leq 1$ as follows from

$$|(\Lambda, U[f_k, g_k]\Psi)| \leq ||\Lambda||\,||\Psi||.$$

We call A the *tag operator*.

It suffices for condition (2) above, that the weak convergence of the unitary operators $U[f_k, g_k]$ be verified for sets $\{\Lambda_i\}$, $\{\Psi_i\}$ of vectors whose finite linear combinations are dense in $\mathfrak{H}$[18]. As such sets, we can take the OFS $\{\Phi[f, g]\}$ itself. Thus condition (2) above is implied by the convergence of $(\Phi[\tilde{f}, \tilde{g}], U[f_k, g_k]\Phi[f, g])$ for all $\tilde{f}, \tilde{g}, f, g \in L^2(R_3)$. In turn, in view of the CCR's and condition (1) above, this convergence is ensured by the convergence of $(\Phi_0, U[f_k + f, g_k + g]\Phi_0)$ for all $f, g \in L^2(R_3)$. Armed with this condition it is trivial to find suitable weakly convergent pair sequences $\{f_k, g_k\}$: We need only ensure that

$$\mathcal{K}\{(f + f_k, f + f_k), (f + f_k, g + g_k),$$
$$(g + g_k, g + g_k)\} \quad (37)$$

converges for all f and g.

For our class of suitable sequences, let us pick any real normalized set of weakly convergent functions, $u_k(\mathbf{x}) \in L^2(R_3)$, $k = 1, 2, \cdots$, i.e., $(u_k, u_k) = 1$, and $(u_k, g) \to 0$ for all $g \in L^2(R_3)$, and set

$$f_k(\mathbf{x}) = pu_k(\mathbf{x}); \qquad g_k(\mathbf{x}) = qu_k(\mathbf{x}), \quad (38)$$

where p and q are arbitrary real numbers. [Such a sequence is manifestly given by an orthonormal set $u_k(\mathbf{x})$, $k = 1, 2, \cdots$.] Then Eq. (37) becomes

$$\mathcal{K}\{(f, f) + 2(f, f_k) + p^2, (f, g) + (f_k, g)$$
$$+ (f, g_k) + pq, (g, g) + 2(g_k, g) + q^2\}, \quad (39)$$

which, in view of the continuity of $\mathcal{K}$ and of the weak convergence of f_k and g_k to zero, converges for all $f, g \in L^2(R_3)$ and all real values p, q, and has the value

$$\mathcal{K}\{(f, f) + p^2, (f, g) + pq, (g, g) + q^2\}. \quad (40)$$

Hence the sequences in (38) define bona fide tag operators A, and for them we have

$$(\Phi_0, U[f, g]A\Phi_0) = \mathcal{K}\{(f, f) + p^2, (f, g) + pq,$$
$$(g, g) + q^2\} = (\Phi[-f, -g], A\Phi_0) = (\Phi[f, g], A\Phi_0). \quad (41)$$

We now observe from the form of this expression that for all $T \in O(R, \infty)$,

[18] A. N. Kolmogorov and S. V. Fomin, *Elements of the Theory of Functions and Functional Analysis*, L. F. Boron, translator (Graylock Press, Rochester, New York, 1957), Vol. 1, p. 90.

$$(\Phi[f, g], A\Phi_0) = (\Phi[Tf, Tg], A\Phi_0)$$
$$= (U[T]\Phi[f, g], A\Phi_0) = (\Phi[f, g], U[T]^{-1}A\Phi_0).$$

From the cyclicity of the CCR representation and the assumed uniqueness of Φ_0 under all $U[T]$, we conclude that

$$A\Phi_0 = a\Phi_0, \tag{42}$$

where a is some scalar depending on p and q, which we call the *tag*. In consequence, in the notation of (29), we find that

$$\mathcal{K}\{X + p^2, Y + pq, Z + q^2\}$$
$$= (\Phi_0, U[f, g]\Phi_0)a$$
$$= \mathcal{K}\{X, Y, Z\}a$$
$$= \mathcal{K}\{X, Y, Z\}\mathcal{K}\{p^2, pq, q^2\};$$

here, in the last relation, we have *evaluated* the tag a by specializing to the case $f = g = 0$. If we multiply this relation by $\mathcal{K}\{p_1^2, p_1q_1, q_1^2\}$, then it follows that

$$\mathcal{K}\{X + X', Y + Y', Z + Z'\}$$
$$= \mathcal{K}\{X, Y, Z\}\mathcal{K}\{X', Y', Z'\}, \tag{43}$$

where $X' = p^2 + p_1^2$, $Y' = pq + p_1q_1$, $Z' = q^2 + q_1^2$. Hence (43) holds true for any points X, Y, Z and X', Y', Z' in the physical domain as defined by (30).

Since $\mathcal{K}$ is continuous and $\mathcal{K}\{0, 0, 0\} = 1$, there is an open, convex neighborhood, $\mathfrak{N}$, about the origin in the physical domain where $\mathcal{K}\{X, Y, Z\} \neq 0$. But then $\mathcal{K}$ never vanishes, for it follows from (43) that for any positive integer n,

$$\mathcal{K}\{nX, nY, nZ\} = (\mathcal{K}\{X, Y, Z\})^n \neq 0$$

for a point $X, Y, Z \in \mathfrak{N}$. Our further discussion is conventional in nature and is conveniently carried out in terms of the everywhere-continuous function $W(X, Y, Z)$ defined by

$$\mathcal{K}\{X, Y, Z\} \equiv e^{-W(X,Y,Z)},$$

which is subject to the normalization condition $W(0, 0, 0) = 0$. Equation (43) then implies that

$$W(X + X', Y + Y', Z + Z') = W(X, Y, Z)$$
$$+ W(X', Y', Z'). \tag{44}$$

For any positive integer n, we find

$$W(nX, nY, nZ) = nW(X, Y, Z),$$

and thus for any positive rational n/m,

$$W(nX/m, nY/m, nZ/m) = (1/m)W(nX, nY, nZ)$$
$$= (n/m)W(X, Y, Z).$$

From the continuity of W it then follows for all real, nonnegative s that

$$W(sX, sY, sZ) = sW(X, Y, Z). \tag{45}$$

We note that any W may be decomposed as

$$W(X, Y, Z) = W(|Y|, Y, |Y|)$$
$$+ W(X - |Y|, 0, 0) + W(0, 0, Z - |Y|);$$

and combining this with (45) we have

$$W(X, \pm|Y|, Z) = |Y| \cdot W(1, \pm 1, 1)$$
$$+ (X - |Y|)W(1, 0, 0)$$
$$+ (Z - |Y|)W(0, 0, 1)$$
$$\equiv AX + B_{\pm}|Y| + CZ.$$

From (44) there follows the condition

$$W(2X, 0, 2Z) = W(X, Y, Z) + W(X, -Y, Z),$$

and it thus follows that $B_+ = -B_- \equiv B$. Hence, we have shown that

$$W(X, Y, Z) = AX + BY + CZ$$

for some complex A, B, and C. In turn we see that

$$\mathcal{K}\{X, Y, Z\} = e^{-AX-BY-CZ}. \tag{46}$$

From Lemma 2.2, it follows that A and C are real while $B = 0$. From the bounded property of $\mathcal{K}$ (i.e., $|\mathcal{K}| \leq 1$) we obtain $A \geq 0$, $C \geq 0$.

Further limits on A and C follow from the fact that we require $\mathcal{K}$ to generate a CCR representation, and are immediate consequences of the analysis in CRT IV and CRT V since each of the present field representations can be constructed as an incomplete tensor product representation. Let us expand each test function as follows:

$$f(\mathbf{x}) = \sum_{n=1}^{\infty} p_n h_n(\mathbf{x}); \qquad p_n = (h_n, f), \tag{47a}$$

$$g(\mathbf{x}) = \sum_{n=1}^{\infty} q_n h_n(\mathbf{x}); \qquad q_n = (h_n, g), \tag{47b}$$

where $\{h_n(\mathbf{x})\}$ is an arbitrary complete orthonormal sequence in $L^2(R_3)$. Then, considered as a function of the sequences $\{p_n\}$ and $\{q_n\}$, each of the relevant kernels are of the product form

$$\mathcal{K}(0, 0; \{p_n\}, \{q_n\}) = \prod_{n=1}^{\infty} \exp\left[-(Ap_n^2 + Cq_n^2)\right].$$

For this function to generate a CCR representation it follows from CRT V that it is necessary and sufficient that

$$\mathcal{K}(0, 0; p, q) \equiv \exp\left[-(Ap^2 + Cq^2)\right] \tag{48}$$

correspond to a CCR for a *single* degree of freedom. It is a consequence of von Neumann's uniqueness theorem[19] that *every* such single-particle representation is expressible in the form

$$\mathcal{K}(0, 0; p, q) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \varphi^*(x + \tfrac{1}{2}q, y)e^{+ipx} \times \varphi(x - \tfrac{1}{2}q, y)\, dx\, dy. \quad (49)$$

A direct consequence of the representation (49) is the square integrability of $\mathcal{K}$ and the constraint

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\mathcal{K}(0, 0; p, q)|^2\, (dp\, dq/2\pi) \leq 1, \quad (50)$$

equality holding if and only if the single-particle representation is irreducible and when $\varphi(x, y) = \varphi_0(x)\varphi_1(y)$, almost everywhere.[20] Applying (50) to the form in (48), we determine the necessary condition $AC \geq \frac{1}{16}$. Adopting this condition on A and C, let us set $C \equiv m/4$, $m > 0$, and $A \equiv \xi/4m$, $\xi \geq 1$ so that

$$\mathcal{K}(0, 0; p, q) = \exp\,[-\tfrac{1}{4}(\xi m^{-1}p^2 + mq^2)]. \quad (51)$$

It is straightforward to show that this kernel can be generated from (49) by the function

$$\varphi(x, y) = [m^2(1 - \zeta^2)/\pi^2]^{\frac{1}{4}} \times \exp\,[-\tfrac{1}{2}m(x^2 + 2\zeta xy + y^2)], \quad (52)$$

where

$$\zeta \equiv (1 - \xi^{-1})^{\frac{1}{2}}, \qquad 0 \leq \zeta < 1. \quad (53)$$

Only when $\zeta = 0$, i.e., $\xi = 1$, does $\varphi(x, y)$ have a product form $\varphi_0(x)\varphi_1(y)$ leading to an irreducible representation; for all $\xi > 1$, there follows $\zeta > 0$ so that the CCR representation is reducible. We take up a further study of the reducible representations subsequently.

It remains to show that the CCR representations of the exponential form (46) actually possess a *unique* state Φ_0 invariant under $U[T]$. For cyclic CCR representations admitting the Euclidean translation group, Araki has shown uniqueness of the invariant state whenever the CCR representation possesses the cluster decomposition property,[21] the heart of which can be summarized by remarking that the operator sequence $\tilde{U}_k \equiv U[T\{k\mathbf{a}, \mathbf{I}\}]$, $\mathbf{a} \neq 0$, converges weakly to the projection operator onto Φ_0. Because of our effort to avoid any actual use of Euclidean invariance, we first set $U_k \equiv U[T_k]$ where $T_k \in O(R, \infty)$, $k = 1, 2, \cdots$, and choose a sequence T_k that converges weakly to zero on $L^2(R_3)$. One such T_k sequence is given as follows: Let $h_n(\mathbf{x})$ be an arbitrary complete orthonormal sequence and expand $f(\mathbf{x})$ as in (47a). Then, we may choose

$$(T_k f)(\mathbf{x}) \equiv \sum_{n=1}^{k} p_{k+1-n}h_n(\mathbf{x}) + \sum_{n=k+1}^{\infty} p_n h_n(\mathbf{x}),$$

which is a symmetric transformation such that $T_k^2 = 1$. It is straightforward to show from (46) that as a consequence of the convergence of the T_k, the operator sequence $\{U_k\}$ converges weakly to the projection operator onto Φ_0. Now let Ψ be an arbitrary vector invariant under U_k, $U_k\Psi = \Psi$, for all k.

Then, for all $\Lambda \in \mathfrak{K}$, we have

$$(\Lambda, \Psi) = (\Lambda, U_k\Psi) = \lim_{k\to\infty} (\Lambda, U_k\Psi) = (\Lambda, \Phi_0)(\Phi_0, \Psi),$$

from which it follows that $\Psi = c\Phi_0$, $c = (\Phi_0, \Psi)$, demonstrating the uniqueness of the invariant state Φ_0. Thus we can summarize the foregoing in

Theorem 2.1. Every CCR representation satisfying (i) and (ii) has a reproducing kernel of the form

$$(\Phi_0, U[f, g]\Phi_0) = \mathcal{K}_{m,\xi}(0, 0; f, g) = \exp\,\{-\tfrac{1}{4}[\xi m^{-1}(f, f) + m(g, g)]\}, \quad (54)$$

where $m > 0$, $\xi \geq 1$. We refer to these representations as the "(m, ξ) representations"; they are irreducible when $\xi = 1$, and reducible when $\xi > 1$.

[*Remark*: We observe that if we *drop* the uniqueness condition on Φ_0 from assumptions (i) and (ii), then the most general cyclic representation has a reproducing kernel of the form

$$(\Phi_0, U[f, g]\Phi_0) = \int \exp\,\{-\tfrac{1}{4}[a(f, f) + 2b(f, g) + c(g, g)]\}d\sigma(a, b, c),$$

where $\pm b$ enters the integral with the same weight and where the measure σ respects the conditions $a > 0$, $c > 0$, and $ac \geq b^2 + 1$, almost everywhere in σ. This result may be obtained as follows: If we denote the tag operator A of Eq. (41) by $A[p^2, pq, q^2]$, then the introduction of a second tag operator shows that

$$\mathcal{K}\{(f, f) + p^2 + p'^2, (f, g) + pq + p'q', (g, g) + q^2 + q'^2\} = (\Phi[f, g], A[p^2, pq, q^2] \times A[p'^2, p'q', q'^2]\Phi_0),$$

[19] J. von Neumann, Math. Ann. 104, 570 (1931). See also the related discussion in CRT IV.
[20] These properties are proved in CRT IV and CRT V.
[21] H. Araki, J. Math. Phys. 1, 492 (1960), Theorem 6.1.

from which we learn (if we set $f = g = 0$) that the kernel itself is *determined* by these few tag operators. Since the various A operators commute and the ones in question are self-adjoint, we can appeal to standard theorems on the spectral representation of self-adjoint semigroups[22(a)] and on the joint spectral representation of commuting operators[22(b)] to determine the form of the integrand above. The parametric restrictions are consequences of the positive definiteness of the Hilbert space inner product.

Our result is a generalization of an earlier one given in Ref. 22(c) for the "universally invariant states," which possess still higher symmetry [essentially, a function only of $(f, f) + (g, g)$] than the "rotationally invariant states" considered here.]

We now show that each of the (m, ξ) representations are *unitarily inequivalent* to one another. From Eqs. (36) and (42) it follows that

$$AU[f, g]\Phi_0 = U[f, g]A\Phi_0 = aU[f, g]\Phi_0;$$

therefore $A = aI$ on a dense set of vectors and hence on the whole Hilbert space. However in this case the tags, a, are *unitary invariants*. Let us assume that a unitary operator V exists such that for all $f_k, g_k \in L^2(R_3)$, $U'[f_k, g_k] = VU[f_k, g_k]V^{-1}$. If f_k, g_k is a sequence satisfying conditions (1) and (2) above for U, then the existence of a weak limit for U' follows from the existence of a weak limit for U, and furthermore

$$\lim U'[f_k, g_k] = A' = VAV^{-1} = VaIV^{-1} = aI.$$

The various tags appropriate to the present examples follow from Theorem 2.1 as

$$a = \mathcal{K}\{p^2, pq, q^2\} = \exp\{-\tfrac{1}{4}[\xi m^{-1}p^2 + mq^2]\}, \quad (55)$$

which are unequal to one another for all p and q for different (m, ξ) pairs. Hence we have established

Theorem 2.2. For the (m, ξ) representations whose reproducing kernels are given in Theorem 2.1 each (m, ξ) pair labels a unitarily inequivalent representation of the CCR's.

III. HAMILTONIAN OPERATORS FOR ROTATIONALLY SYMMETRIC MODELS

We now take up the question of the introduction of dynamics in the form of an evolution operator $U(t) = \exp(-it\mathcal{H})$, which satisfies assumption (iii) of Sec. I, so as to verify Eq. (25). Let $\{U[T]\}'$ denote the set of all bounded operators that commute with all $U[T]$, $T \in O(R, \infty)$; by (iii) $U(t) \in \{U[T]\}'$. Now any $\mathfrak{G} \in \{U[T]\}'$ obviously has matrix elements $(\Phi[f', g'], \mathfrak{G}\Phi[f, g])$ which are a function of the ten scalar invariants $(f', f'), \cdots, (f', g), \cdots, (g, g)$. Our first step below is to show that in fact if $\mathfrak{G} \in \{U[T]\}'$, then

$$\begin{aligned}(\Phi[f', g'], \mathfrak{G}\Phi[f, g]) &= A\{(f', f), (f', g), (g', f), (g', g)\} \\ &\times (\Phi[f', g'], (\Phi_0)(\Phi_0, \Phi[f, g]) \\ &= C\{(f', f), (f', g), (g', f), (g', g)\} \\ &\times \mathcal{K}_{m,\xi}(f', g'; f, g), \end{aligned} \quad (56)$$

the second form following from the first. Suppose now that $\Phi[f, g] \subset \mathfrak{D}_{\mathcal{H}}$, the domain of $\mathcal{H}$, then (56) predicts that

$$\begin{aligned}(\Phi[f', g'], \mathcal{H}\Phi[f, g]) &= G\{(f', f), (f', g), (g', f), (g', g)\} \\ &\times \mathcal{K}_{m,\xi}(f', g'; f, g). \end{aligned} \quad (57)$$

It is a straightforward consequence of (8), for τ real and $e = e(\mathbf{x}) \in L^2(R_3)$, that

$$\begin{aligned}(\Phi[f', g'], e^{-i\tau\varphi(e)}\mathcal{H}e^{i\tau\varphi(e)}\Phi[f, g]) &= G\{(f' + \tau e, f + \tau e), (f' + \tau e, g), \\ &(g', f + \tau e), (g', g)\}\ \mathcal{K}_{m,\xi}(f', g'; f, g). \end{aligned} \quad (58)$$

Under further domain restrictions, we take a partial derivative of (58) with respect to τ, and then set $\tau = 0$ so as to obtain the matrix elements of $-i[\varphi(e), \mathcal{H}]$. Next we take (14) into account and note that

$$(\Phi[f', g'], \pi(e)\Phi[f, g]) = \tfrac{1}{2}[(e, f' + f) + im(e, g' - g)]\mathcal{K}_{m,\xi}(f', g'; f, g).$$

As a consequence, if $a = (f', f)$, $b = (f', g)$, $c = (g', f)$ and $d = (g', g)$, we learn that

$$\left\{(e, f' + f)\frac{\partial}{\partial a} + (e, g)\frac{\partial}{\partial b} + (e, g')\frac{\partial}{\partial c}\right\}G\{a, b, c, d\} = \tfrac{1}{2}[(e, f' + f) + im(e, g' - g)] \quad (59)$$

for all f', g', f, g and all e. Choose f, f', g, and g' all nonzero and linearly independent and choose e orthogonal to any three of them in turn. From such a resultant set of equations it follows that the most general solution of (59) has the form

$$\begin{aligned}G\{a, b, c, d\} &= \tfrac{1}{2}[a - im(b - c) + m^2 d + F\{d\}]. \\ &= \tfrac{1}{2}[(f' + img', f - img) + F\{(g', g)\}]. \end{aligned} \quad (60)$$

In this determination, F remains arbitrary and

[22] (a) Reference 16, p. 395; (b) Ref. 16, p. 290; (c) I. E. Segal, Illinois J. Math 6, 500 (1962), Theorem 1'.

we must appeal to additional properties to fix F. For example, from $\mathfrak{K}\Phi_0 = 0$ it follows that $G\{0, 0, 0, 0\} = 0$, so that $F\{0\} = 0$. But more important is the requirement that $\mathfrak{K}$ really be a bona fide self-adjoint operator. This requirement forces the *identical vanishing* of F, i.e., $F \equiv 0$, in the irreducible cases ($\xi = 1$). It might be supposed that only one or possibly a few functions F would be admissible when $\xi > 1$, but that is not the case as we shall see. We now fill in the essential steps in the foregoing outline.

Case of Irreducible CCR Representation

For convenience let us introduce the "normalization"

$$N = (\Phi_0, \Phi[f, g]) = \exp\{-\tfrac{1}{4}[m^{-1}(f, f) + m(g, g)]\}$$

and the complex field $h(\mathbf{x}) = f(\mathbf{x}) - img(\mathbf{x})$. Then it is a consequence of (16) that we may write

$$(\Phi[\tilde{f}, \tilde{g}], \Phi[f, g]) = \tilde{N}N \exp[\tfrac{1}{2}m^{-1}(\tilde{h}^*, h)]. \quad (61)$$

It is immediately clear that we can now introduce a bosonlike Fock-space representation,[23]

$$\mathfrak{H} = \sum_{n=0}^{\infty} \oplus \mathfrak{H}_n \quad (62)$$

in which

$$\Phi[f, g] = N \sum_{n=0}^{\infty} \oplus [h(\mathbf{x}_1) \cdots h(\mathbf{x}_n)] \quad (63)$$

with inner product (61). Consequently, any $\mathfrak{G} \in \{U[T]\}'$ has matrix elements of the form

$$(\Phi[\tilde{f}, \tilde{g}], \mathfrak{G}\Phi[f, g]) = \tilde{N}N \sum_{n=0}^{\infty} \frac{1}{n!(2m)^n} b_n(\tilde{h}^*, h)^n \quad (64)$$

for an arbitrary uniformly bounded set of complex b_n. Any possible term in the sum (64) of the form $(\tilde{h}^*, \tilde{h}^*)(h, h)$, etc. is prohibited because it does not correspond to matrix elements of a bounded operator. (Stated otherwise, the decomposition

$$U[T] = \sum_{n=0}^{\infty} \oplus U_n[T]$$

determined by (63) is a decomposition into mutually inequivalent irreducible representations, which is in fact the case. In consequence $\{U[T]\}'$ is Abelian.[24]) Equation (64) establishes (56) for the $(m, 1)$ representations and furthermore shows in this case that

$$A\{(\tilde{f}, f), (\tilde{g}, g), (\tilde{g}, f), (\tilde{g}, g)\} = A\{(\tilde{f} + im\tilde{g}, f - img)\}$$

$$C\{(\tilde{f}, f), (\tilde{f}, g), (\tilde{g}, f), (\tilde{g}, g)\} = C\{(\tilde{f} + im\tilde{g}, f - img)\}.$$

So long as $\Phi[f, g] \subset \mathfrak{D}_{\mathfrak{K}}$, it follows from these relations that

$$G\{(f', f), (f', g), (g', f), (g', g)\} = G\{(f' + img', f - img)\}.$$

On comparison with (60) we learn that

$$F = \text{constant} = 0.$$

It remains to exhibit a self-adjoint operator $\mathfrak{K}$ with the proper matrix elements that satisfies (iii). But this operator is clearly the analog of the Harmonic oscillator. In particular, if $b_n = e^{-inmt}$ in (64), then we are assured[25] of the existence of a self-adjoint $\mathfrak{K}$ such that

$$(\Phi[f', g'], \exp(-it\mathfrak{K})\Phi[f, g]) = \exp[\tfrac{1}{2}m^{-1}(e^{-imt} - 1)(f' + img', f - img)] \times \mathfrak{K}_m(f', g'; f, g). \quad (65)$$

The remaining conditions of (iii) as well as the fulfillment of the necessary domain conditions to validate the preceding calculations follows immediately from Eq. (65). We summarize these results in

Theorem 3.1. For the $(m, 1)$ representations the only Hamiltonian $\mathfrak{K}$ that fulfills (iii) is the free field RS model whose matrix elements are

$$(\Phi[f', g'], \mathfrak{K}\Phi[f, g']) = \tfrac{1}{2}(f' + img', f - img)\mathfrak{K}_m(f', g'; f, g). \quad (66)$$

Case of Reducible CCR Representation

Once again we let N denote a "normalization",

$$N = (\Phi_0, \Phi[f, g]) = \exp\{-\tfrac{1}{4}[\xi m^{-1}(f, f) + m(g, g)]\}.$$

But for efficiency we wish to examine a class of Fock-space representations simultaneously. For that purpose let us introduce

$$u(\mathbf{x}) \equiv \xi^{\frac{1}{2}} \cos(\theta + \alpha) f(\mathbf{x}) - im \cos(\theta)\, g(\mathbf{x}), \quad (67a)$$

[23] Yu. V. Novozhilov and A. V. Tulub, *Method of Functionals in the Quantum Theory of Fields* (Gordon and Breach, New York, 1961); H. Araki and E. J. Woods, J. Math. Phys. 4, 637 (1963). For emphasis on the analyticity aspects see I. E. Segal, Illinois J. of Math. 6, 500 (1962); *Mathematical Problems of Relativistic Physics* (American Mathematical Society, Providence, Rhode Island, 1963), Chap. VI; V. Bargmann, Proc. Nat. Acad. Sci. U. S. 48, 199 (1962); See also CRT V, Sec. 3E.

[24] M. A. Naimark, Ref. 7, p. 287.

[25] F. Riesz and B. Sz.-Nagy, Ref. 16, p. 383.

$$v(\mathbf{x}) \equiv \xi^{\frac{1}{2}} \sin(\theta + \alpha) f(\mathbf{x}) - im \sin(\theta)\, g(\mathbf{x}), \tag{67b}$$

where θ is an arbitrary real angle, and

$$\cos\alpha \equiv \xi^{-\frac{1}{2}} < 1,$$
$$\sin\alpha = (1 - \xi^{-1})^{\frac{1}{2}} \equiv \zeta > 0.$$

It follows from these definitions that

$$m^{-1}[(\tilde{u}^*, u) + (\tilde{v}^*, v)] = \xi m^{-1}(\tilde{f}, f) + m(\tilde{g}, g) + i[(\tilde{f}, g) - (\tilde{g}, f)],$$

which holds independently of θ. Consequently we have

$$(\Phi[\tilde{f}, \tilde{g}], \Phi[f, g]) = \tilde{N}N \times \exp\{\tfrac{1}{2}m^{-1}[(\tilde{u}^*, u) + (\tilde{v}^*, v)]\}. \tag{68}$$

Again we introduce a Fock-space representation[23] but now we require a "two boson field" form.[26] That is, we set

$$\mathfrak{H} = \sum_{n,p=0}^{\infty} \oplus \mathfrak{H}^{\theta}_{n,p}, \tag{69}$$

the decomposition depending on the choice of θ in (67), and for which

$$\Phi[f, g] = N \sum_{n,p=0}^{\infty} \oplus [u(\mathbf{x}_1) \cdots u(\mathbf{x}_n) v(\mathbf{y}_1) \cdots v(\mathbf{y}_p)], \tag{70}$$

the inner product being given by (68). For any θ this decomposition makes plausible the form of matrix elements for the most general bounded operator $\mathfrak{B} \in \{U[T]\}'$ as

$$(\Phi[\tilde{f}, \tilde{g}], \mathfrak{B}\Phi[f, g]) = \tilde{N}N \sum_{n,p=0}^{\infty} \frac{1}{n!p!(2m)^{n+p}} \times \sum_{r=0}^{n} \sum_{s=0}^{p} b_{nr,ps}(\tilde{u}^*, u)^{n-r}(\tilde{u}^*, v)^r(\tilde{v}^*, u)^s(\tilde{v}^*, v)^{p-s} \tag{71}$$

for suitable uniformly bounded complex coefficients $b_{nr,ps}$. Since we will not work with this general form we leave the precise set of coefficients unspecified. As before conceivable terms in the sum like $(\tilde{u}^*, \tilde{u}^*)\cdot(u, u)$, $(\tilde{u}^*, \tilde{v}^*)(u, v)$, etc., are not permitted as they do not correspond to matrix elements of bounded operators. {In the present case, the decomposition

$$U[T] = \sum_{n,p=0}^{\infty} \oplus U_{n,p}[T]$$

afforded by (70) is such that the representations

$$U_S[T] = \sum_{n+p=S} \oplus U_{n,p}[T]$$

are disjoint for different S (no subrepresentation of one is equivalent to a subrepresentation of the other), but the $U_S[T]$ representations are reducible. Each $U_S[T]$ is decomposed into a finite direct sum of irreducibles, some of which are equivalent, by reduction of

$$\mathfrak{H}_S = \sum_{n+p=S} \oplus \mathfrak{H}_{n,p}$$

under the permutation group. In consequence $\{U[T]\}'$ is not Abelian, but every self-adjoint operator in, or associated with $\{U[T]\}'$ has pure point spectrum.} On recognizing the definition of u and v from (67) we note that Eq. (71) establishes the validity of (56) in the reducible case.

A special class of operators $\mathfrak{B}_{\theta,\lambda} \in \{U[T]\}'$ for each θ and $\lambda \geq 0$ is determined by

$$\mathfrak{B}_{\theta,\lambda}\Phi[f, g] = N \sum_{n,p=0}^{\infty} \oplus e^{-n\lambda m} u(\mathbf{x}_1) \cdots u(\mathbf{x}_n) \times v(\mathbf{y}_1) \cdots v(\mathbf{y}_p).$$

It follows that $\mathfrak{B}_{\theta,\lambda} = \exp(-\lambda\mathfrak{K}_\theta)$, where $\mathfrak{K}_\theta$ is a bona fide positive (unbounded) self-adjoint operator.[27] Clearly we have

$$(\Phi[\tilde{f}, \tilde{g}], \exp(-\lambda\mathfrak{K}_\theta)\Phi[f, g]) = \tilde{N}N \exp\{\tfrac{1}{2}m^{-1}[e^{-\lambda m}(\tilde{u}^*, u) + (\tilde{v}^*, v)]\} = \exp[\tfrac{1}{2}m^{-1}(e^{-\lambda m} - 1)(\tilde{u}^*, u)]\mathcal{K}_{m,\xi}(\tilde{f}, \tilde{g}; f, g).$$

In particular, if $\theta = 0$, Eq. (67a) leads to $u(\mathbf{x}) = f(\mathbf{x}) - img(\mathbf{x})$. Thus there exists a self-adjoint operator $\mathfrak{K}_0$ such that

$$(\Phi[f', g'], e^{-\lambda\mathfrak{K}_0}\Phi[f, g]) = \exp[\tfrac{1}{2}m^{-1}(e^{-\lambda m} - 1) \times (f' + img', f - img)]\mathcal{K}_{m,\xi}(f'g'; f, g).$$

Also of interest is the case $\theta = \frac{1}{2}\pi - \alpha$, for which $u(\mathbf{x}) = -im\zeta g(\mathbf{x})$ according to (67a). If we denote this $\mathfrak{K}_\theta$ by $\mathfrak{W}$, then we are assured the existence of a positive self-adjoint operator $\mathfrak{W}$ such that

$$(\Phi[f', g'], \exp(-\lambda\mathfrak{W})\Phi[f, g]) = \exp[\tfrac{1}{2}m(e^{-\lambda m} - 1)\zeta^2(g', g)]\mathcal{K}_{m,\xi}(f', g'; f, g). \tag{72}$$

We shall use the two operators $\mathfrak{K}_0$ and $\mathfrak{W}$ to construct our Hamiltonian. Again we do not elaborate on simple domain questions all of which are easily verified.

[26] Related constructions have been given by H. Araki and E. J. Woods, J. Math. Phys. 4, 637 (1963). They are special cases of construction of CCR representations by "contraction," i.e., singular transformations on the test-function space, as discussed in CRT V, Sec. 2E.

[27] F. Riesz and B. Sz.-Nagy, Ref. 16, p. 395.

We note first that

$$-(\partial/\partial\lambda)(\Phi[f', g'], e^{-\lambda\mathcal{K}_0}\Phi[f, g])\,|_{\lambda=0}$$
$$= (\Phi[f', g'], \mathcal{K}_0\Phi[f, g])$$
$$= \tfrac{1}{2}(f' + img', f - img)\mathcal{K}_{m,\xi}(f', g'; f, g). \quad (73)$$

Secondly we define, for an arbitrary self-adjoint operator A the "factorial operator", for $n \geq 1$, by

$$\mathfrak{F}[A^{(n)}] \equiv A(A - I)(A - 2I) \cdots (A - [n - 1]I).$$

It is then straightforward to show that

$$(\Phi[f', g'], \mathfrak{F}[(\mathcal{W}/m)^{(n)}]\Phi[f, g])$$
$$= \{\tfrac{1}{2}\zeta^2 m(g', g)\}^n \mathcal{K}_{m,\xi}(f', g'; f, g). \quad (74)$$

Since the spectrum of $(\mathcal{W}/m)$ is 0, 1, 2, 3, $\cdots$ it follows that

$$\mathfrak{F}[(\mathcal{W}/m)^{(n)}] \geq 0$$

for it has the spectrum

$$0, n!, (n + 1)!, (n + 2)!/2!, (n + 3)!/3!, \cdots .$$

For simplicity, we restrict our attention to those operator polynomials

$$\mathcal{U}\left\{\left(\frac{\mathcal{W}}{m}\right)\right\} \equiv \frac{1}{2}\sum_{n=1}^{N}\left(\frac{2}{m}\right)^n v_n \mathfrak{F}\left[\left(\frac{\mathcal{W}}{m}\right)^{(n)}\right], \quad (75)$$

where v_n are real and where $\mathcal{U}\{(\mathcal{W}/m)\} > 0$ whenever $\mathcal{W} > 0$. In terms of the spectrum of this operator, we require that

$$\frac{1}{2}\sum_{n=1}^{N}\left(\frac{2}{m}\right)^n v_n \frac{q!}{(q - n)!} > 0; \quad q = 1, 2, 3, \cdots, \quad (76)$$

which puts a kind of positivity condition on the $\{v_n\}$. In particular $v_1 > 0$ and $v_N > 0$. Equation (76) is manifestly fulfilled if furthermore $v_n \geq 0$, $n = 2, \cdots N - 1$.

If $\{v_n\}$ fulfills the positivity condition (76), then let us define the associated polynomial

$$V\{x\} \equiv \sum_{n=1}^{N} v_n x^n.$$

It then follows that

$$(\Phi[f', g'], \mathcal{U}\{(\mathcal{W}/m)\}\Phi[f, g])$$
$$= \tfrac{1}{2}V\{\zeta^2(g', g)\}\mathcal{K}_{m,\xi}(f', g'; f, g). \quad (77)$$

Finally consider the operator

$$\mathcal{K}_V \equiv \mathcal{K}_0 + \mathcal{U}\{(\mathcal{W}/m)\} \geq 0, \quad (78)$$

defined on $\{\Phi[f, g]\}$, with matrix elements

$$(\Phi[f', g'], \mathcal{K}_V\Phi[f, g]) = \tfrac{1}{2}[(f' + img', f - img)$$
$$+ V\{\zeta^2(g', g)\}]\mathcal{K}_{m,\xi}(f', g'; f, g). \quad (79)$$

Since $\mathcal{K}_V$, as defined on $\{\Phi[f, g]\}$ by (79) is symmetric and nonnegative, it follows that there exists[28] a self-adjoint operator—which we also call $\mathcal{K}_V$—such that $\mathcal{K}_V \geq 0$, and which has the matrix elements given by (79).

We need only prove uniqueness of the ground state Φ_0 belonging to the extended $\mathcal{K}_V$ to complete our construction. Recall[28] that $\mathfrak{D}_{\mathcal{K}_V} \subset \mathfrak{E}_V \subset \mathfrak{H}$, where $\mathfrak{E}_V$ consists of all vectors $\Psi \in \mathfrak{H}$ that are limits of Cauchy sequences Ψ_n in the norm $|\Lambda|_V \equiv (\Lambda, \mathcal{K}_V\Lambda)^{\frac{1}{2}}$. In particular this requires that Ψ_n is a Cauchy sequence in *both* the norms $|\Lambda|_0 \equiv (\Lambda, \mathcal{K}_0\Lambda)^{\frac{1}{2}}$ and $|\Lambda|_1 \equiv (\Lambda, \mathcal{U}\{(\mathcal{W}/m)\}\Lambda)^{\frac{1}{2}}$. If moreover Ψ satisfies $\mathcal{K}_V\Psi = 0$, then in addition $|\Psi_n|_V \to 0$, which implies that both $|\Psi_n|_0 \to 0$ and $|\Psi_n|_1 \to 0$. However it is easy to see from the properties of $\mathcal{K}_0$ that $|\Psi_n - \Psi_m|_0 \to 0$ and $|\Psi_n|_0 \to 0$ if and only if $||\mathcal{K}_0(\Psi_n - \Psi_m)|| \to 0$ and $||\mathcal{K}_0\Psi_n|| \to 0$. Thus in the notation of (69) it is necessary for $\mathcal{K}_V\Psi = 0$ that

$$\Psi \in \sum_{p=0}^{\infty} \oplus \mathfrak{H}^0_{0,p}. \quad (80)$$

A similar analysis applied to the "$\mathcal{U}$-metric", $|\ |_1$, shows for $\mathcal{K}_V\Psi = 0$ it is necessary that

$$\Psi \in \sum_{p=0}^{\infty} \oplus \mathfrak{H}^\theta_{0,p}, \quad (81)$$

where $\theta = \frac{1}{2}\pi - \alpha$ as before, critical use being made of (76). We now prove that the only Ψ consistent with (80) and (81) is a multiple of Φ_0.

First assume Ψ satisfies (80). Then there is a sequence of symmetric $\psi_0(\mathbf{y}_1, \cdots, \mathbf{y}_p) \in L^2(R_{3p})$ such that

$$(\Phi[f, g], \Psi) = N\sum_{p=0}^{\infty}\frac{1}{p!}\left(\frac{\xi^{\frac{1}{2}}\zeta}{2m}\right)^p$$
$$\times \int f(\mathbf{y}_1) \cdots f(\mathbf{y}_p)\psi_0(\mathbf{y}_1, \cdots, \mathbf{y}_p)\, d^{3p}y \quad (82)$$

since $v(\mathbf{y}) = \xi^{\frac{1}{2}}\zeta f(\mathbf{y})$ when $\theta = 0$. That is, apart from N, *this function is totally independent of* $g(\mathbf{x})$. Now assume Ψ satisfies (81). Then there is a sequence of symmetric $\psi_\theta(\mathbf{y}_1, \cdots, \mathbf{y}_p) \in L^2(R_{3p})$ such that

$$(\Phi[f, g], \Psi) = N\sum_{p=0}^{\infty}\frac{1}{p!(2m)^p}$$
$$\times \int v^*(\mathbf{y}_1) \cdots v^*(\mathbf{y}_p)\psi_\theta(\mathbf{y}_1, \cdots, \mathbf{y}_p)\, d^{3p}y, \quad (83)$$

where

$$v(\mathbf{y}) = \xi^{\frac{1}{2}}f(\mathbf{y}) - i(m/\xi^{\frac{1}{2}})g(\mathbf{y}).$$

[28] F. Riesz and B. Sz.-Nagy, Ref. 16, p. 329. We do not examine possible distinctions due to other extension methods.

The only possible way for the latter series to be independent of $g(\mathrm{y})$ for all $f, g \in L^2(R_3)$ is that only the $p = 0$ term contributes. That is, $\Psi = c\Phi_0$, c a constant, as was to be shown. This result is not true if $v_1 = 0$ in (75). We summarize our results in

Theorem 3.2. For each (m, ξ) representation, $\xi > 1$, there exists a self-adjoint operator $\mathcal{K}_V$ satisfying assumption (iii) with matrix elements

$$(\Phi[f', g'], \mathcal{K}_V\Phi[f, g]) = \tfrac{1}{2}[(f' + img', f - img) + V\{\zeta^2(g', g)\}]\mathcal{K}_{m,\xi}(f', g'; f, g), \quad (84)$$

$\zeta^2 = 1 - \xi^{-1}$, for each polynomial

$$V\{x\} = \sum_{n=1}^{N} v_n x^n,$$

which is positive in the sense of (76).

In conclusion we note the specialization of (84),

$$(\Phi[f', 0], \mathcal{K}_V\Phi[f, 0]) = \tfrac{1}{2}(f', f)\mathcal{K}_{m,\xi}(f', 0; f, 0),$$

which is consistent with Araki's general results.[29] In Araki's theory, where it is assumed that Φ_0 is cyclic for the operators $W[f]$ alone, these matrix elements essentially determine $\mathcal{K}_V$. However in the reducible cases ($\xi > 1$) neither Φ_0, nor any vector is cyclic for the $W[f]$ (or the $V[g]$) alone.

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It is a pleasure to thank J. McKenna for countless conversations concerning continuous representations which, almost everywhere, have had a measurable impact on the approach adopted in this paper.

[29] H. Araki, J. Math. Phys. 1, 492 (1960), Sec. 8.

Matrix Representation of the Angular Momentum Projection Operator

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Formulas are obtained which give the matrix representation, relative to a product basis, of the projection operator for the total angular momentum of a system. If the individual angular momenta are not too large, the matrix elements depend upon a small number of parameters, independent of the number of angular momenta coupled. Recurrence relations between elements and symmetry properties of elements are derived. These results enable one to perform the vector coupling of a large number of angular momenta in a relatively simple fashion. The connection between the matrix elements and vector coupling coefficients is discussed. Several important special cases are treated in detail.

I. INTRODUCTION

THE standard quantum mechanical problem of coupling N commuting angular momenta

$$\mathbf{J} = \sum_{i=1}^{N} \mathbf{J}_i \tag{1}$$

to give simultaneous eigenvectors of J^2 and J_z with eigenvalues $j(j+1)$ and m, respectively, (units with $\hbar = 1$ will be used throughout) can be treated in many ways. The conventional approach[1] is to perform successive binary couplings of the constituent angular momenta, using the appropriate Clebsch–Gordan, or Wigner, coefficients at each stage. Different coupling schemes lead to different complete, orthonormal sets of eigenvectors, related to each other by unitary transformations. For small N, these transformation matrices may be expressed in terms of well known quantities[1] such as the Racah coefficients or the $6j$-symbols for $N = 3$, and the $9j$-symbols for $N = 4$.

Since there frequently is no physical basis for selecting one coupling scheme over another, some arbitrariness is introduced into constructing the eigenvectors.

If N is large, the above procedure becomes unwieldy because of the large number of couplings involved. Löwdin and his co-workers have developed an alternative approach using projection operators, which has been applied to a variety of atomic and molecular problems.[2-7] The operator

$$P_j = \prod_{\substack{k \\ (k \neq j)}} \frac{J^2 - k(k+1)}{j(j+1) - k(k+1)} \tag{2}$$

projects that component which has total angular momentum j out of any state vector for the system. In (2), k goes over all values of angular momentum except the value j. The numerator in the product annihilates these components. The denominator assures that P_j leaves unchanged any eigenvector of J^2 with quantum number j, or equivalently, that P_j is an idempotent

$$P_j^2 = P_j. \tag{3}$$

To construct simultaneous eigenvectors of J^2 and J_z, one normally operates on a product vector[8]

$$\left| \prod_{i=1}^{N} j_i m_i \right\rangle = \prod_{i=1}^{N} |j_i m_i\rangle, \tag{4}$$

composed of simultaneous eigenvectors of J_i^2 and J_{iz} with quantum numbers j_i and m_i. The above state is an eigenvector of J_z with eigenvalue

$$m = \sum_{i=1}^{N} m_i \tag{5}$$

but it is not of J^2. Since J^2, and hence P_j, commutes with J_z and the individual J_i^2, the projected vector has the set $j_1, j_2, \cdots, j_N, j, m$ as good quantum numbers. To obtain a complete set of eigenvectors with these quantum numbers, one projects all possible products of the form (4) with the given values for j_i and with m_i values satisfying (5). Since the number of possible products is, in general, greater than the number of independent vectors specified by the above quantum numbers (i.e., the number of multiplets for the value j arising from the vector coupling), the set of projected vectors will not be independent. However, it has been shown by Löwdin[5]

[1] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton University, Princeton, New Jersey, 1957).
[2] P.-O. Löwdin, Phys. Rev. **97**, 1509 (1955).
[3] P.-O. Löwdin, Advan. Phys. **5**, 1 (1956).
[4] P.-O. Löwdin, Rev. Mod. Phys. **34**, 520 (1962).
[5] P.-O. Löwdin, Rev. Mod. Phys. **36**, 966 (1964).
[6] R. Fieschi and P.-O. Löwdin, "Atomic State Wave Functions Generated by Projection Operators," Technical Note from the Quantum Chemistry Group of Uppsala University (1957).
[7] A. Rotenberg, J. Chem. Phys. **39**, 512 (1963).
[8] One could also use other state vectors for the system, e.g. Slater determinants. See Ref. 6.

that, because of Eq. (3), these vectors can be orthonormalized in a relatively simple manner.[9] Different orderings of the projected functions during the orthonormalization lead to different bases. This is equivalent to the arbitrariness in coupling scheme in the conventional method.

Löwdin[5] has shown that (2) may be rewritten, when acting on an eigenvector of J_z with eigenvalue $m \geq 0$, as

$$P_j = P_{jm} = \frac{(2j+1)(j+m)!}{(j-m)!} \sum_{k=0} \frac{(-)^k J_-^{j-m+k} J_+^{j-m+k}}{k!\,(2j+1+k)!}, \tag{6}$$

where

$$J_\pm = J_x \pm iJ_y \tag{7}$$

are the usual raising and lowering operators. An additional suffix m has been added to P_j to emphasize that (6) is valid only when acting on a state of definite m. In most applications, the sum in (6) is finite, since continued raisings eventually annihilate the state vector. Equation (6) is particularly useful when operating on the product states (4), since it can be expressed in terms of raising and lowering operators for the individual angular momenta by using the multinomial theorem.

Section II presents a new derivation of Eq. (6) for the projection operator, which, in contrast to that of Ref. 5, does not start from the product form (2). It is shown that (6) is valid for all m, rather than only for $m \geq 0$. In addition, the method of proof given here appears more promising for the analogous problem for other Lie groups, viz., to find that operator which projects a vector of definite weight onto a particular irreducible representation.[10]

In Sec. III, an expression is derived for an arbitrary element of the matrix representation of P_j in terms of the product basis (4). Although it has not been extensively used, this representation appears to have several advantages. Physical results, being expectation values, frequently can be expressed directly in terms of the matrix elements. In addition, because of certain symmetry properties, many elements in the representation are numerically equal. Alternative expressions for the elements, which take advantage of the symmetries, are derived in Sec. IV. These formulas are particularly useful for problems in which the individual j_i are small. In such cases, the matrix elements depend on a small number of parameters; this number is independent of how many angular momenta are coupled. A special case has been considered in Ref. 11, in which it was shown, for a system of an arbitrary number of angular momenta with $j_i \leq 1$, that the diagonal matrix elements depend upon only four parameters.

For the case $N = 2$, the matrix elements are simply related to the Clebsch–Gordan and $3j$ symbols. This connection is considered in Sec. V. Relations between different matrix elements are considered in Sec. VI and some important special cases of the general formulas are discussed in Sec. VII.

II. DERIVATION OF FORMULA FOR P_{jm}

Let $|m\rangle$ be an arbitrary eigenvector of J_z with eigenvalue m and $|j, m\rangle$ an arbitrary simultaneous eigenvector of J^2 and J_z with quantum numbers j and m, respectively. Consider first the special case $m = j$. If one can find a linear operator P_{jj} satisfying the conditions

$$J_z P_{jj} |j\rangle = jP_{jj} |j\rangle, \tag{8}$$

$$J_+ P_{jj} |j\rangle = 0, \tag{9}$$

$$P_{jj} |j, j\rangle = |j, j\rangle, \tag{10}$$

then that operator is the required projection operator. Because of the relation

$$J^2 = J_- J_+ + J_z^2 + J_z, \tag{11}$$

Eqs. (8) and (9) ensure that the projected vector is an eigenvector of J^2 and J_z with the required quantum numbers. Equation (10) shows that P_{jj} is an idempotent.

Consider next a general infinite series, in which the terms are products formed from the generators J_+, J_- and J_z of SU_2, taken in an arbitrary order and each an arbitrary number of times. Because of the commutation relations

$$[J_+, J_-] = 2J_z, \qquad [J_z, J_\pm] = \pm J_z, \tag{12}$$

each term can be reordered so that all raising operators appear to the right and all lowering operators to the left (or vice versa); i.e., the most general series formed from the generators may be written as

$$S = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \sum_{r=0}^{\infty} a_{pqr} J_-^p J_z^q J_+^r. \tag{13}$$

Then suppose that this series operates only on eigenstates of J_z. Since J_+ operating on such a state gives another eigenstate of J_z, one can replace J_z every-

[9] The author has derived a procedure for selecting a subset of the product functions such that their projections are complete and independent, although still not orthogonal. Since it is not related to the main body of this paper, this theorem will be presented elsewhere.

[10] The author has found the analog of Eq. (6) for the group SU_n, for the case where the weight of the vector equals the highest weight of the irreducible representation.

[11] J. Shapiro, Nuovo Cimento Suppl. 18, 40 (1960).

where by an eigenvalue, and the above series reduces to

$$S_m = \sum_{p=0}^{\infty} \sum_{r=0}^{\infty} b_{pr} J_-^p J_+^r. \tag{14}$$

Let us try to find a solution P_{ij} of Eqs. (8)–(10) of the form (14). Equation (8) states that m is unchanged by the operator, i.e., only the terms with $p = r$ survive in (14). This gives

$$P_{ij} = \sum_{r=0}^{\infty} c_r J_-^r J_+^r. \tag{15}$$

To apply (9), note that (12) leads to

$$[J_+, J_-^r] = J_-^{r-1} \cdot 2J_z + [J_+, J_-^{r-1}]J_-.$$

By iterating this result and using (12), one obtains

$$\begin{aligned}[J_+, J_-^r] &= \sum_{i=0}^{r-1} J_-^{r-1-i}(2J_z)J_-^i \\ &= J_-^{r-1} \sum_{i=0}^{r-1} (2J_z - 2i) \\ &= rJ_-^{r-1}(2J_z - r + 1).\end{aligned} \tag{16}$$

Using (15) and (16) in (9) leads to

$$\begin{aligned}0 &= \sum_{r=0}^{\infty} C_r J_+ J_-^r J_+^r \, |j\rangle \\ &= \sum_{r=0}^{\infty} C_r J_-^r J_+^{r+1} \, |j\rangle \\ &\quad + \sum_{r=1}^{\infty} r C_r J_-^{r-1}(2J_z - r + 1)J_+^r \, |j\rangle.\end{aligned}$$

In the first sum replace r by $r - 1$ and in the second sum set $J_z = j + r$, its eigenvalue. This gives

$$\sum_{r=1}^{\infty} [C_{r-1} + r(2j + 1 + r)C_r]J_-^{r-1} J_+^r \, |j\rangle = 0,$$

which is satisfied if the coefficients obey the recurrence relation

$$r(2j + 1 + r)C_r + C_{r-1} = 0, \quad r = 1, 2, \cdots. \tag{17}$$

Iteration of (17) leads to

$$C_r = \frac{(-)^r(2j + 1)!}{r!\,(2j + 1 + r)!} C_0, \tag{18}$$

so that

$$P_{ij} = C_0(2j + 1)! \sum_{r=0}^{\infty} \frac{(-)^r J_-^r J_+^r}{r!\,(2j + 1 + r)!}.$$

The normalization factor C_0 is determined by Eq. (10). Since $J_+ \, |jj\rangle = 0$, only the $r = 0$ term survives, leading to $C_0 = 1$ and Eq. (6) with $m = j$ for P_{ij}.

For a general value of m, one can write

$$P_{im} = kJ_-^{i-m} P_{ij} J_+^{i-m}, \tag{19}$$

i.e., raise m to j, then project, and then lower back to m. Note that both the raising and lowering operations give nonzero results for that component of $|m\rangle$ which survives the projection, and do not change its j-value. The constant k is determined by the condition, analogous to (10), that

$$P_{im} \, |jm\rangle = |jm\rangle. \tag{20}$$

Because of (10), this leads to

$$1 = k\langle jm| \, J_-^{i-m} J_+^{i-m} \, |jm\rangle = k \, ||J_+^{i-m} \, |jm\rangle||^2. \tag{21}$$

The matrix element in (21) can be evaluated from the well known relations

$$\begin{aligned}J_+ \, |jm\rangle &= [(j - m)(j + m + 1)]^{\frac{1}{2}} \, |j, m + 1\rangle, \\ J_- \, |jm\rangle &= [(j + m)(j - m + 1)]^{\frac{1}{2}} \, |j, m - 1\rangle,\end{aligned} \tag{22}$$

giving

$$k = (j + m)!/(j - m)!\,(2j)!. \tag{23}$$

Substituting (23) into (19), one immediately obtains Eq. (6) for P_{jm}. Although the Dirac phase convention[12] has been used in (22), it is clear from (21) that the answer is independent of this choice.

The entire derivation could have been carried out starting with the choice $m = -j$ instead of $m = j$ and interchanging J_+ and J_- everywhere. This leads to the alternative expression

$$P_{jm} = \frac{(2j + 1)(j - m)!}{(j + m)!} \sum_{r=0} (-)^r \frac{J_+^{j+m+r} J_-^{j+m+r}}{r!\,(2j + 1 + r)!}, \tag{24}$$

i.e., the result obtained by replacing m by $-m$ and interchanging J_+ and J_- in (6). The two expressions (6) and (24) are equal to each other (see Sec. IV), and both are valid for all m.

III. MATRIX REPRESENTATION OF THE PROJECTION OPERATOR

Consider the matrix element

$$M = \left\langle \prod_{i=1}^{N} j_i m_i' \middle| \, P_{jm} \, \middle| \prod_{i=1}^{N} j_i m_i \right\rangle \tag{25}$$

of the projection operator between two product vectors of the form of Eq. (4). Since P_j commutes with the individual J_i^2 and with J_z, this representation is diagonal in the j_i and has nonzero elements only if

[12] P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford University Press, New York, 1947), 3rd ed.

$$\sum_{i=1}^{N} m_i = \sum_{i=1}^{N} m_i' = m. \tag{26}$$

Substituting (6) into (25) gives

$$M = \frac{(2j+1)(j+m)!}{(j-m)!} \sum_{r=0}^{\infty} \frac{(-)^r M_r}{r!\,(2j+1+r)!}, \tag{27}$$

where

$$M_r = \langle \pi j_i m_i' |\, J_-^{j-m+r} J_+^{j-m+r} \,| \pi j_i m_i \rangle. \tag{28}$$

By setting

$$J_\pm = \sum_{i=1}^{N} J_{i\pm}, \tag{29}$$

and by using the multinomial theorem for the powers appearing in (28), it follows that

$$M_r = [(j-m+r)!]^2 \times \sum_{s_1,\cdots,s_N} \sum_{t_1,\cdots,t_N} \left[\prod_{i=1}^{N} \frac{\langle j_i m_i' |\, J_{i-}^{s_i} J_{i+}^{t_i} \,| j_i m_i \rangle}{s_i!\, t_i!} \right], \tag{30}$$

where $\sum s_i = \sum t_i = j - m + r$. The limits on the sums in (30) are

$$0 \le s_i \le j_i - m_i', \qquad 0 \le t_i \le j_i - m_i,$$

since otherwise the single-particle matrix elements are zero. In addition, since these elements are zero unless $m_i' + s_i = m_i + t_i$, half of the sums in (30) may be eliminated by introducing indices

$$k_i = j_i - m_i' - s_i = j_i - m_i - t_i. \tag{31}$$

These quantities have limits

$$0 \le k_i \le \min\,(j_i - m_i',\ j_i - m_i) \tag{32}$$

and satisfy the relation

$$\sum_{i=1}^{N} k_i = \sum_{i=1}^{N} (j_i - m_i - t_i) = \bar{j} - j - r, \tag{33}$$

where

$$\bar{j} = \sum_{i=1}^{N} j_i \tag{34}$$

is the algebraic sum of the j_i, i.e., $\bar{j}$ is the maximum possible value of j that can arise from coupling the given individual angular momenta. Equation (30) becomes

$$M_r = [(j-m+r)!]^2 \times \sum_{k_1,\cdots,k_N} \left[\prod_{i=1}^{N} \frac{\langle j_i m_i' |\, J_{i-}^{j_i - m_i' - k_i} J_{i+}^{j_i - m_i - k_i} \,| j_i m_i \rangle}{(j_i - m_i - k_i)!\,(j_i - m_i' - k_i)!} \right] \tag{35}$$

where $\sum k_i = \bar{j} - j - r$. This can be written in a concise form as follows. Define quantities

$$f_{k_i}^{i} = \frac{\langle j_i m_i' |\, J_{i-}^{j_i - m_i' - k_i} J_{i+}^{j_i - m_i - k_i} \,| j_i m_i \rangle}{(j_i - m_i - k_i)!\,(j_i - m_i' - k_i)!} \tag{36}$$

and polynomials

$$p^i = (f_0^i)^{-1} \sum_{k_i} f_{k_i}^{i} x^{k_i}. \tag{37}$$

These polynomials depend only upon the quantum numbers j_i, m_i, and m_i' associated with angular momentum number i, and are normalized to have a constant term of unity. Equation (35) then can be written as

$$M_r = [(j-m+r)!]^2 \left(\prod_{i=1}^{N} f_0^i \right) a_{\bar{j}-j-r}, \tag{38}$$

where

$$\sum_s a_s x^s = \prod_{i=1}^{N} p^i, \tag{39}$$

i.e., the quantity a appearing in (38) is the coefficient of $x^{\bar{j}-j-k}$ in the product of polynomials in (39).

The quantities f can be evaluated by using (22) leading to

$$f_{k_i}^{i} = \left[\binom{2j_i}{j_i - m_i} \binom{2j_i}{j_i - m_i'} \right]^{\frac{1}{2}} \times \frac{(j_i - m_i)!\,(j_i - m_i')!\,(2j_i - k_i)!}{(j_i - m_i - k_i)!\,(j_i - m_i' - k_i)!\,k_i!\,(2j_i)!}. \tag{40}$$

It follows that

$$f_0^i = \left[\binom{2j_i}{j_i - m_i} \binom{2j_i}{j_i - m_i'} \right]^{\frac{1}{2}} \tag{41}$$

and the polynomials are the hypergeometric functions

$$p^i = F[-(j_i - m_i), -(j_i - m_i'), -2j_i, -x]. \tag{42}$$

Substituting (38) into (27) gives for the complete matrix element

$$M = \left(\prod_{i=1}^{N} f_0^i \right) \frac{(2j+1)(j+m)!}{(j-m)!} \times \sum_{r=0}^{\infty} (-)^r \frac{[(j-m+r)!]^2 a_{\bar{j}-j-r}}{r!\,(2j+1+r)!}. \tag{43}$$

Finally, noting that

$$\sum_{r=0}^{\infty} (-)^r \frac{[(j-m+r)!]^2}{r!\,(2j+1+r)!} x^r = \frac{[(j-m)!]^2}{(2j+1)!} \times F(j-m+1,\ j-m+1,\ 2j+2,\ -x)$$

and using (39), (41), and (42), one can rewrite (43) as

$$M = \binom{2j}{j-m}^{-1} \left[\prod_{i=1}^{N} \binom{2j_i}{j_i - m_i} \binom{2j_i}{j_i - m_i'} \right]^{\frac{1}{2}} b_{\bar{j}-j}, \tag{44}$$

where

$$\sum_r b_r x^r = F(j - m + 1, j - m + 1, 2j + 2, -x) \times \prod_{i=1}^{N} F[-(j_i - m_i), -(j_i - m_i'), -2j_i, -x]. \quad (45)$$

The use of the Dirac phase convention in (22) has led to real matrix elements. The effect of a different choice may be seen as follows. Since the result of operating with the combination $J_{i-}J_{i+}$ is unchanged [Eq. (11)], the $f_{k_i}^i$ of (36) will be multiplied by a phase factor which depends only on i, and not on k_i, and which is unity if $m_i = m_i'$. Equation (37) shows that the polynomials p^i are unchanged, since they involve ratios of $f_{k_i}^i$ with the same i. From (43) it follows that diagonal matrix elements are unchanged (i.e., real for all choices of phase), whereas off-diagonal elements will be multiplied by an overall phase factor, because of the product of the f_0^i. The result for diagonal elements also follows from (3), which shows that they may be written as the norm of a vector. Thus diagonal matrix elements are real and positive.

One interesting feature of (44) and (45) is that individual angular momenta for which $m_i = m_i' = j_i$ enter into M only through the quantity $\bar{\jmath}$, since the binomial coefficients and the hypergeometric function are unity in this case. Indeed, the hypergeometric function is unity if either $m_i = j_i$ or $m_i' = j_i$. These simplifications, together with other properties of the matrix elements, will be considered in the next section.

IV. ALTERNATIVE FORMULAS FOR THE MATRIX ELEMENTS

An explicit formula for the matrix elements can be obtained by expanding the hypergeometric functions in (45). This usually is not the simplest procedure. One can rewrite (44) and (45) in forms which take advantage of the symmetry properties of the elements. Furthermore, as will be shown in section VI, recurrence relations may be derived which express a given matrix element in terms of simpler elements.

In obtaining these results, the following well known properties of the hypergeometric functions[13] will be used:

$$F(a, b, c, z) = F(b, a, c, z), \quad (46)$$

$$= (1-z)^{c-a-b}F(c-a, c-b, c, z) \quad (47)$$

$$= (1-z)^{-a}F(a, c-b, c, z/(z-1)), \quad (48)$$

$$\frac{d^n}{dz^n} F(a, b, c, z) = \frac{\Gamma(a+n)\Gamma(b+n)\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c+n)} \times F(a+n, b+n, c+n, z), \quad (49)$$

$$c(1-z)F(a, b, c, z) - cF(a-1, b, c, z) + (c-b)zF(a, b, c+1, z) = 0. \quad (50)$$

Two symmetry properties of the matrix elements are evident immediately. First, consider the set of all nonzero matrix elements for fixed j, j_1, j_2, $\cdots$, j_N [i.e., those elements with different sets m_i, m_i' which satisfy (26)]. Among these, there will be elements which differ only in interchanges of some of the m_i with the corresponding m_i'. Equations (44) and (45) show that these elements are equal because of (46). In other words, the value of a matrix element depends solely upon the pairs (m_i, m_i'), independent of their order, provided that (26) is satisfied.

Second, if (47) is applied to all hypergeometric functions appearing in (45), the total power of $1 - z = 1 + x$ drops out because of (26), and one obtains

$$\sum_r b_r x^r = F(j + m + 1, j + m + 1, 2j + 2, -x) \times \prod_{i=1}^{N} F[-(j_i + m_i), -(j_i + m_i'), -2j_i, -x], \quad (51)$$

i.e., just (45) with all projection quantum numbers replaced by their negatives. Since (44) also is invariant under these changes in sign, one obtains

$$\langle \pi j_i, m_i' | P_{jm} | \pi j_i, m_i \rangle = \langle \pi j_i, -m_i' | P_{j,-m} | \pi j_i, -m_i \rangle. \quad (52)$$

Equation (51) also is obtained if the derivation of Sec. III is carried out starting with (24) for the projection operator, so that the symmetry property (52) proves the equivalence of the two formulas (6) and (24) for P_{jm}.

Equation (52) may be obtained more directly as follows. Equation (2) shows that P_j commutes with the unitary operator[1]

$$R_{\hat{n}}(\theta) = \exp[i\theta \mathbf{J} \cdot \hat{n}] \quad (53)$$

for a rotation through an angle θ about an axis specified by the unit vector $\hat{n}$. Thus one has, for any rotation

$$\langle \pi j_i m_i' | P_{jm} | \pi j_i m_i \rangle = \langle \pi j_i m_i' | R^\dagger P_{jm} R | \pi j_i m_i \rangle. \quad (54)$$

Taking the rotation through π about the y axis and using the simple form of the rotation matrices[1] in this case, one obtains (52) after a short calculation.

[13] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953,) Vol. I, especially pp. 101–106.

The formulas for the matrix elements may be rewritten in a form which includes, among others, the above two symmetry properties. Because of (47), one has, for any m,

$$F(j-m+1, j-m+1, 2j+2, -x) = (1+x)^{m-|m|} \times F(j-|m|+1, j-|m|+1, 2j+2, -x). \quad (55)$$

To rewrite the product in (45), define, for each i,

$$p_i = \max(|m_i|, |m_i'|), \quad q_i = |m_i + m_i'| - p_i. \quad (56)$$

From (56) it follows that

$$|q_i| \leq p_i \leq j_i, \quad (57)$$

Using (46) and (47), one can set

$$F[-(j_i - m_i), -(j_i - m_i'), -2j_i, -x] = F[-(j_i - p_i), -(j_i - q_i), -2j_i, -x] \quad \text{if} \quad m_i + m_i' \geq 0$$

$$= (1+x)^{p_i+q_i} F[-(j_i - p_i), -(j_i - q_i), -2j_i, -x] \quad \text{if} \quad m_i + m_i' < 0. \quad (58)$$

Using these results, (44) and (45) become

$$M = \binom{2j}{j-|m|}^{-1} \left[\prod_{i=1}^{N} \binom{2j_i}{j_i - p_i}\binom{2j_i}{j_i - q_i}\right]^{\frac{1}{2}} b_{\bar{j}-j} \quad (59)$$

$$\sum_r b_r x^r = (1+x)^{k-|m|} \times F(j-|m|+1, j-|m|+1, 2j+2, -x) \times \prod_{i=1}^{N} F[-(j_i - p_i), -(j_i - q_i), -2j_i, -x], \quad (60)$$

where

$$k = m + \sum_{(m_i + m_i' < 0)} (p_i + q_i).$$

Since

$$m = \tfrac{1}{2}\sum_i (m_i + m_i') = \tfrac{1}{2} \sum_{(m_i+m_i' \geq 0)} (p_i + q_i) - \tfrac{1}{2} \sum_{(m_i+m_i' < 0)} (p_i + q_i),$$

one can write k as a sum over all i

$$k = \frac{1}{2}\sum_{i=1}^{N} (p_i + q_i). \quad (61)$$

Equations (59)–(61) show that all individual angular momenta with the same values of j_i, p_i, and q_i enter into the matrix element in exactly the same way. It is convenient to divide the N angular momenta into subsets $S = S(j_s, p_s, q_s)$ such that all elements of a particular subset have the same values of j_i, p_i, and q_i. Let $n_s = n(j_s, p_s, q_s)$ be the number of elements in the subset S. Clearly

$$\sum_s n_s = N. \quad (62)$$

From (56) it follows that the subset $S(j_s, p_s, q_s)$ includes all individual angular momenta for which one of the following is satisfied.

(a) $j_i = j_s \quad m_i = p_s \quad m_i' = q_s$

(b) $j_i = j_s \quad m_i = q_s \quad m_i' = p_s$

(c) $j_i = j_s \quad m_i = -p_s \quad m_i' = -q_s$

(d) $j_i = j_s \quad m_i = -q_s \quad m_i' = -p_s.$

Equation (34), and (59)–(61) can be written in terms of sums and products over subsets

$$M = \binom{2j}{j-|m|}^{-1} \prod_s \left[\binom{2j_s}{j_s - p_s}\binom{2j_s}{j_s - q_s}\right]^{n_s/2} \cdot b_{\bar{j}-j}, \quad (63)$$

$$\sum_r b_r x^r = (1+x)^{k-|m|} \times F(j-|m|+1, j-|m|+1, 2j+2, -x) \times \prod_s \{F[-(j_s - p_s), -(j_s - q_s), -2j_s, -x]\}^{n_s}, \quad (64)$$

$$\bar{j} = \sum_s j_s n_s, \qquad k = \tfrac{1}{2}\sum_s (p_s + q_s) n_s. \quad (65)$$

For each S, the numbers j_s, p_s, q_s are known, so that the dependence of the matrix element on any subset S is given by the single number n_s. Since those n_s for which $p_s = |q_s| = j_s$ enter only through the definitions (65) of $\bar{j}$ and k, it is convenient to consider the matrix elements to be functions of $\bar{j}$ and k, rather than of these n_s. Eqs. (63) and (64) then show that b and M depend on the following parameters:

$$b_{\bar{j}-j} = b_{\bar{j}-j}(j, |m|, \bar{j}, k, \{n_s \mid p_s < j_s\}), \quad (66)$$

$$M = M(j, |m|, \bar{j}, k, \{n_s \mid |q_s| < j_s\}). \quad (67)$$

By parameterizing in this fashion, one takes advantage of the fact that certain matrix elements with different values of N are equal.

Since the remainder of the calculation of M is trivial, let us consider the quantity $b_{\bar{j}-j}$. The parameterization of (66) is not minimal. For example, consider those sets S for which $p_s = j_s - 1$. One has

$$F[-1, -(j_s - q_s), -2j_s, -x] = 1 + \tfrac{1}{2}(1 - q_s/j_s)x. \quad (68)$$

There are many such sets S, allowed by Eq. (57), with the same ratio of q_s to j_s. Equations (64) and (68) show that $b_{\bar{j}-j}$ depends only upon the sum of the corresponding n_s. For instance, all sets with $p_s = j_s - 1$ and $q_s = 0$ give $F = 1 + \frac{1}{2}x$. Such a set occurs for every integral $j_s > 0$. The sets with

$p_s = j_s - 1$ are particularly easy to handle in evaluating $b_{\bar{\jmath}-j}$, since the powers of the hypergeometric functions appearing in (64) can be expanded by the binomial theorem.

If the maximum value of j_i is small, the set of n_s entering (66) or (67) is correspondingly small, independent of the number of individual angular momenta coupled. For example, if all $j_i \leq \frac{3}{2}$, the only $n(j_s, p_s, q_s)$ that enter into $b_{\bar{\jmath}-j}$ are $n(1, 0, 0)$, $n(\frac{3}{2}, \frac{1}{2}, \frac{1}{2})$ and $n(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2})$, because of the condition (57).

One additional simplification may be introduced into the expressions for M. Using (47) and (49), one may write

$$
\begin{aligned}
&F(j-|m|+1, j-|m|+1, 2j+2, -x) \\
&\quad = \frac{(-)^{j-|m|}(2j+1)!}{[(j-|m|)!]^2(j+|m|+1)!}\frac{d^{j-|m|}}{dx^{j-|m|}} \\
&\qquad \times F(1, 1, j+|m|+2, -x), \\
&\quad = \frac{(-)^{j-|m|}(2j+1)!}{[(j-|m|)!]^2(j+|m|+1)!}\frac{d^{j-|m|}}{dx^{j-|m|}} \\
&\qquad \times [(1+x)^{j+|m|} \\
&\qquad \times F(j+|m|+1, j+|m|+1, j+|m|+2, -x)], \\
&\quad = \frac{(-)^{j-|m|}(2j+1)!}{(j-|m|)!\,(j+|m|+1)!} \\
&\qquad \times \sum_{i=0}^{j-|m|}\left[\frac{1}{i!\,(j-|m|-i)!}\frac{d^i}{dx^i}(1+x)^{j+|m|}\right. \\
&\qquad \left.\times \frac{d^{j-|m|-i}}{dx^{j-|m|-i}}\right. \\
&\qquad \times F(j+|m|+1, j+|m|+1, j+|m|+2, -x)], \\
&\quad = (2j+1)\binom{2j}{j-|m|} \\
&\qquad \times \sum_{i=0}^{j-|m|}\left[\frac{(-)^i[(2j-i)!]^2}{i!\,(j-|m|-i)!\,(j+|m|-i)!\,(2j+1-i)!}\right. \\
&\qquad \times (1+x)^{j+|m|-i} \\
&\qquad \left.\times F(2j+1-i, 2j+1-i, 2j+2-i, -x)\right], \\
&\quad = (2j+1)\binom{2j}{j-|m|}(1+x)^{-j+|m|} \\
&\qquad \times \sum_{i=0}^{j-|m|}\frac{(-)^i[(2j-i)!]^2 F(1,1,2j+2-i,-x)}{i!\,(j-|m|-i)!\,(j+|m|-i)!\,(2j+1-i)!}.
\end{aligned}
\tag{69}
$$

From (50) one has

$$
\begin{aligned}
&F(1, 1, c, -x) \\
&= \frac{c-1}{c-2}\left[\frac{1+x}{x}F(1, 1, c-1, -x) - \frac{1}{x}\right].
\end{aligned}
\tag{70}
$$

Upon substitution into (69) and hence into (64), the last term of (70), with $c = 2j + 2 - i$, leads to a highest power of x of

$$
\begin{aligned}
&k - |m| - j + |m| - 1 + \sum_s (j_s - p_s)n_s \\
&\qquad = \bar{\jmath} - j - 1 - \tfrac{1}{2}\sum_s (p_s - q_s)n_s < \bar{\jmath} - j.
\end{aligned}
$$

Since this term does not contribute to the matrix element, it may be dropped. As the factor $(1 + x)/x$ in (70) does not change the highest power, this argument may be repeated, allowing the substitution

$$
\begin{aligned}
&F(1, 1, 2j+2-i, -x) \\
&\quad \to (2j+1-i)\left(\frac{1+x}{x}\right)^{2j-i}F(1, 1, 2, -x)
\end{aligned}
\tag{71}
$$

in each term in (69).[14] The sum then can be performed, leading to

$$
\begin{aligned}
&F(j-|m|+1, j-|m|+1, 2j+2, -x) \\
&\to (2j+1)\binom{2j}{j-|m|}^2\frac{(1+x)^{j+|m|}}{x^{2j}}F(1, 1, 2, -x) \\
&\quad \times F\left[-(j-|m|), -(j+|m|), -2j, \frac{x}{1+x}\right] \\
&= (2j+1)\binom{2j}{j-|m|}^2\frac{(1+x)^{2|m|}}{x^{2j}}F(1, 1, 2, -x) \\
&\quad \times F[-(j-|m|), -(j-|m|), -2j, -x]
\end{aligned}
\tag{72}
$$

to be substituted into (64). Equation (48) has been used in the last step.

The last hypergeometric function in (72) is exactly of the form of those in the product in (64) with

$$
j_s = j \qquad p_s = q_s = |m|. \tag{73}
$$

Thus we add an extra particle with j_s, p_s, q_s given by (73) to the appropriate group S and consider the coupling of $N + 1$ particles. Let N_s be the number of particles in the augmented sets S (i.e. $N_s = n_s$ except for the set (73), for which $N_s = n_s + 1$). Define

$$
\bar{J} = \bar{\jmath} + j = \sum_s j_s N_s, \tag{74}
$$

$$
K = k + |m| = \tfrac{1}{2}\sum_s (p_s + q_s)N_s. \tag{75}
$$

With these new definitions, substitution of (72) into (63) gives

$$
M = (2j+1)Z, \tag{76}
$$

where

$$
Z = \prod_s\left[\binom{2j_s}{j_s - p_s}\binom{2j_s}{j_s - q_s}\right]^{N_s/2}C_J, \tag{77}
$$

$$
\begin{aligned}
&\sum_r C_r x^r = (1+x)^K F(1, 1, 2, -x) \\
&\quad \times \prod_s \{F[-(j_s - p_s), -(j_s - q_s), -2j_s, -x]\}^{N_s}.
\end{aligned}
\tag{78}
$$

Comparison of (77) and (78) with (63) and (64) shows that the quantity Z is just the matrix element

[14] Note that $F(1, 1, 2, -x) = \log(1 + x)/x$.

for the coupling of the augmented set of $N + 1$ particles to give $j = 0$. This will be discussed further in the next section. Since the quantum numbers j and $|m|$ have been incorporated into the N_s, the quantities C and Z depend on two less parameters than the corresponding quantities b and M, i.e.,

$$C_J = C_J(\bar{J}, K, \{N_s \mid p_s < j_s\}), \tag{79}$$

$$Z = Z(\bar{J}, K, \{N_s \mid |q_s| < j_s\}). \tag{80}$$

One final change can be made in (77) and (78). The same argument that led to (71) shows that the substitution

$$(1 + x)^K F(1, 1, 2, -x) \rightarrow (K + 1)^{-1} x^K F(1, 1, K + 2, -x) \tag{81}$$

does not change the matrix element, so that one can write

$$Z = \frac{1}{K+1} \prod_s \left[\binom{2j_s}{j_s - p_s} \binom{2j_s}{j_s - q_s} \right]^{N_s/2} d_{J-K} \tag{82}$$

$$\sum_r d_r x^r = F(1, 1, K + 2, -x) \times \prod_s \{F[-(j_s - p_s), -(j_s - q_s), -2j_s, -x]\}^{N_s}. \tag{83}$$

V. RELATION OF MATRIX ELEMENTS TO VECTOR COUPLING COEFFICIENTS

Equation (76) between M and Z is an extension to N angular momenta of the relationship between the Clebsch–Gordan (CG) coefficients, which couple two angular momenta to give a resultant J, and the $3 - j$ symbols, which enter into the coupling of three angular momenta to give zero.[1] To see this, consider the matrix elements M for the coupling

$$\mathbf{J}_1 + \mathbf{J}_2 = \mathbf{J}.$$

In this case, since the coupled state vector $|j_1 j_2 j m>$ is nondegenerate, one can write

$$P_{jm} = |j_1 j_2 j m\rangle\langle j_1 j_2 j m|. \tag{84}$$

It follows that

$$M = \langle j_1 m_1' j_2 m_2' | P_{jm} | j_1 m_1 j_2 m_2 \rangle = \langle j_1 m_1' j_2 m_2' \mid j_1 j_2 j m\rangle\langle j_1 j_2 j m \mid j_1 m_1 j_2 m_2\rangle. \tag{85}$$

Assuming the usual phase conventions, the CG coefficients are real. Equation (85) shows that M is the product of two CG coefficients, with the same values of j_1, j_2, and j and with

$$m_1 + m_2 = m_1' + m_2' = m. \tag{86}$$

The $3 - j$ symbols are defined by[1]

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-)^{j_1 - j_2 - m_3}}{\sqrt{2j_3 + 1}} \langle j_1 m_1 j_2 m_2 \mid j_1 j_2 j_3, -m_3\rangle. \tag{87}$$

From (76), (85), and (87) one obtains the result

$$Z = \begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & -m \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}. \tag{88}$$

The various symmetry properties of the $3 - j$ symbols,[1] if applied to (88), lead to invariance properties of Z that are obvious from (82) and (83). These symmetry properties must be applied to both factors in (88), since this equation is meaningful only if the order of j_1, j_2, j_3 and the sign of m are the same in both factors. This result suggests that our final formula for the matrix element may be the most symmetrical possible.

Calais[15] has obtained the general formula for the CG coefficients by projection operator techniques. This can also be done using the expressions derived here. The phases of the CG coefficients are usually defined by the condition that those coefficients with $m_1 = j_1$ are real and positive. Since this is also true for diagonal matrix elements, it follows from (85) that

$$\langle j_1 m_1 j_2 m_2 \mid j_1 j_2 j m\rangle = \frac{\langle j_1 j_1 j_2, m - j_1 | P_{jm} | j_1 m_1 j_2 m_2\rangle}{\langle j_1 j_1 j_2, m - j_1 | P_{jm} | j_1 j_1 j_2, m - j_1\rangle^{\frac{1}{2}}}. \tag{89}$$

For this particular case, where one is adding only two angular momenta, it is most convenient to use Eqs. (44) and (45) for the matrix elements. Setting $\bar{j} = j_1 + j_2$, one obtains for the numerator in (89)

$$b^N_{j_1+j_2-j} = \frac{(2j+1)!\,(j_2 - m_2)!\,(j_1 + j_2 - m)!}{[(j-m)!]^2 (2j_2)!} \times \sum_{\substack{r,t \\ (r+t=j_1+j_2-j)}} \frac{(-)^t [(j - m + t)!]^2 (2j_2 - r)!}{t!\,(2j + 1 + t)!\,r!\,(j_2 - m_2 - r)!\,(j_1 + j_2 - m - r)!}$$

$$= (-)^{j_1+j_2-j} \frac{(2j+1)!\,(j_2 - m_2)!\,(j_1 + j_2 - m)!}{[(j-m)!]^2 (2j_2)!} \times \sum_r \frac{(-)^r (j_1 + j_2 - m - r)!\,(2j_2 - r)!}{r!\,(j_1 + j_2 + j + 1 - r).\,(j_1 + j_2 - j - r)!\,(j_2 - m_2 - r)!}. \tag{90}$$

[15] J.-L. Calais, Technical Note No. 25 from the Quantum Chemistry Group of Uppsala University (1959).

The sum in (90) goes over the values

$$0 \leq r \leq \min (j_2 - m_2, j_1 + j_2 - j). \tag{91}$$

For the denominator in (89), one has $m_2 = m - j_1$, and (90) becomes, after setting $r = j_1 + j_2 - j - s$,

$$b^D_{j_1+j_2-j} = \frac{(2j+1)!}{(2j_2)!}\left[\frac{(j_1+j_2-m)!}{(j-m)!}\right]^2 \sum_s \frac{(-)^s(j+j_2-j_1+s)!}{s!\,(j_1+j_2-j-s)!\,(2j+1+s)!}$$

$$= \frac{(2j+1)!}{(2j_2)!}\left[\frac{(j_1+j_2-m)!}{(j-m)!}\right]^2 \frac{(2j_1)!\,(j+j_2-j_1)!}{(j_1+j_2-j)!\,(j_1-j_2+j)!\,(j_1+j_2+j+1)!}. \tag{92}$$

The summation in (92) has been performed using the relation[13]

$$F(a, b, c, 1) = \Gamma(c)\Gamma(c-a-b)/\Gamma(c-a)\Gamma(c-b). \tag{93}$$

Evaluating the matrix elements by (44) and substituting into (89), one obtains the following formula for the CG coefficients:

$$\langle j_1 m_1 j_2 m_2 \mid j_1 j_2 j m\rangle = (-)^{j_1+j_2-j}$$

$$\times \left[\frac{(2j+1)(j_1+j_2-j)!\,(j_1-j_2+j)!\,(j_1+j_2+j+1)!\,(j+m)!\,(j_2-m_2)!}{(j+j_2-j_1)!\,(j-m)!\,(j_1-m_1)!\,(j_1+m_1)!\,(j_2+m_2)!}\right]^{\frac{1}{2}}$$

$$\times \sum_r \frac{(-)^r(j_1+j_2-m-r)!\,(2j_2-r)!}{r!\,(j_1+j_2+j+1-r)!\,(j_1+j_2-j-r)!\,(j_2-m_2-r)!}. \tag{94}$$

Equation (94) can readily be shown to be equivalent to the formulas appearing in the literature.[1]

The author has obtained, by the use of projection operators, the general formula of Racah[16] for the $6-j$ symbols. This derivation has not been included in this paper because it does not use the matrix representation.

VI. RELATIONS BETWEEN MATRIX ELEMENTS

In many applications, one needs the matrix elements M or Z for a range of values of the parameters. When this is so, the computations are simplified by using relations which connect different matrix elements. For the quantity Z, these relations follow immediately by expanding one of the factors in (78) as a power series. Each resulting term can then be put in the form of (77) and (78) (for different values of the parameters) and identified with a matrix element. For example, a power x^n in the series has the effect of changing $\bar{J}$ into $\bar{J} - n$. Similar considerations can be used in (64) to obtain relations on M.

By expanding a factor $1 + x$ in (78), one obtains

$$Z(\bar{J}, K, \{N_s\}) = Z(\bar{J}, K-1, \{N_s\}) + Z(\bar{J}-1, K-1, \{N_s\}), \tag{95}$$

which gives an element with value K in terms of elements with the value $K - 1$, for fixed values of the N_s.

Relations in which a particular N_t is decreased by one may be obtained by expanding a corresponding hypergeometric function in (78). Direct expansion gives

$$Z(\bar{J}, K, \{N_s\}) = \left[\frac{(j_t-p_t)!\,(j_t-q_t)!}{(j_t+p_t)!\,(j_t+q_t)!}\right]^{\frac{1}{2}} \sum_{\lambda=0}^{j_t-p_t} \frac{(2j_t-\lambda)!\,Z(\bar{J}-\lambda, K, \{N_s-\delta_{ts}\})}{\lambda!\,(j_t-p_t-\lambda)!\,(j_t-q_t-\lambda)!}. \tag{96}$$

Another useful result comes from using (48) and then expanding as a power series in $x/(1+x)$; this gives

$$Z(\bar{J}, K, \{N_s\}) = \left[\frac{(j_t-p_t)!\,(j_t+q_t)!}{(j_t+p_t)!\,(j_t-q_t)!}\right]^{\frac{1}{2}} \sum_{\lambda=0}^{j_t-p_t} \frac{(-)^\lambda(2j_t-\lambda)!\,Z(\bar{J}-\lambda, K+j_t-p_t-\lambda, \{N_s-\delta_{ts}\})}{\lambda!\,(j_t-p_t-\lambda)!\,(j_t+q_t-\lambda)!}. \tag{97}$$

[16] G. Racah, Phys. Rev. **62**, 438 (1942).

In (95)–(97) the set $\{N_s\}$ does not include those subsets for which $|q_s| = j_s$. Even though they may have equal values for all N_s, different terms in (95)–(97) correspond to matrix elements in which different numbers of angular momenta are coupled.

VII. SPECIAL CASES

In many problems, the expressions for the matrix elements simplify because the values of the parameters are restricted. Some of these special cases are considered in this section.

1. Diagonal Matrix Elements

Some calculations, such as that of isotopic spin statistical weights in Ref. 11, involve only diagonal matrix elements. It has been shown that these elements are real and positive. Since all angular momenta have $q = p$, there is no square root in (82), and the set $N_s = N(j_s, p_s)$ entering into Z is the same as that entering into d, namely, those for which $0 \leq p_s < j_s$. Furthermore, $\bar{J}$ and K are no longer independent, since (74) and (75) give

$$K = \bar{J} - \sigma, \tag{98}$$

where

$$\sigma = \sum_s (j_s - p_s)N(j_s, p_s) \tag{99}$$

involves only those N_s entering into the matrix elements Z_D. Thus one has

$$Z_D = Z_D(\bar{J}, \{N(j_s p_s) \mid 0 \leq p_s < j_s\}). \tag{100}$$

For example, if all angular momenta (including j) have $j_i \leq \frac{3}{2}$, the quantities Z_D depend only upon the three parameters $\bar{J}$, $N(1, 0)$ and $N(\frac{3}{2}, \frac{1}{2})$, independent of the number of angular momenta coupled.

For a general diagonal element, Eqs. (82) and (83) become

$$Z_D = \frac{1}{\bar{J} - \sigma + 1} \prod_s \binom{2j_s}{j_s - p_s}^{N(j_s,p_s)} \cdot d_\sigma, \tag{101}$$

$$\sum_r d_r x^r = F(1, 1, \bar{J} - \sigma + 2, -x) \times \prod_s \{F[-(j_s - p_s), -(j_s - p_s), -2j_s, -x]\}^{N(j_s,p_s)}. \tag{102}$$

For an equation between matrix elements to involve only diagonal elements, every term must satisfy (98). Of the relations derived in Sec. VI, this condition is obeyed only by (97), which becomes

$$Z_D(\bar{J}, \{N_s\}) = \sum_{\lambda=0}^{j_i - p_i} \frac{(-)^\lambda (2j_i - \lambda)!\, Z_D(\bar{J} - \lambda, \{N_s - \delta_{is}\})}{\lambda!\,(j_i - p_i - \lambda)!\,(j_i + p_i - \lambda)!}. \tag{103}$$

Equations (98)–(103) have been used by J.N.-S. Wong and the author to extend the tables of[11] for the construction of isotopic spin statistical weights to include particles with I spins up to $\frac{5}{2}$. These results will be published in a separate article.

2. Matrix Elements with $|m| = j$

Although j enters the symmetric quantity Z in the same way as all other angular momenta, this case (named by Löwdin "the principal case") enters into calculations often enough to merit separate discussion. Wavefunctions for arbitrary m can be constructed from those for $|m| = j$ by application of the raising or lowering operators. In addition, physical results frequently are independent of m. For example, the energy of a rotationally invariant system is independent of the projection quantum number of the total angular momentum.

When $|m| = j$, the corresponding N_s does not enter into (82) and (83), so that one can set $N_s = n_s$, $\bar{J} = \bar{\jmath} + j$ and $K = k + j$, giving

$$Z(\bar{\jmath} + j, k + j, \{n_s\}) = \frac{1}{k + j + 1} \prod_s \left[\binom{2j_s}{j_s - p_s}\binom{2j_s}{j_s - q_s}\right]^{n_s/2} d_{\bar{\imath}-k}, \tag{104}$$

$$\sum_r d_r x^r = F(1, 1, k + j + 2, -x) \times \prod_s \{F[-(j_s - p_s), -(j_s - q_s), -2j_s, -x]\}^{n_s}. \tag{105}$$

Equations (104) and (105) express Z in terms of the original set of N angular momenta. Equation (76) is equivalent to the relation

$$M(j, |m| = j, \bar{\jmath}, k, \{n_s\}) = (2j + 1)M(0, 0, \bar{\jmath} + j, k + j, \{n_s\}) \tag{106}$$

between the matrix elements M.

3. Matrix Elements for j near $\bar{\jmath}$

When the difference $\bar{\jmath} - j$ is small, the elements may be evaluated directly from (44) and (45). For example, by evaluating b_0 and b_1 in (45), one obtains for the cases $j = \bar{\jmath}$ and $j = \bar{\jmath} - 1$ the results

$$M(j = \bar{\jmath}) = \binom{2j}{j - m}^{-1} \left[\prod_{i=1}^{N} \binom{2j_i}{j_i - m_i}\binom{2j_i}{j_i - m_i'}\right]^{\frac{1}{2}}, \tag{107}$$

$$M(j=\bar{j}-1)=\binom{2j}{j-m}^{-1}\left[\prod_{i=1}^{N}\binom{2j_i}{j_i-m_i}\binom{2j_i}{j_i-m_i'}\right]^{\frac{1}{2}} \times\left[\sum_{i=1}^{N}\frac{(j_i-m_i)(j_i-m_i')}{2j_i}-\frac{(j-m+1)^2}{2j+2}\right]. \quad (108)$$

4. Matrix Elements when $p_s = j_s$ for Nearly All N_s

Equation (83) simplifies in this case, since most of the hypergeometric functions become unity. It should be remembered, however, that a nonzero N_s will enter Z if $|q_s| < j_s$, even though $p_s = j_s$, because of the binomial coefficients in (82). We consider a few simple cases.

a. All $p_s = j_s$

The product in (83) becomes unity, so that

$$d_{J-K} = (-)^{J-K}(K+1)!\,(\bar{J}-K)!/(\bar{J}+1)!, \quad (109)$$

$$Z = (-)^{J-K}\frac{K!\,(\bar{J}-K)!}{(\bar{J}+1)!}\prod_s\binom{2j_s}{j_s-q_s}^{N_s/2}. \quad (110)$$

b. All $p_s = j_s$, except $s = t$, for which $N_t = 1$

Using (110) in (96) and (97), one obtains the two equivalent results

$$Z = (-)^{J-K}K! \times\left[\frac{(j_t-p_t)!\,(j_t-q_t)!}{(j_t+p_t)!\,(j_t+q_t)!}\right]^{\frac{1}{2}}\prod_{(s\neq t)}\binom{2j_s}{j_s-q_s}^{N_s/2} \times\sum_{\lambda=0}^{j_t-p_t}\frac{(-)^\lambda(2j_t-\lambda)!\,(\bar{J}-K-\lambda)!}{\lambda!\,(j_t-p_t-\lambda)!\,(j_t-q_t-\lambda)!\,(\bar{J}+1-\lambda)!} \quad (111)$$

and

$$Z = (-)^{J-K-j_t+p_t}(\bar{J}-K-j_t+p_t)! \times\left[\frac{(j_t-p_t)!\,(j_t+q_t)!}{(j_t+p_t)!\,(j_t-q_t)!}\right]^{\frac{1}{2}}\prod_{(s\neq t)}\binom{2j_s}{j_s-q_s}^{N_s/2} \times\sum_{\lambda=0}^{j_t-p_t}\frac{(-)^\lambda(2j_t-\lambda)!\,(K+j_t-p_t-\lambda)!}{\lambda!\,(j_t-p_t-\lambda)!\,(j_t+q_t-\lambda)!\,(\bar{J}-\lambda+1)!}. \quad (112)$$

One special case contained in (111) or (112) is the coupling of N spin $\frac{1}{2}$ particles to give a total spin s and projection m. Taking t to be the particle with $j_t = s$ and $p_t = q_t = |m|$, the binomial coefficients and the square root in (112) reduce to unity. One can set

$$\bar{J} = \bar{s}+s, \quad K = \bar{s}+|m|-\beta, \quad (113)$$

where

$$N = 2\bar{s}, \quad \beta = \tfrac{1}{2}\sum_s(j_s-q_s)n_s = \tfrac{1}{2}n(\tfrac{1}{2},\tfrac{1}{2},-\tfrac{1}{2}). \quad (114)$$

Clearly β is the number of pairs of spin flips in going from the initial to the final state in the matrix element. From (112) one obtains

$$M(s,m,\bar{s},\beta) = (-)^\beta(2s+1)\beta! \times\sum_{\lambda=0}^{s-|m|}\frac{(-)^\lambda(2s-\lambda)!\,(\bar{s}+s-\beta-\lambda)!}{\lambda!\,(s-m-\lambda)!\,(s+m-\lambda)!\,(\bar{s}+s+1-\lambda)!}. \quad (115)$$

In this case, the projected state vectors take the simple form

$$P_{sm}\,|\prod\tfrac{1}{2},m_i\rangle = \sum_\beta\{M(s,m,\bar{s},\beta)\sum_{m_i'(\beta)}|\prod_i\tfrac{1}{2},m_i'\rangle\}. \quad (116)$$

For each term in (116), the inner sum is to be taken over all possible sets of m_i' leading to the specified value β for the number of pairs of spin flips.

A formula which is equivalent to (115) has been derived by Sasaki and Ohno.[17] Special cases of (115) have been obtained by several authors[2,18,19] and used to find the spin projection of a Slater determinant.

c. All $p_s = j_s$ except $s = r$, for which $p_r = j_r - 1$ and N_r is arbitrary

In this case (68) and (83) give

$$\sum d_i x^i = F(1,1,K+2,-x)[1+(j_r-q_r)x/2j_r]^{N_r}. \quad (117)$$

Using the binomial theorem in the second factor, one obtains

$$d_{J-K} = \sum_{\substack{\lambda,\mu\\(\lambda+\mu=\bar{J}-K)}}(-)^\lambda\left[\binom{N_r}{\mu}\Big/\binom{K+1+\lambda}{K+1}\right]\left(\frac{j_r-q_r}{2j_r}\right)^\mu = (-)^{J-K}\sum_{\mu=0}^{N_r}\left[\binom{N_r}{\mu}\Big/\binom{\bar{J}+1-\mu}{K+1}\right]\left(-\frac{j_r-q_r}{2j_r}\right)^\mu \quad (118)$$

and from (82)

$$Z = \frac{(-)^{\bar{J}-K}}{K+1}(2j_r)^{N_r/2}\prod_s\binom{2j_s}{j_s-q_s}^{N_s/2} \times\sum_{\mu=0}^{N_r}\left[\binom{N_r}{\mu}\Big/\binom{\bar{J}+1-\mu}{K+1}\right]\left(-\frac{j_r-q_r}{2j_r}\right)^\mu. \quad (119)$$

[17] F. Sasaki and K. Ohno, J. Math. Phys. 4, 1140 (1963).
[18] J. K. Percus and A. Rotenberg, J. Math. Phys. 3, 928 (1962).
[19] R. Pauncz, Technical Note No. 82 from the Quantum Chemistry Group of Uppsala University (1962).

One special case contained in (119) is the coupling of N particles, all with $j_i \leq 1$, to give a total angular momentum satisfying either $j \leq 1$ or $|m| = j$. Under these conditions, only $N_1 = N(1, 0, 0)$ and $N_2 = N(1, 1, 0)$ enter into (119). The quantity N_2 enters only through the binomial coefficient and N_1 has $p_1 = j_1 - 1$, so we set $r = 1$. Equation (119) becomes

$$Z = \frac{(-)^{\bar{J}-K}2^{N_1+N_2/2}}{K+1} \times \sum_{\mu=0}^{N_1}\left[\binom{N_1}{\mu}\Big/\binom{\bar{J}+1-\mu}{K+1}\right]\left(-\frac{1}{2}\right)^{\mu}$$

$$= \frac{(-)^{\bar{J}-K-N_1}2^{N_2/2}}{K+1} \times \sum_{\nu=0}^{N_1}\left[\binom{N_1}{\nu}(-2)^{\nu}\Big/\binom{\bar{J}+1-N_1+\nu}{K+1}\right]. \quad (120)$$

A formula for arbitrary values of j and m is obtained by substituting (120) with $\bar{J} = \bar{j}$, $K = k$ and $N_r = n_r$ into either (96) or (97) for $j_i = j$ and $p_i = q_i = |m|$. The diagonal elements for this case have been treated in Ref. 11, in which an alternative expression was derived. For diagonal elements one has $n_2 = 0$ and $k = \bar{j} - n_1$.

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Solution of an Atomic Integral Containing Three Odd Powers of Interelectronic Separation Coordinates

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(Received 25 January 1965)

A wavefunction expressed as a linear combination of terms each involving only one interelectronic separation coordinate requires the solution of matrix elements of the Hamiltonian which contain three odd powers of the interelectronic separation coordinates. This paper discusses in detail the integration of $\int\int\int \rho_1^k\rho_2^m\rho_3^n\rho_{23}\rho_{13}^{-1}\rho_{12}\exp -(a\rho_1 + b\rho_2 + c\rho_3)d\tau_1 d\tau_2 d\tau_3$.

INTRODUCTION

With the advent of high-speed electronic digital computers it has only recently[1-3] become feasible to extend the correlated wave functions of Hylleraas,[4] and James and Coolidge[5] to atoms with more than three electrons. By employing interelectronic separation coordinates the aforementioned authors were able to converge rather quickly to the experimentally determined ground-state energies via a variational procedure.

By considering interelectronic separations individually one can construct a total wavefunction whose terms each involve only one of the $\frac{1}{2}N(N-1)$ possible interelectronic separation coordinates of an N-electron atom. In this way the most involved energy matrix elements merely require the solution of three-electron integrals.

It is the purpose of this paper to discuss the solution of that three-electron integral containing three odd powers of the interelectronic separation coordinates.

FORMULATION

Neglecting nuclear motion, the nonrelativistic Hamiltonian for many-electron atoms with the energy in units of $e^2/2a_0$ is given by

$$H = \sum_i -\nabla_i^2 - (2Z/\rho_i) + \Big(\sum_{j>i} 2/\rho_{ij}\Big). \quad (1)$$

The N-electron wavefunction is

$$\phi = \sum_i c(i)\Big(\prod_{j=1}^{N}\rho_j^{k(j,i)}\Big) \times \exp -\Big(\prod_{j=1}^{N}\alpha(i,j)\rho_j\Big)\prod_{j>l}^{N}\rho_{lj}^{m(l,j,i)}. \quad (2)$$

In each of the i-terms of Eq. (2), only one ρ_{ij} is used and we restrict m values for that coordinate to be 0, 1, or 2. With these limitations, three odd

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One special case contained in (119) is the coupling of N particles, all with $j_i \leq 1$, to give a total angular momentum satisfying either $j \leq 1$ or $|m| = j$. Under these conditions, only $N_1 = N(1, 0, 0)$ and $N_2 = N(1, 1, 0)$ enter into (119). The quantity N_2 enters only through the binomial coefficient and N_1 has $p_1 = j_1 - 1$, so we set $r = 1$. Equation (119) becomes

$$Z = \frac{(-)^{\bar{J}-K}2^{N_1+N_2/2}}{K+1} \times \sum_{\mu=0}^{N_1}\left[\binom{N_1}{\mu}\Big/\binom{\bar{J}+1-\mu}{K+1}\right]\left(-\frac{1}{2}\right)^{\mu}$$

$$= \frac{(-)^{\bar{J}-K-N_1}2^{N_2/2}}{K+1} \times \sum_{\nu=0}^{N_1}\left[\binom{N_1}{\nu}(-2)^{\nu}\Big/\binom{\bar{J}+1-N_1+\nu}{K+1}\right]. \quad (120)$$

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powers of interelectronic separation coordinates may occur in only one way, viz.

$$I = \int_{\tau_1}\int_{\tau_2}\int_{\tau_3} \rho_1^k \rho_2^m \rho_3^n \rho_{23}\rho_{13}^{-1}\rho_{12}\, e^{-(a\rho_1+b\rho_2+c\rho_3)}\, d\tau_1\, d\tau_2\, d\tau_3. \tag{3}$$

Multiplying by $\rho_{23}\rho_{12}/\rho_{23}\rho_{12}$ and expanding by the law of cosines with the definition

$$J(k, m, n, l, j) = \int_{\tau_1}\int_{\tau_2}\int_{\tau_3} \rho_1^k \rho_2^m \rho_3^n \rho_{23}^{-1}\rho_{13}^{-1}\rho_{12}^{-1} \cos^l\theta_{23} \cos^j\theta_{12}\, e^{-(a\rho_1+b\rho_2+c\rho_3)}\, d\tau_1\, d\tau_2\, d\tau_3, \tag{4}$$

we have

$$\begin{aligned} I = {} & J(k+2, m+2, n, 0, 0) + J(k, m+4, n, 0, 0) + J(k+2, m, n+2, 0, 0) \\ & + J(k, m+2, n+2, 0, 0) - 2J(k+1, m+3, n, 1, 0) \\ & + J(k+1, m+1, n+2, 1, 0) + J(k+2, m+1, n+1, 0, 1) \\ & + J(k, m+3, n+1, 0, 1) + 4J(k+1, m+2, n+1, 1, 1). \end{aligned} \tag{5}$$

By the Neumann expansion

$$\rho_{ij}^{-1} = \sum_{p=0} \frac{\rho_{ij<}^p}{\rho_{ij>}^{p+1}} P_p(\cos\theta_{ij}), \tag{6}$$

where $\rho_{ij<}$ is the smaller of the distances ρ_i, ρ_j to the ith and jth particles and $\rho_{ij>}$ is the corresponding larger distance and P_p (cos θ_{ij}) is the Legendre polynomial whose argument is the cosine of the angle between ρ_i and ρ_j, hence,

$$\begin{aligned} & J(k, m, n, l, j) \\ & = \sum_p \sum_q \sum_r \int_{\tau_1}\int_{\tau_2}\int_{\tau_3} \frac{\rho_{23<}^p}{\rho_{23>}^{p+1}} \frac{\rho_{13<}^q}{\rho_{13>}^{q+1}} \frac{\rho_{12<}^r}{\rho_{12>}^{r+1}} \\ & \times \rho_1^k \rho_2^m \rho_3^n e^{-(a\rho_1+b\rho_2+c\rho_3)} \cos^l\theta_{23} \cos^j\theta_{12} \\ & \times P_p(\cos\theta_{23}) P_q(\cos\theta_{13}) P_r(\cos\theta_{12})\, d\tau_1\, d\tau_2\, d\tau_3. \end{aligned} \tag{7}$$

If now we measure θ_1, and θ_3 to ρ_2 and ϕ_1, and ϕ_3 on a plane perpendicular to ρ_2, then in this system of coordinates

$$\begin{aligned} \theta_{23} &\to \theta_3, \\ \theta_{12} &\to \theta_1, \\ \theta_{13} &\to \theta_{13}, \\ \phi_1 &\to \psi_1, \\ \phi_3 &\to \psi_3, \\ \phi_2 &\to \psi_2. \end{aligned}$$

By the addition theorem for Legendre polynomials, we may write in our new coordinates

$$\begin{aligned} P_q(\cos\theta_{13}) = {} & P_q(\cos\theta_1) P_q(\cos\theta_3) + 2 \sum_{m=1}^{q} \frac{(q-m)!}{(q+m)!} \\ & \times P_q^m(\cos\theta_1) P_q^m(\cos\theta_3) \cos m(\psi_1 - \psi_3), \end{aligned} \tag{8}$$

and since the ψ_i integrations are 0 to 2π the summation vanishes upon integration over ψ_1 and ψ_3, hence our integral becomes

$$\begin{aligned} & J(k, m, n, l, j) \\ & = 8\pi \sum_p \sum_q \sum_r \iiiint \frac{\rho_{23<}^p}{\rho_{23>}^{p+1}} \frac{\rho_{13<}^q}{\rho_{13>}^{q+1}} \frac{\rho_{12<}^r}{\rho_{12>}^{r+1}} \\ & \times \rho_1^k \rho_2^m \rho_3^n e^{-(a\rho_1+b\rho_2+c\rho_3)} P_p(\cos\theta_3) P_q(\cos\theta_3) \\ & \times P_r(\cos\theta_1) P_q(\cos\theta_1) \cos^l\theta_3 \cos^j\theta_1 \sin\theta_1 \sin\theta_2 \\ & \times \sin\theta_3 \rho_1^2 \rho_2^2 \rho_3^2\, d\rho_1\, d\rho_2\, d\rho_3\, d\theta_1\, d\theta_2\, d\theta_3 \end{aligned} \tag{9}$$

and the coordinates have been separated.

Consider the angular integration

$$\sum_p \sum_q \int_0^\pi P_p(\cos\theta_3) P_q(\cos\theta_3) \cos^l\theta_3 \sin\theta_3\, d\theta_3. \tag{10}$$

Let $x = \cos\theta_3$, $dx = -\sin\theta_3 d\theta$, $x = -1$ for $\theta_3 = \pi$, $x = 1$ for $\theta_3 = 0$, hence we have

$$\sum_p \sum_q \int_{-1}^{+1} P_p(x) P_q(x) x^l\, dx, \tag{11}$$

and for the particular problem solved here, $l = 0$ or 1. For $l = 0$, we have

$$\begin{aligned} & \sum_p \sum_q \int_{-1}^{+1} P_p(x)_q P(x)\, dx \\ & = \sum_p \sum_q \frac{2}{2p+1} \delta_{p,q} \quad \text{or} \quad \sum_q \frac{2}{2q+1}. \end{aligned} \tag{12}$$

For $l = 1$ consider

$$(2p+1)xP_p(x) = (p+1)P_{p+1}(x) + pP_{p-1}(x)$$

or

$$\begin{aligned} xP_p(x) = {} & (1/2p+1) \\ & \times \{(p+1)P_{p+1}(x) + pP_{p-1}(x)\}; \end{aligned} \tag{13}$$

hence for $l = 1$, we have

$$\sum_p \sum_q \frac{1}{2p+1}\left\{\int_{-1}^{+1}(p+1)P_{p+1}(x)P_q(x)\,dx + \int_{-1}^{+1} pP_{p-1}(x)P_q(x)\,dx\right\}$$
$$= \sum_p \sum_q \frac{1}{2p+1}\left\{(p+1)\frac{2}{2q+1}\delta_{p+1,q} + \frac{2p}{2q+1}\delta_{p-1,q}\right\}$$
$$= \sum_q \left[\left(\frac{1}{2(q-1)+1}\frac{((q-1)+1)}{2q+1}\frac{2}{2q+1}\right) + \left(\frac{1}{2(q+1)+1}\frac{(q+1)}{2q+1}\frac{2}{2q+1}\right)\right]$$
$$= \sum_q \frac{2}{(2q+1)}\left(\frac{q}{2q-1} + \frac{q+1}{2q+3}\right) \tag{14}$$

with $p = q-1, q+1$ respectively.

Hence p, r occurring in Eq. 7 depend upon l, j and are functions of q; hence we may calculate the radial integral in terms of p, r define

$$K(k,m,n,p,r) = \int_{\rho_1}^{\infty}\int_{\rho_2}^{\infty}\int_{\rho_3}^{\infty} \frac{\rho_{23<}^{p}}{\rho_{23>}^{p+1}}\frac{\rho_{13<}^{q}}{\rho_{13>}^{q+1}}\frac{\rho_{12<}^{r}}{\rho_{12>}^{r+1}}\rho_1^k\rho_2^m\rho_3^n e^{-(a\rho_1+b\rho_2+c\rho_3)}\rho_1^2\rho_2^2\rho_3^2\,d\rho_1\,d\rho_2\,d\rho_3. \tag{15}$$

Let us perform the integrations in the following manner:

(1) Integrate ρ_2 between the limits (a) $0 \to \rho_{13<}$ (b) $\rho_{13<} \to \rho_{15>}$ (c) $\rho_{13>} \to \infty$.

(2) Integrate ρ_3 between the limits (a) $0 \to \rho_1$ (b) $\rho_1 \to \infty$.

Our integral becomes

$$K(k,m,n,p,r) = \int_0^{\infty}\rho_1^{k+2}e^{-a\rho_1}\,d\rho_1\Bigg[\int_0^{\rho_1}\rho_3^{n+2}e^{-c\rho_3}\,d\rho_3$$
$$\times\left\{\frac{\rho_{23<}^{p}}{\rho_{23>}^{p+1}}\frac{\rho_{13<}^{q}}{\rho_{13>}^{q+1}}\frac{\rho_{12<}^{r}}{\rho_{12>}^{r+1}}\left(\int_0^{\rho_{13<}}\rho_2^{m+2}e^{-b\rho_2}\,d\rho_2 + \int_{\rho_{13<}}^{\rho_{13>}}\rho_2^{m+2}e^{-b\rho_2}\,d\rho_2 + \int_{\rho_{13>}}^{\infty}\rho_2^{m+2}e^{-b\rho_2}\,d\rho_2\right)\right\}$$
$$+\int_{\rho_1}^{\infty}\rho_3^{n+2}e^{-c\rho_3}\,d\rho_3\left\{\frac{\rho_{23<}^{p}}{\rho_{23>}^{p+1}}\frac{\rho_{13<}^{q}}{\rho_{13>}^{q+1}}\frac{\rho_{12<}^{r}}{\rho_{12>}^{r+1}}\left(\int_0^{\rho_{13<}}\rho_2^{m+2}e^{-b\rho_2}\,d\rho_2 + \int_{\rho_{13<}}^{\rho_{13>}}\rho_2^{m+2}e^{-b\rho_2}\,d\rho_2 + \int_{\rho_{13>}}^{\rho_{13<}}\rho_2^{m+2}e^{-b\rho_2}\,d\rho_2\right)\right\}\Bigg]. \tag{16}$$

The ordering of ρ_1, ρ_2 and ρ_3 from least to greatest in each of the 6 integrations is (from left to right)

	least	middle	greatest
1	ρ_2	ρ_3	ρ_1
2	ρ_3	ρ_2	ρ_1
3	ρ_3	ρ_1	ρ_2
4	ρ_2	ρ_1	ρ_3
5	ρ_1	ρ_2	ρ_3
6	ρ_1	ρ_3	ρ_2;

hence our integral becomes

$$K(k,m,n,p,r) = \int_0^{\infty}\rho_1^{k-q-r}e^{-a\rho_1}\,d\rho_1\int_0^{\rho_1}\rho_3^{n+1-p+q}e^{-c\rho_3}\,d\rho_3\int_0^{\rho_3}\rho_2^{m+2+p+r}e^{-b\rho_2}\,d\rho_2$$
$$+\int_0^{\infty}\rho_1^{k-q-r}e^{-a\rho_1}\,d\rho_1\int_0^{\rho_1}\rho_3^{n+2+p+q}e^{-c\rho_3}\,d\rho_3\int_{\rho_1}^{\infty}\rho_2^{m+1-p+r}e^{-b\rho_2}\,d\rho_2$$
$$+\int_0^{\infty}\rho_1^{k+1-q+r}e^{-a\rho_1}\,d\rho_1\int_0^{\rho_1}\rho_3^{n+2+p+q}e^{-c\rho_3}\,d\rho_3\int_{\rho_1}^{\infty}\rho_2^{m-p-r}e^{-b\rho_2}\,d\rho_2$$
$$+\int_0^{\infty}\rho_1^{k+1-r+q}e^{-a\rho_1}\,d\rho_1\int_{\rho_1}^{\infty}\rho_3^{n-p-q}e^{-c\rho_3}\,d\rho_3\int_0^{\rho_1}\rho_2^{m+2+p+r}e^{-b\rho_2}\,d\rho_2$$
$$+\int_0^{\infty}\rho_1^{k+2+q+r}e^{-a\rho_1}\,d\rho_1\int_{\rho_1}^{\infty}\rho_3^{n-p-q}e^{-c\rho_3}\,d\rho_3\int_{\rho_1}^{\rho_3}\rho_2^{m+1-r+p}e^{-b\rho_2}\,d\rho_2$$
$$+\int_0^{\infty}\rho_1^{k+2+q+r}e^{-a\rho_1}\,d\rho_1\int_{\rho_1}^{\infty}\rho_3^{n+1-q+p}e^{-c\rho_3}\,d\rho_3\int_{\rho_3}^{\infty}\rho_2^{m-p-r}e^{-b\rho_2}\,d\rho_2$$

by means of the definition

$$W(k, m, n, a, b, c) = \int_0^\infty dx \int_x^\infty dy \int_y^\infty dz\, x^k y^m z^n e^{-(ax+by+cz)}, \tag{17}$$

where $x < y < z$ and by reference to the scheme below Eq. (14) we may write our integral as

$$\begin{aligned} K(k, m, n, p, r) = {} & W(m + 2 + p + r, n + 1 - p + q, k - q - r, b, c, a) \\ & + W(n + 2 + p + q, m + 1 - p + r, k - q - r, c, b, a) \\ & + W(n + 2 + p + q, k + 1 - q + r, m - p - r, c, a, b) \\ & + W(m + 2 + p + r, k + 1 - r + q, n - p - q, b, a, c) \\ & + W(k + 2 + q + r, m + 1 - r + p, n - p - q, a, b, c) \\ & + W(k + 2 + p + r, n + 1 - q + p, m - p - r, a, c, b). \end{aligned} \tag{18}$$

Now p, r take on the values of $q \pm l$, $q \pm j$ respectively, where l, j are each either 0 or 1. Hence we have that

$$\begin{aligned} K(k, m, n, q \pm l, q \pm j) = {} & W(m + 2 + 2q \pm l \pm j, n + 1 \mp l, k - 2q \mp j, b, c, a) \\ & + W(n + 2 + 2q \pm l, m + 1 \mp l \pm j, k - 2q \mp j, c, b, a) \\ & + W(n + 2 + 2q \pm l, k + 1 \pm j, m - 2q \mp l \mp j, c, a, b) \\ & + W(m + 2 + 2q \pm l \pm j, k + 1 \mp j, n - 2q \mp l, b, a, c) \\ & + W(k + 2 + 2q \pm j, m + 1 \mp j \pm l, n - 2q \mp l, a, b, c) \\ & + W(k + 2 + 2q \pm j, n + 1 \pm l, m - 2q \mp l \mp j, a, c, b). \end{aligned} \tag{19}$$

(1) We note that q occurs in the same manner in all of these expressions.

(2) We may drop the cumbersome $\pm$ notation by the simple substitutions $L = l + 2$, $J = j + 2$, altering the total index accordingly.

Hence define

$$\begin{aligned} DDC(K, M, N, A, B, C, L, J, q) = {} & W(M - 2 + 2q + L + J, N + 3 - L, K - 2q + 2 - J, B, C, A) \\ & + W(N + 2q + L, M + 1 - L + J, K - 2q + 2 - J, C, B, A) \\ & + W(N + 2q + L, K - 1 + J, M + 4 - L - J - 2q, C, A, B) \\ & + W(M - 2 + 2q + L + J, K + 3 - J, N - 2q + 2 - L, B, A, C) \\ & + W(K + 2q + J, M + 1 - J + L, N - 2q + 2 - L, A, B, C) \\ & + W(K + 2q + J, N - 1 + L, M - 2q + 4 - L - J, A, C, B). \end{aligned} \tag{20}$$

Combining our angular and radial integrations in Eq. (3), we have finally

$$\begin{aligned} I = {} & 64\pi^3 \sum_q \frac{1}{(2q+1)^2} \Big\{ [DDC(K+2, M+2, N, A, B, C, 2, 2, q) \\ & + DDC(K, M+4, N, A, B, C, 2, 2, q) + DDC(K+2, M, M+2, A, B, C, 2, 2, q) \\ & + DDC(K, M+2, N+2, A, B, C, 2, 2, q)] - \frac{2q}{(2q-1)} [DDC(K+1, M+3, N, A, B, C, 1, 2, q) \\ & + DDC(K+1, M+1, N+2, A, B, C, 1, 2, q) + DDC(K+2, M+1, N+1, A, B, C, 2, 1, q) \\ & + DDC(K, M+3, N+1, A, B, C, 2, 1, q)] - \frac{2(q+1)}{(2q+3)} [DDC(K+1, M+3, N, A, B, C, 3, 2, q) \\ & + DDC(K+1, M+1, N+2, A, B, C, 3, 2, q) + DDC(K+2, M+1, N+1, A, B, C, 2, 3, q) \end{aligned}$$

$$+ DDC(K, M+3, N+1, A, B, C, 2, 3, q)] + \frac{4q^2}{(2q-1)^2} DDC(K+1, M+2, N+1, A, B, C, 1, 1, q)$$

$$+ \frac{4(q+1)^2}{(2q+3)^2} DDC(K+1, M+2, N+1, A, B, C, 3, 3, q) + \frac{4q(q+1)}{(2q-1)(2q+3)}$$

$$\times_i [DDC(K+1, M+2, N+1, A, B, C, 1, 3, q) + DDC(K+1, M+2, N+1, A, B, C, 3, 1, q)]\Big\}. \tag{21}$$

The convergence of this series is guaranteed if each of the W's converges as $q \to \infty$.

Consider

$$W_q = \int_0^\infty \rho_1^{k+2q} e^{-a\rho_1}\, d\rho_1 \int_{\rho_1}^\infty \rho_2^m e^{-b\rho_2}\, d\rho_2 \times \int_{\rho_2}^\infty \rho_3^{n+2q} e^{-c\rho_3}\, d\rho_3,$$

which is the general form of all of the W's. This may be written as

$$W_q = \int_0^\infty \rho_3^{n-2q} e^{-c\rho_3}\, d\rho_3 \int_0^{\rho_3} \rho_2^m e^{-b\rho_2}\, d\rho_2 \times \int_0^{\rho_3} \rho_1^{k+2q} e^{-a\rho_1}\, d\rho_1.$$

Expand the exponentials in a Taylor series; then

$$W_q = \sum_\alpha \frac{(-1)^\alpha}{a^\alpha \alpha!\,(k+2q+\alpha+1)} \int_0^\infty \rho_3^{n-2q} e^{-c\rho_3}\, d\rho_3 \int_0^{\rho_3} \rho_2^{m+k+2q+\alpha+1} e^{-b\rho_2}\, d\rho_2$$

$$= \sum_{\alpha,\beta} \frac{(-1)^\alpha (-1)^\beta (k+m+n+\alpha+\beta+2)!}{a^\alpha b^\beta \alpha!\,\beta!\,(k+2q+\alpha+1)(m+k+2q+\alpha+\beta+2) c^{k+m+n+\alpha+\beta+3}}.$$

Thus, convergence of the W's is guaranteed if the expression converges for $q = 0$ since q appears only in the denominator of this expression. The convergence for $q=0$ is guaranteed if $k+m+n \geq -2$, $k+m \geq -1$, $k > 0$, which conditions obtain for the W's involved here.

Contributions to the Quantization Problem in General Relativity*

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It is possible to quantize most classical field theories by identifying the group of canonical transformations which maintain the covariance properties with a group of unitary transformation in Hilbert space which has the same commutator algebra. The commutators among the canonical field variables are equal to the Dirac delta function times a factor which may be zero. But in the general theory of relativity the classical group of the canonical transformations which maintain the covariance properties of the theory has an invariance subgroup. The ambiguities thus introduced by the usual process of quantization can be avoided by the use of the Dirac quantization procedure for theories with constraints. We establish an analogy between classical Dirac brackets and commutators, and fix an intrinsic coordinate system. This choice of local intrinsic coordinate conditions leads to commutators among the canonical field variables of the general theory of relativity which depend upon the Dirac delta function and its first seven derivatives.

I. THE QUANTIZATION OF FIELD THEORIES WITH CONSTRAINTS

THE formulations of quantum theories of fields other than the gravitational field have received general acceptance among physicists. However, the general theory of relativity has not been quantized satisfactorily except in the linear approximation.[1] The principal obstacle to the quantization of the general theory of relativity by the mathematical procedures used for constructing the quantized forms of other classical field theories is the difficulty in the establishment of a workable analogy between the commutators among quantum operators and the Poisson brackets among the classical field variables corresponding to these operators. In a covariant classical theory there is a group of canonical transformations which maintain the covariance properties. The transformations in this group carry one physical state into another. The transition to a quantized theory is accomplished by identifying the group of canonical transformations with a group of unitary transformations in Hilbert space which has the same commutator algebra.

This analogy will break down if the classical group of canonical transformations contains a subgroup which maps a physical state into the same physical state defined in a different representation.[2] Such a subgroup is called an invariance subgroup. If the invariance group has the dimensions of a function space, the transformations which belong to it have generators which vanish.[3] These generators of the transformations of the invariance subgroup have the form of algebraic or differential relations among the field variables. (For electromagnetism, the best known example of such a theory, this constraint is the condition that the momentum conjugate to the scalar potential vanishes everywhere.) These are first-class constraints in Dirac's terminology.[4] Their Poisson brackets with the Hamiltonian and with each other vanish if the constraints are satisfied.

To fix a coordinate system we must introduce additional constraints among the canonical variables. These additional constraints cannot commute with each other or with the first-class constraints. All the constraints must therefore be regarded as second-class constraints when the coordinate system is fixed.

For a theory which contains second-class constraints Dirac[4,5] has introduced a new type of classical commutator bracket which vanishes for all such constraints. The Dirac bracket is defined in terms of the Poisson bracket by the expression

$$\{M, N\}^* = \{M, N\} + \iint \{M, C^A(x')\} F_{AB}(x', x'') \times \{N, C^B(x'')\}\, d^3x'\, d^3x'', \qquad (I.1)$$

where the summation is extended over all second-class constraints and where $F_{AB}(x, x')$ is defined:

$$\int \{C^A(x), C^B(x')\} F_{BC}(x, x'')\, d^3x = \delta^A_C \delta(x', x''). \qquad (I.2)$$

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[1] W. Pauli and M. Fierz, Helv. Phys. Acta 12, 297 (1939).

[2] P. G. Bergmann and I. Goldberg, Phys. Rev. 98, 531 (1955).

[3] J. L. Anderson and P. G. Bergmann, Phys. Rev. 83, 1018 (1951).

[4] P. A. M. Dirac, Can. J. Math. 2, 129 (1950); 3, 1 (1951).

[5] P. A. M. Dirac, Proc. Roy. Soc. (London) A246, 326 and 333 (1958); Phys. Rev. 114, 924 (1959).

For the general theory of relativity, an analogy between Poisson brackets and commutators would give

$$[\mathbf{g}_{\mu\nu}, \mathbf{g}'_{\rho\sigma}] = [\mathbf{p}^{\mu\nu}, \mathbf{p}^{\rho\sigma\prime}] = 0, \quad [\mathbf{g}_{\mu\nu}, \mathbf{p}^{\rho\sigma\prime}] = \delta^{\rho\sigma}_{\mu\nu}\delta(x, x'), \tag{I.3}$$

where

$$\delta^{\rho\sigma}_{\mu\nu} = \tfrac{1}{2}(\delta^{\rho}_{\mu}\delta^{\sigma}_{\nu} + \delta^{\rho}_{\nu}\delta^{\sigma}_{\mu}). \tag{I.4}$$

We will show that they must be modified to Dirac brackets (I.1) by the addition of a term of the form

$$\iint [\mathbf{M}, \mathbf{C}^{A\prime\prime}]\mathbf{F}_{AB}(x'', x''')[\mathbf{N}', \mathbf{C}^{B\prime\prime\prime}]\, d^3x''\, d^3x''' \tag{1.5}$$

on the right side of Eq. (I.3), where $\mathbf{M}$ and $\mathbf{N}$ are the operators corresponding to two classical quantities M and N. Since C^A contains derivatives of the field variables, $[\mathbf{M}, \mathbf{C}^{A\prime}]$ contains derivatives of the Dirac delta function $\delta(x, x')$., Hence, the commutators of the general theory of relativity contain derivatives of $\delta(x, x')$.

II. DIRAC'S REDUCTION OF THE CANONICAL VARIABLES

Dirac[5] has stated the field equations of the general theory of relativity in a form which does not depend upon certain of the canonical variables. This reduction of the canonical variables also makes possible a relatively simple statement of the physical system on an initial space-like hypersurface, whose metric is g_{mn}. In showing this simplification of the statement of the problem, we shall use these notations, most of which are employed by Dirac: e^{mn} is defined by $e^{mn}g_{nr} = \delta^m_r$. $l^\rho = (g^{00})^{-\frac{1}{2}}g^{0\rho}$ are the components of the unit vector normal to the spacelike hypersurface whose metric is g_{mn}. It follows that $g^{\mu\nu} = e^{\mu\nu} + l^\mu l^\nu$, where $e^{0\mu} = 0$.

$$K^2 = -\det g_{mn}.$$

$p = g_{mn}p^{mn}$, where $p^{\mu\nu} = \partial\mathfrak{L}/\partial g_{\mu\nu,0}$ is the canonical momentum conjugate to $g_{\mu\nu}$.

S_{mn} is the three-dimensional Ricci tensor of the spacelike hypersurface whose metric is g_{mn}, and S is the scalar curvature of this hypersurface.

The symbol / denotes the covariant derivative with respect to the three-dimensional metric g_{mn}.

Greek indices from the first part of the alphabet are the indices of a set of four scalars; these indices run from 0 to 3. Greek indices from iota onward are coordinate indices in four-dimensional space. Small Latin indices run from 1 to 3. Capital Latin indices are defined as they are introduced. The Einstein summation convention holds in all cases.

We shall call "D-invariant" any functional, defined on a given three-dimensional hypersurface imbedded in a four-dimensional Riemann–Einstein manifold, whose transformation law with respect to curvilinear infinitesimal coordinate transformations involves only the $\delta x^\mu = \xi^\mu$, but not their partial derivatives normal to the hypersurface. Peres has shown[6] that a D-invariant functional of the metric tensor and its partial derivatives of finite orders may be represented as a functional of g_{mn}, p^{mn} only, provided that the field equations are satisfied. This theorem will be useful in the calculations of the Dirac brackets among the canonical variables on the initial hypersurface.

The freedom of choice of four coordinate conditions can be used to write the canonical variables g_{mn}, p^{mn} in intrinsic coordinates. Géhéniau and Debever,[7] following a suggestion by Kretschmann,[8] have shown that, when the field equations are satisfied, in general exactly four algebraically independent scalars can be constructed algebraically from the components of the curvature tensor of the Riemann–Einstein manifold. More precisely, if the space has no physical symmetries, i.e., if no Killing vector field can be defined in it and if it has no other "special" structure,[9] then the four scalars are independent. Komar[10] has proposed the introduction of a set of intrinsic coordinates $f^\gamma(A^\alpha)$, four scalar functions of the Géhéniau–Debever scalars. Following him, we introduce the four coordinate conditions

$$F^\gamma = f^\gamma(A^\alpha) - x^\gamma = 0. \tag{II.1}$$

For the time being, the functions f^γ need not be specified.

Several authors[11] have shown that the Géhéniau–Debever scalars are D-invariant. The Komar coordinate conditions (II.1) can therefore be satisfied on the initial hypersurface whose metric is g_{mn}.

III. INITIAL CONDITIONS

Since the coordinate conditions (II.1) can be imposed only upon a space without special symmetry properties, we shall consider only such spaces

[6] A. Peres, Nuovo Cimento 18, 32 (1960).
[7] J. Géhéniau and R. Debever, Bull. Acad. Roy. Belg. Cl. Sci. 42, 144, 252, 313, and 608 (1956); Helv. Phys. Acta Suppl. 4, 101 (1956).
[8] E. Kretschmann, Ann. Physik 53, 575 (1917).
[9] F. A. E. Pirani, Phys. Rev. 105, 1089 (1957).
[10] A. Komar, Phys. Rev. 111, 1182 (1958).
[11] A. Peres, Nuovo Cimento 18, 32 (1960); P. G. Bergmann and A. Komar, Phys. Rev. Letters 4, 432 (1960).

in the following discussion. The problem will be stated on a spacelike initial hypersurface, the general relativistic analog of an initial time $t = t_0$. If the solution is required to propagate itself from this initial hypersurface, then the commutators among the canonical variables on this hypersurface will continue to be valid when projected into the future in accordance with the development of the physical system as described by the Hamiltonian field equations. The determination of the commutators among the canonical field variables at different points in space should therefore begin with the determination of these commutators at different points on an initial hypersurface whose metric is g_{mn}.

We have stated the problem in such a way that $p^{0\mu} = 0$ and that $g_{0\mu}$ are arbitrary functions of the remaining canonical variables. These twelve remaining canonical variables g_{mn}, p^{mn} are defined on the initial spacelike hypersurface and are linked by eight constraints, including the coordinate conditions (II.1), which reduce the number of independent canonical variables to four.

The initial conditions for this problem are now completely specified. If the metric of the space is $g_{\mu\nu}$, the description of the problem on the initial hypersurface consists of:

(1) Six canonical field variables of position g_{mn}, which are the metric of this initial hypersurface.

(2) Six canonical field variables of momentum p^{mn}.

(3) Four "Hamiltonian" constraints $\mathcal{H}_L = \mathcal{H}_r = 0$, where

$$\mathcal{H}_L = K^{-1}(p_{mn}p^{mn} - \tfrac{1}{2}p^2) - KS,$$
$$\mathcal{H}_r = -2p_r{}^s{}_{/s}.$$

(4) Four coordinate conditions $f^\gamma(A^\alpha) - x^\gamma = 0$, which together with the "Hamiltonian" constraints form a set of eight second-class constraints. (Since $\mathcal{H}_L$ and $\mathcal{H}_r$ do not commute with the coordinate conditions, they must now be considered as second-class constraints in a theory with our choice of fixed coordinates.)

The Dirac bracket between any two of these twelve canonical variables will be taken to be the classical analog of the commutator between the corresponding quantum operators. The commutators among g_{mn} and p^{mn} on the initial spacelike hypersurface can then in principle be calculated.

Since $\mathcal{H}_r$ generates a translation in the x^r direction on the initial hypersurface, we can write

$$\int \{F^\gamma, \mathcal{H}_r'\}\, d^3x' = f^\gamma{}_{,r} = \delta^\gamma_r, \qquad \text{(III.1)}$$

$$\int \{F^\gamma, \mathcal{H}_L'\}\, d^3x' = l^\gamma = (g^{00})^{-\frac{1}{2}} g^{0\gamma}, \qquad \text{(III.2)}$$

in keeping with the role of $\mathcal{H}_L$ as the generator of a translation along the unit vector normal to the initial hypersurface. Equation (III.2) yields in principle the position variables $g_{0\mu}$ as functions of the twelve canonical variables g_{mn}, p^{mn}.

IV. THE CANONICAL VARIABLES IN INTRINSIC COORDINATES

We have fixed an intrinsic coordinate system with the help of the coordinate conditions (II.1). These intrinsic coordinate conditions can be formulated entirely in terms of quantities intrinsic to the initial hypersurface, because the Géhéniau–Debever scalars are functions of the twelve canonical variables g_{mn}, p^{mn}. Though this fact may be established by direct computation, it follows from the invariant (and hence D-invariant) nature of these scalars. The Géhéniau–Debever scalars may be written:

$$\begin{aligned} A^0 &= A_{mn}A^{mn} + B_{mn}B^{mn}, \\ A^1 &= -2A_{mn}B^{mn}, \\ A^2 &= A_{mn}(A^m{}_r\, A^{rn} + 3B^m{}_r\, B^{rn}), \\ A^3 &= -B_{mn}(3A^m{}_r\, A^{rn} + B^m{}_r\, B^{rn}), \end{aligned} \qquad \text{(IV.1)}$$

where

$$\begin{aligned} A_{mn} &= 2S_{mn} + K^{-2}(pp_{mn} - 2p_{mr}p^r{}_n), \\ B_{mn} &= -2K^{-1}\epsilon^{rs}{}_{(m}p_{n)r/s}. \end{aligned} \qquad \text{(IV.2)}$$

The two three-dimensional tensors A_{mn}, B_{mn} are obtained from the four-dimensional Weyl tensor by multiplying the various subscripts of that tensor by $e_\alpha{}^\mu = \delta_\alpha{}^\mu$ and by l^μ, respectively, and by multiplying skew symmetric index pairs $[kl]$ by the Levi-Cività tensor $\epsilon^{[kl]}{}_m$. The components of A_{mn} are then those that contain zero or two factors $\epsilon^{[kl]}{}_m$, whereas the components of B_{mn} contain one factor $\epsilon^{[kl]}{}_m$. We shall use the terms "even" and "odd" to characterize tensors in which $\epsilon^{[kl]}{}_m$ occurs as a factor an even or odd number of times, respectively. It now becomes possible to calculate the elements of F_{AB} of Eq. (I.5), and to determine the form which (I.1) has for various choices of functionals of the canonical variables M, N.

These functionals will be given one of the following forms in order to obtain the Dirac brackets among the dynamical variables of the general theory of relativity:

$$M(x) = \int g_{mn}' k^{mn}(x, x')\, d^3x', \tag{IV.3}$$

$$M(x) = \int p^{mn\prime} \lambda_{mn}(x, x')\, d^3x'. \tag{IV.4}$$

The quantities k^{mn} and λ_{mn} will be called density functions. After $\{M, N'\}^*$ is calculated, the commutators among local functions can be obtained by setting $k^{mn}(x, x') = k^{mn}\delta(x, x')$ and $\lambda_{mn}(x, x') = l_{mn}\delta(x, x')$ where k^{mn} and l_{mn} are constants.

Equation (I.1) can be written

$$\{M, N\}^* = \{M^*, N\}, \tag{IV.5}$$

where

$$M^* = M - \iint \{M, C^{A\prime}\} \times F_{AB}(x', x'')C^{B\prime\prime}\, d^3x'\, d^3x''. \tag{IV.6}$$

We can thus define functionals M^* of the canonical variables in terms of the old functionals M and the matrix F_{AB} defined by (I.2). Equation (IV.6) can be written more compactly if we define

$$\gamma_B(x, x') = -\int \{M, C^{A\prime}\}F_{AB}(x', x'')\, d^3x'. \tag{IV.7}$$

It is then possible to write

$$M^*(x) = M(x) + \int \gamma_A(x, x')C^A(x')\, d^3x'. \tag{IV.8}$$

If the constraints are satisfied, these starred functionals are equal to the unstarred functionals. However, if the coefficients γ_A are determined from the condition

$$\{M^*, C^{A\prime}\} = 0, \tag{IV.9}$$

then the Poisson brackets among the starred functionals are identical with the Dirac brackets among the starred or unstarred functionals. Provided always that the coordinate conditions (II.1) are satisfied, all functions and functionals of g_{mn}, p^{mn}, being expressed in intrinsic coordinates, are observables.[12]

We can write

$$\{M^*, N^{*\prime}\} = \left\{M^*, N' + \int \gamma_A(x', x'')C^{A\prime\prime}\, d^3x''\right\} = \{M^*, N'\} + \int \gamma_A(x', x'')\{M^*, C^{A\prime\prime}\}\, d^3x''. \tag{IV.10}$$

But it follows from (IV.9) that the second term on the right of (IV.10) vanishes. Therefore $\{M^*, N^{*\prime}\} = \{M^*, N'\}$. This expression will henceforth be called a "starred bracket," and written $\{M, N'\}^*$.

We shall next calculate the starred canonical variables corresponding to the unstarred variables g_{mn}, p^{mn}. The Poisson brackets among these starred canonical variables are identical with the Dirac brackets among the corresponding unstarred variables. If the starred brackets are then made commutators, the quantization of the general theory of relativity will in principle have been accomplished.

The starred canonical variables are

$$g_{mn}{}^* = g_{mn} + \int (\epsilon^r(x, x')\mathfrak{H}_r' + \epsilon^L(x, x')\mathfrak{H}_L' + \gamma_\alpha(x, x')F^{\alpha\prime})\, d^3x', \tag{IV.11}$$

$$p^{mn*} = p^{mn} + \int (\bar{\epsilon}^r(x, x')\mathfrak{H}_r' + \bar{\epsilon}^L(x, x')\mathfrak{H}_L' + \bar{\gamma}_\alpha(x, x')F^{\alpha\prime})\, d^3x'. \tag{IV.12}$$

The conditions (IV.9) require the following expressions for the coefficients ϵ^r, ϵ^L, and γ_α:

$$\gamma_r(x, x') = \{\mathfrak{H}_r, M'\}, \tag{IV.13}$$

$$\gamma_0(x, x') = l^{0\prime}(\{\mathfrak{H}_L, M'\} - l^{r\prime}\gamma_r(x, x')), \tag{IV.14}$$

$$\epsilon^L(x, x') = -l^{0\prime}\left(\{F^0, M'\} + \int \gamma_\rho(x, x'')\{F^{0\prime}, F^{\rho\prime\prime}\}\, d^3x''\right), \tag{IV.15}$$

$$\epsilon^r(x, x') = -\epsilon^L(x, x')l^{r\prime} - \{F^r, M'\} - \int \gamma_\sigma(x, x'')\{F^{r\prime}, F^{\sigma\prime}\}\, d^3x''. \tag{IV.16}$$

The Dirac bracket may now be written:

$$\begin{aligned}\iint \{M, N'\}^*\, d^3x\, d^3x'' &= \iint \{M, N'\}\, d^3x\, d^3x' \\ &- \iiint \{M, H_\gamma''\}J^\gamma{}_\alpha''\{A^{\alpha\prime\prime}, N'\}\, d^3x\, d^3x'\, d^3x'' \\ &+ \iiint \{M, A^{\alpha\prime\prime}\}J^\gamma{}_\alpha''\{H_\gamma'', N'\}\, d^3x\, d^3x'\, d^3x'' \\ &+ \iiiint \{M, H_\gamma''\}J^\gamma{}_\alpha''\{A^{\alpha\prime\prime}, A^{\beta\prime\prime\prime}\} \\ &\times J^\delta{}_\beta'''\{N', H_\delta'''\}\, d^3x\, d^3x'\, d^3x''\, d^3x''',\end{aligned} \tag{IV.17}$$

where

$$J^\gamma{}_\alpha = \partial f^\gamma/\partial A^\alpha, \qquad H_\rho = l_\rho\mathfrak{H}_L + e_\rho{}^r\mathfrak{H}_r. \tag{IV.18}$$

[12] Reference 10, Sec. 1. The references cited in this paper provide fuller discussions of the concept of observables in the general theory of relativity. Cf. also P. G. Bergmann and A. Komar, Coll. Intern. CNRS 91, 309 (1962).

The choices of M and N' as functionals of the canonical variables of the general theory of relativity fall into three combinations:

$$(1)\quad M = \int g_{mn}''k^{mn}\,\delta(x, x'')\,d^3x'',$$

$$N' = \int g_{rs}''k^{rs}\,\delta(x', x'')\,d^3x''.$$

$$(2)\quad M = \int g_{mn}''k^{mn}\,\delta(x, x'')\,d^3x'',$$

$$N' = \int p^{rs\prime\prime}l_{rs}\,\delta(x', x'')\,d^3x''.$$

$$(3)\quad M = \int p^{mn\prime\prime}l_{mn}\,\delta(x, x'')\,d^3x'',$$

$$N' = \int p^{rs\prime\prime}l_{rs}\,\delta(x', x'')\,d^3x''.$$

V. THE HIGHEST DIFFERENTIAL ORDER OF $\delta(x, x')$ IN THE EXPANSION OF THE DIRAC BRACKETS

If Eq. (IV.17) is evaluated for each pair of canonical variables of the general theory of relativity, the Dirac brackets among these variables will be obtained. If, for particular choices of M and N', integrations by parts are performed on the right side of (IV.17) so that the density function part of N' is left undifferentiated, then

$$\iint \{M, N'\}^*\,d^3x\,d^3x'$$

can be written as a sum of several terms, each of which contains a different order of differentiation of the density function part of M. If the density functions are each set equal to a constant times $\delta(x, x')$, and the indicated double integration is performed, then the following result can be anticipated:

$$[\mathbf{M}, \mathbf{N}']^* = {}_0F\,\delta(x, x') + {}_1F^i\,\delta_{,i}(x, x') + {}_2F^{ij}\,\delta_{,ij}(x, x') + \cdots \qquad (V.1)$$

where the coefficients ${}_0F$, ${}_1F^i$, ${}_2F^{ij}$, etc., depend upon the choice of M and N'.

The expansion (V.1) of $[\mathbf{M}, \mathbf{N}']^*$ has a finite number of terms, which may be determined for each particular choice of M and N' from an examination of (IV.17). Since A^α contains up to second derivatives of g_{mn}, and up to first derivatives of p^{mn}, the factor $[\mathbf{A}^\alpha'', \mathbf{A}^{\beta\prime\prime\prime}]$ will, after integration by parts over either x'' or x''', contain up to third derivatives of $[\mathbf{g}_{mn}'', \mathbf{p}^{rs\prime\prime\prime}]$ and hence of $\delta(x'', x''')$. [This result is obtained through use of the identity $(\partial/\partial x)\delta(x, x') = -(\partial/\partial x')\delta(x, x')$.] Since $\mathfrak{IC}_r$ contains up to first derivatives of g_{mn} and p^{mn}, and $\mathfrak{IC}_L$ contains up to second derivatives of g_{mn}, we can similarly expect $[\mathbf{g}_{mn}, \mathbf{H}_\gamma']$ to contain up to first derivatives of $\delta(x, x')$, and $[\mathbf{p}^{mn}, \mathbf{H}_\gamma']$ to contain up to second derivatives of $\delta(x, x')$. If the last term on the right-hand side of (IV.17) is integrated by parts so that all the derivatives of the second density function are transferred to the first density function; then the last term in the expansion (V.1) will contain the fifth derivative of $\delta(x, x')$ for combination 1, the sixth derivative of $\delta(x, x')$ for combination 2, and the seventh derivative of $\delta(x, x')$ for combination 3.

It can be shown that, for combination 1, ${}_5F^{(tuvwx)}$ vanishes if and only if

$$\begin{aligned} &J^\gamma{}_0 J^\delta{}_0 - J^\gamma{}_1 J^\delta{}_1 = 0,\\ &J^\gamma{}_0 J^\delta{}_3 - J^\gamma{}_1 J^\delta{}_2 = 0,\\ &J^\gamma{}_0 J^\delta{}_3 - J^\gamma{}_2 J^\delta{}_1 = 0,\\ &J^\gamma{}_0 J^\delta{}_2 - J^\gamma{}_1 J^\delta{}_3 = 0,\\ &J^\gamma{}_0 J^\delta{}_2 - J^\gamma{}_3 J^\delta{}_1 = 0,\\ &J^\gamma{}_2 J^\delta{}_2 - J^\gamma{}_3 J^\delta{}_3 = 0. \end{aligned} \qquad (V.2)$$

For combination 2, ${}_6F^{(tuvwxy)}$ vanishes if and only if conditions (V.2) are met for $\delta = 0$.

For combination 3, ${}_7F^{(tuvwxyz)}$ vanishes if and only if

$$(J^0{}_0)^2 - (J^0{}_1)^2 = 0,\quad J^0{}_0 J^0{}_2 - J^0{}_1 J^0{}_3 = 0,\quad J^0{}_0 J^0{}_3 - J^0{}_1 J^0{}_2 = 0,\quad (J^0{}_2)^2 - (J^0{}_3)^2 = 0. \qquad (V.3)$$

Calculation shows that conditions (V.2) are met only if the determinant of $J^\gamma{}_\alpha$ vanishes. However, the Jacobian of the intrinsic coordinates as functions of the Géhéniau–Debever scalars cannot be singular, as the transformation between the intrinsic coordinates and the initially chosen set of curvilinear coordinates must be reversible. The coefficients of the highest differential order of the Dirac delta function cannot be made to vanish for classes I and II.

Conditions (V.3) are satisfied if

$$\frac{\partial f^0}{\partial A^0} = \pm\frac{\partial f^0}{\partial A^1},\qquad \frac{\partial f^0}{\partial A^2} = \pm\frac{\partial f^0}{\partial A^3}. \qquad (V.4)$$

If conditions (V.4) or any other nontrivial solution of (V.3) are made on the intrinsic coordinates, ${}_7F^{(tuvwxyz)}$ vanishes.

VI. CONCLUSIONS

It has been shown that the commutators between two different canonical variables of the general theory of relativity at different points on a spacelike hypersurface must contain derivatives of the Dirac delta function $\delta(x, x')$. The commutator between two position variables g_{mn}, g_{rs} contains up to the fifth derivative of $\delta(x, x')$ for the choice of intrinsic coordinates which we have made. The commutator between a position variable g_{mn} and a momentum variable p^{rs} contains up to the sixth derivative of $\delta(x, x')$. The coefficients of these highest derivatives of $\delta(x, x')$ cannot be made equal to zero by any particular choice of intrinsic coordinates. The commutator between two momentum variables p^{mn}, p^{rs} contains up to the seventh derrivative of $\delta(x, x')$, but the coefficient of this derivative can be made to vanish for some choices of intrinsic coordinates.

The quantized general theory of relativity thus assumes a mathematical form far more complex than that of any other quantum theory. This complexity is in part the result of our choice of intrinsic coordinates, a choice that was originally determined by the desire to formulate coordinate conditions purely locally, and with the lowest differential order available. It would appear that an essential simplification could be brought about only in the context of an entirely different approach.

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On the Complete Unitarity Equations for Pion–Pion Scattering

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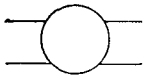
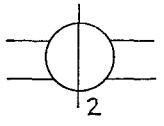
The off-the-mass-shell equations for pion–pion scattering in the lowest approximation of the complete unitarity formalism of Taylor are discussed. It is shown that if the vertex-function renormalization constant is taken to be zero, the equations have no (nonzero) solution. These equations are equivalent to certain bootstrap equations, which thus also have no solution. Both systems are discussed in the case where the renormalization constant is not put equal to zero.

1. INTRODUCTION

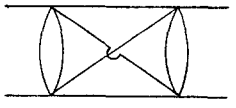
WE discuss the equations for pion–pion scattering arising in the off-the-mass-shell formalism developed by Taylor.[1] In this formalism, a diagram such as the two-particle amplitude

$M =$ 

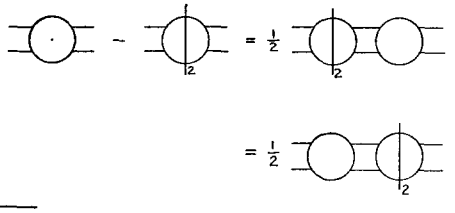
represents the sum of all perturbation graphs with the same number of legs and consistent with the interaction being discussed; this is the content of the "vacuous" complete unitarity hypothesis, cf. T3. We consider also diagrams such as

$M_2 =$ 

which represents the sum of those perturbation graphs such as

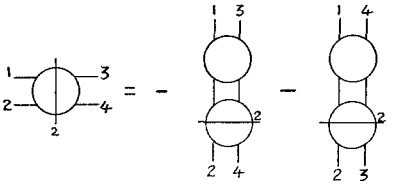


which cannot be divided into disconnected parts by a line across the 1–2 channel. Complete unitarity then gives the following equation, which we may regard as a more precise definition of M_2:



(1)

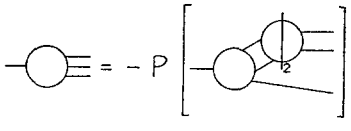
as well as equations defining other "cutless" amplitudes which we will not need in this paper. Equation (1), which we will refer to as the Bethe–Salpeter equation, is thus independent of any approximation. In order to get another equation one performs a "cut-structure analysis" (T3) followed by an approximation (n-cut approximation nCA) in which one considers only generalized graphs having less than n cuts in at least one channel (T3). In this paper we shall be concerned only with the lowest or 2CA approximation, in which the propagators are uncorrected, and the relevant cut-structure equation is



(2)

The pair of nonlinear integral equations (1), (2), describe, then, pseudoscalar pions (*inter alia*, questions of isospin are neglected), and satisfy unitarity and crossing symmetry up to the three-particle threshold (T5, Appendix). They will still require a vertex-function renormalization (T1, T2), which has to be carried out by differentiation (T5), thus giving rise to the constant λ in (2) which we imagine for the moment to be a constant of integration.

We can write (2) in the form



(3)

in which case we have a bootstrap system for pseudoscalar pions (T6).

After defining some notation we will discuss the Bethe–Salpeter equation in Sec. 2, and the cut-structure equation for $\lambda = 0$ in Sec. 3. From this discussion it will follow that for $\lambda = 0$, the 2CA and bootstrap systems have no solutions. In Sec. 4 we

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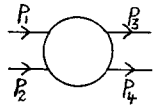
[1] J. G. Taylor, "On the Field Equations I–VI," to be published *en bloc* in Nuovo Cimento. We refer to the nth of these as Tn. Matters concerning renormalization are discussed in T1 and T2; the cut-structure analysis and the nCA approximation appear in T3; T5 contains some observations on the 2CA equations discussed in this paper, and in T6 there is a discussion of some bootstrap equations in the off-the-mass-shell formalism. Equations from these papers are referred to as, e.g., Eq. (IV.3) for Paper IV, Eq. (3).

shall outline the difficulties of the case $\lambda \neq 0$. In Sec. 5 we discuss the relevance of these results to bootstraps in general.

We shall use an argument based on the theory of Banach algebras (Appendix IV) which we have discussed elsewhere (in Ref. 2; but the details will be independent of that reference). In fact, the method can be considerably generalized; cf. remarks in Ref. 3. In the appendices, however, we sketch an analytical method by which, under more restrictive assumptions, we can get the same results (Appendix I); this method is somewhat generalized in Appendix II, and in Appendix III we discuss the relationship between these analytical methods and the more general method.

We shall write $M(1234)$ as shorthand for $M(p_1p_2p_3p_4)$, with the sign convention

$M(p_1p_2p_3p_4)$ corresponds to 

so that each bubble will conserve momentum according to

$$p_1 + p_2 - p_3 - p_4 = 0;$$

then the two equations become

$$M(1234) - M_2(1234) = -k \int \frac{M(1256)M_2(5643)\delta^4(1+2-5-6)\, d5\, d6}{(p_5^2 - m^2 + i\epsilon)(p_6^2 - m^2 + i\epsilon)}, \tag{4}$$

$$M_2(1234) = -k \int \frac{M(1356)M_2(5624)\delta^4(1+3-5-6)\, d5\, d6}{(p_5^2 - m^2 + i\epsilon)(p_6^2 - m^2 + i\epsilon)} - k(3 \leftrightarrow 4) + \lambda. \tag{5}$$

It will be necessary to discuss the detailed forms of (4) and (5) only in the appendices, and we will therefore write them in the more anschaulich form

$$M - M_2 = -kMM_2 \quad \text{(Bethe–Salpeter equation)}, \tag{6}$$

$$M_2 = -kP(MM_2) \quad \text{(cut-structure equation)}, \tag{7}$$

where P represents the permutations and addition made explicitly in (5). Here k is a constant with the pure imaginary value

$$k = i/2(2\pi)^4. \tag{8}$$

2. THE BETHE–SALPETER EQUATION

TCP defines a natural involution (Def. IV.2) under which M is invariant:

$$M(1234) = \bar{M}(3412).$$

Let us embed Eq. (6) into any Banach algebra with identity satisfying the following additional condition, which is actually rather weak (footnote 4): all elements of the form $I + a^* a$ shall be invertible.

Then because of the indentity $(I + ia)(I - ia) = I + a^2$, $I - ia$ is also invertible for Hermitian a, and we can solve the equation in the form

$$M_2 = M/(I - kM). \tag{9}$$

This proves what we "knew" already, namely that M and M_2 commute. In this framework, then, we can be sure that (6) does define M_2 properly; and once we have (9), there is nothing more to be done with the Bethe–Salpeter equation. In this sense (cf. footnote 4) the assumptions of this section are weaker than those of the next.

3. THE CUT-STRUCTURE EQUATION: CASE $\lambda = 0$.

Here we shall take the following framework (footnote 3): a commutative Banach algebra with involution satisfying

$$|a^*a| = |a^*|\,|a|.$$

This framework is much more general than the one in Appendix I, and since we proved the commutativity under weaker analytic assumptions in the last section, it is really only the assumption about the norm that is new. Then we can apply the Gel'fand–Neumark theorem and get characters satisfying (footnote 5)

$$a(x) - b(x) = -ka(x)b(x), \qquad b(x) = -kP[a(x)b(x)] \tag{10}$$

[2] M. M. Broido, "On 'Homogeneous' Equations," Cambridge University preprint (to be published). We shall refer to this paper as B.

[3] This is discussed in general terms in Sec. 4 of Ref. 2. A more explicit choice of framework would rest largely on the possession of some definite information about the high-energy behavior of the equations. We do not know very much about this, though it seems that constant behavior would be self-consistent (cf. T5) and consistent with experiment.

Remarks added during preparation (February 1965)[4] The argument can be greatly extended in scope and realistic high-energy behavior explicitly included (cf. remarks in Appendix II) by using the technique of locally multiplicatively-convex algebras (E. A. Michael, Mem. Am. Math. Soc. It is also possible to give a much more detailed treatment of the involutions, avoiding some difficulties which arise in the text in connection with the reality properties of the propagators in this off-the-mass-shell method; we will go into this in detail elsewhere.

[4] See Definition IV.7 in Appendix IV, and remarks after it.

[5] See Theorem IV. 6. in Appendix IV. The relevance to the general method is discussed in Ref. 2, Sec. 4(c).

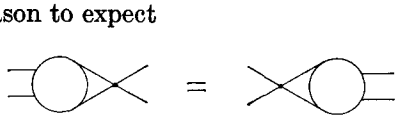
at each maximal ideal x; we must still determine what is meant by the transformation P in this situation. Now because M is Hermitian, $a(x)$ is real; and because M is invariant under the permutations, so is $a(x)$. This is because the Gel'fand isomorphism must preserve the structure of the Banach space, regarded as a representation module for the permutation group (the identical argument is often used implicitly in representation-theoretic discussions of quantum mechanics) and in particular must take an invariant element into an invariant element. But since $b(x)$ is a function of $a(x)$ by (9) or (10), the permutations reduce to phase transformations at each maximal ideal x. Both permutations satisfy $U^2 = 1$, so their phases can only be ± 1 and the cut-structure equation takes the form

$$b(x) = 2ka(x)b(x)f(x), \tag{11}$$

where $f(x)$ is a function taking only the values 0 or ± 1. Considering each point x separately we see at once that the equations have only one solution with real a, namely zero. [The situation and the last part of the argument are analogous to that arising from Eq. (6) of B.] This proves the assertion that there are no solutions.

4. DISCUSSION OF THE CUT-STRUCTURE EQUATION FOR $\lambda \neq 0$.

Suppose first of all that the framework is the same as in Sec. 3. The coupling constant would then give rise to a Hermitian element, since it has at least as much symmetry as M. Equation (11) will then become $b(x) = c(x) + 2a(x)b(x)f(x)$ with $f(x)$ taking the values 1 and 0 only, and where $c(x)$ is the function arising from λ and is real. Again, it is not difficult to see that there is no solution at all with real $a(x)$. If one converts the problem to one about operator algebras in Hilbert space (see B) one realizes that this is not surprising, since it corresponds to performing the vertex-function renormalization by subtraction of a constant, and this is not expected to succeed. Another way of looking at it is that there is no reason to expect



We now sketch some of the issues involved in the corresponding noncommutative problem. We imagine the equations as operator equations in Hilbert space again. A "coupling constant" (cf. Sec. 5 below) of the form $\lambda = C(12)C(34)$ will obviously be an operator of rank 1. But in a multiplication like the one in (4) the integral would not coverge for $C(12) =$ const. If we imagined λ as an unbounded linear operator (generalizing the framework) it could not even be self-adjoint (footnote 6), and would probably be quite inaccessible to Hilbert-space methods. Of course one might try another form for the function $C(12)$ to represent the high-energy behavior, (since this is not expected to be given accurately by 2CA) but the whole problem would then be very sensitive to the choice of this function (footnote 7). This state of affairs is unsatisfactory; we hope to return to these points in a later paper.

5. APPLICATIONS TO BOOTSTRAPS

The bootstrap equation (3) is as we mentioned before simply another way of writing (2), and is not an analytic continuation of (2). It is pointed out in T6 that the "coupling constants" appearing in bootstraps of this kind can be expected to be momentum-dependent, vanishing only on the mass shell; for this reason we have mentioned momentum-dependent coupling constants in Sec. 4. Several people have followed the suggestion of Salam (Ref. 8) that one ought to put the vertex-function renormalization constant equal to zero. The bootstrap system we have dealt with is the pseudoscalar meson equivalent of Salam's; and we have shown that it has no solution. We feel that this confirms the conjecture of T6 that the renormalization constant can vanish only on the mass shell. Taylor has succeeded in establishing a similar result for a (mathematically) simplified model (Ref. 9) with Euclidean metric and finite momentum-space cutoff, using fixed-point methods.

6. CONCLUSIONS

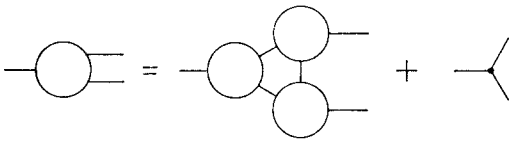
We have shown within very wide assumptions that the 2CA equations and the bootstrap system for pseudoscalar particles both have no nontrivial solution in the case where the vertex-function renormalization constant vanishes. We have discussed the significance of these results within the nCA formalism. The bootstrap result is also interesting in that the bootstrap (1), (3) is a far less crude approximation than most bootstrap systems, say than the scalar meson bootstrap (T6)

[6] This follows from the von Neumann spectral theorem. See F. Riesz and B. Sz.-Nagy, *Lectures on Functional Analysis* (Budapest, 1952), Sec. 120.

[7] This is clearest when one performs an iteration process, though for these equations nothing much is known about whether this would converge or not.

[8] A. Salam, Nuovo Cimento **25**, 244 (1962).

[9] J. G. Taylor (private communication).



(which could perhaps be dealt with by the Galois-theoretic considerations of B, Sec. 2, (b2), and to which we will return). Although it might be possible to deal with the equations for $\lambda \neq 0$ as they stand, we feel that the renormalization is a real necessity and that the quantities appearing in the re-integrated equations are not well defined. In such a case, one will probably be forced to treat the differentiated equations in all their glory. We hope to discuss this problem in a later paper.

ACKNOWLEDGMENTS

It is a great pleasure to thank Dr. J. G. Taylor for a number of stimulating discussions, particularly on bootstraps. I also wish to thank the DSIR for a grant.

APPENDIX 1

In this Appendix we derive the results of the paper using a simple analytical technique based on the resemblance of the multiplication MM_2 to the multiplication of operators represented by kernels in spaces of L^2 type. It is well known how such square-summable kernels may be approximated in norm by operators of finite rank; this procedure is analogous to Fourier analysis of functions of two variables, and we shall refer to it simply as Fourier analysis. We will deal here only with the case where the coupling constant is zero.

Unfortunately the resemblance to multiplication of kernels is not a complete one because of the presence of the delta function conserving the momentum. In fact as we see at once from Eq. (4), the multiplication MM_2 can be written without subsidiary conditions (with some abuse of notation) in the form

$$(MM_2)(xyz) = \int M(xyw)M_2(xwz)\, du\,(xw)$$

where

$$x = p_1 + p_2 = p_5 + p_6 = p_3 + p_4$$
$$y = p_1 - p_2$$
$$w = p_5 - p_6$$
$$z = p_3 - p_4$$

and the measure $u(xw)$ (which will not concern us further) takes into account the propagators. The multiplication is really quite complicated—pointwise in x, and similar to that for Fredholm kernels only in y and z. If we wish to attack the problem by Fourier analysis directly, we will have to deal with these two sets of variables separately. However it turns out that because of the particular algebraic structure of the problem we can obtain all the information we need from the kernel-type part of the multiplication alone. We will thus consider the variable x as simply a parameter and will write

$$(MM_2)(xyz) = \int M(xyw)M_2(xwz)\, du_x(w) \tag{13}$$

and will focus our attention on the variables y, z, w. For "most" values of x (in a sense we shall not bother to define exactly) we assume that there is a square-summability condition in the other variables:

$$|M|_x = \int |M(xyz)|^2\, d\, |u_x(y)|\, d\, |u_x(z)| < \infty \tag{14}$$

and similarly for M_2. Then if for each value of x, $A^x_i(y)$ is an orthonormal sequence of real-valued functions, complete in the sense of the scalar product

$$\int A^x_i(y)A^x_j(y)\, du_x(y) = \delta_{ij}, \tag{15}$$

we obtain for each value of x the Fourier expansions

$$\begin{aligned} M(xyz) &= a^x_{ij}A^x_i(y)A^x_j(z) \\ M_2(xyz) &= b^x_{ij}A^x_i(y)A^x_j(z) \end{aligned} \tag{16}$$

(summation convention only on lower suffices)

which will be unique and will converge to the required value u_x — p.p. in each variable y and z; and by virtue of (14) we have

$$\sum_{ij} |a^x_{ij}|^2 < \infty \quad \text{etc.} \tag{17}$$

Then we can regard the quantities a^x_{ij} as matrices indexed by the lower suffices for each value of the upper suffix. In particular, for the multiplication (13) we obtain ordinary matrix multiplication:

$$\begin{aligned} &M(xyw)M_2(xwz)\, du_x(w) \\ &\quad = \int a^x_{ik}A^x_i(y)A^x_k(w)b^x_{jl}A^x_j(w)A^x_l(z)\, du_x(w) \\ &\quad = a^x_{ik}b^x_{kl}A^x_i(y)A^x_l(z). \end{aligned}$$

Thus when we multiply through by say $A^x_p(y)A^x_q(z)$ and integrate over y and z, we obtain the correspondences

$$\begin{aligned} M &\to a^x_{ij} \\ MM_2 &\to a^x_{ik}b^x_{kj} \end{aligned} \tag{18}$$

so we can now drop all the suffices and write the two equations in the form (where the type of multiplication is understood)

$$\begin{aligned} a - b &= -kab, \\ b &= -kP[ab], \end{aligned} \tag{19}$$

where we must now determine the exact form of the operator P. Under TCP and under permutations of the variables in Eqs. (1), (2), the symmetry properties of M pass under (18) to a, as is obvious when we write

$$a^z{}_{ij} = \int M(xyz)A^z{}_i(y)A^z{}_j(z)\, du_z(y)\, du_z(z) \tag{20}$$

because of course in (20) we change only the variables of M and not those of the other quantities in the integration. In other words a is a Hermitian matrix and is invariant under the permutations in P. Then we can solve the Bethe–Salpeter equation in (19) in the form

$$b = a/(I - ka) \tag{21}$$

as in any other kind of matrix algebra: see Neumark, Ref. 10, Sec. 23.1, Lemma 1).

The cut-structure equation does not diagonalize in so obvious a way because the separation into two types of multiplication [Eq. (13)] is not crossing-symmetric. Since

$$(MM_2)(1234) = a^x{}_{ik}b^x{}_{kj}A^x{}_i(y)A^x{}_j(z)$$

we will have (we must now write everything explicitly)

$$(MM_2)(1234) = a^{1+3}{}_{ik}b^{1+3}{}_{kj}A^{1+3}{}_i(1 - 3)A^{1+3}{}_j(2 - 4)$$

and the cut-structure equation becomes [cf. (20)]

$$b^x{}_{pq} = -k \int a^{1+3}{}_{ik}b^{1+3}{}_{kj}A^{1+3}{}_i(1 - 3)A^{1+3}{}_j(2 - 4) \times A^x{}_p(y)A^x{}_q(f)\, du_x(y)\, du_x(f) - (\text{other term}). \tag{22}$$

By (21) we can assume that the $a^x{}_{ij}$ are diagonal for all x. They are then all real, and the last equation is of the form

$$b^x{}_p = -k \sum \int b^y{}_q K_q(x, y)\, dy - (\text{other term}),$$

where we have written $b^x{}_p$ for the p' the diagonal term; the $K_q(x, y)$ are real. But because k is pure imaginary, this last equation is inconsistent unless the b's are zero. But then also the a's are zero by (21).

[10] We can use the criterion in M. A. [Newmark] Neumark, *Normed Rings* (Moscow, 1958). Cf. comments in Ref. (2).

Thus this construction is not a precise parallel to the use of the Gel'fand–Neumark theorem in the main part of the paper. It might be supposed that it is more general in view of the lack of restrictions on the x dependence in (13). This is not so, because crossing symmetry will force us to reimpose similar conditions, as we see from Eq. (22), where there is an implicit integration over just such a variable.

APPENDIX II

In this Appendix we discuss the range of validity of the treatment in Appendix I and enlarge this range somewhat by a generalization.

The condition (14) is unrealistic for two reasons:

(a) For each value of x, there is a value of y for which $u_x(y)$ is singular—this is simply the mass shell. This would be innocuous if it were not for the modulus signs in (14), which arise from the use of the Schwartz inequality. With (14) as it stands we have to put $M = 0$ at these points in order to make the integral converge; but in that case there is scattering only off the mass shell and none on it! There seems to be little doubt that this could be overcome by the use of distribution theory, but since the conditions imposed in the body of the paper are so much more general we do not feel this would be worth the loss of clarity in what is after all only an illustration. Still, we have to admit that we have not been able to formulate explicitly a realistic set of conditions in closed form which imply the conditions used in the main part of the paper. This restriction will remain in the discussion below.

(b) Behavior for large values of the variables. Because the integral

$$\int \frac{d^4p}{(p^2 - m^2)^2}$$

is logarithmically divergent at infinity, the variables cannot approach nonzero constant values there. However (14) is even more restrictive than it need be, and we will now remove this unnecessary restriction. The point is that in the original equations [say (4), (5)], not more than one multiplication occurs in each term. Thus we may generalize (14) to

$$|M|_{g,x} = \int g^x(y)\, |M(xyz)|^2\, d\, |u_x(y)|\, d\, |u_x(z)| < \infty,$$

where the real function $g^x(y)$ satisfies $0 < g^x(y) \leq 1$ for each x. Then we will regard our kernels not as maps of a Hilbert space into itself but as maps say from the space spanned by the basis functions $A^x{}_i(y)$

into that spanned by the functions

$$B^x{}_i(y) = g^x(y)^{-\frac{1}{2}} A^x{}_i(y).$$

Then in order to get an algebra we take the isomorphism between the two spaces defined by $VB_i = A_i$, under which circumstances the multiplication in the equations corresponds to something of the form $(P, Q) \to PVQ$, and when we come to calculate the Fourier components we obtain equations which we can write in an obvious notation:

$$c - d = -kcvd \quad \text{etc.},$$

where v is the "Fourier matrix" corresponding to V. Regarded as an operator $\ell^2 \to \ell^2$, v is Hermitian-positive and bounded [we omit the details, which can be checked by inspection of the matrix elements using expressions corresponding and analogous to (20)]. Denoting by $v^{\frac{1}{2}}$ the Hermitian-positive square root (Ref. 11) and putting $a = v^{\frac{1}{2}}cv^{\frac{1}{2}}$, etc. we get an equation $a - b = -kab$, and so on as before, also for the other equation.

The transformation $c \to v^{\frac{1}{2}}cv^{\frac{1}{2}}$ is not invertible, although it is an algebraic isomorphism into (the inverse image of v is the identity, and products go into products with suitable conventions). In order actually to carry out such an inversion, consider the set of operators of Hilbert–Schmidt type on ℓ^2 with the multiplication

$$(r, s) \to rvs,$$

where v has no zero eigenvalue. We add an identity in the usual way: call the resulting algebra $V(\ell^2)$. This does not alter the representations (Ref. 12). The algebra $V(\ell^2)$, regarded as a semigroup with involution, now satisfies the requirements of the Nagy Hauptsatz (Ref. 13) so there exists an extension of ℓ^2 in which we have a representation of $V(\ell^2)$, i.e., with multiplication.

$$(r', s') \to r's'$$

with

$$pr\,r' = r \quad \text{etc.}$$

In order to get back to where we started from, we can use the minimal condition attached to the Hauptsatz and then take the isomorphism theorem for simple Hilbert algebras. (Appendix IV, Theorem IV.4).

[11] "Hermitian positive square root"—see, for instance, Riesz–Sz.-Nagy, Ref. 6, Sec. 104, where an existence and uniqueness theorem are given.
[12] Reference 10, Sec. 10.3, Theorem V.
[13] B. Sz.-Nagy, Acta. Sci. Math. Szeged 15, 104 (1954).

APPENDIX III

From the point of view of the general method it does not matter in the slightest which norm we take. This is brought out more effectively by the following theorem (see Ref. 10 Sec. 12, Corollary 2 to Theorem 1): If two semisimple commutative Banach algebras are algebraically isomorphic, they are also topologically isomorphic.

For the case $\lambda = 0$ we proved in Sec. 2 that the systems must be commutative; even for $\lambda \neq 0$, M and M_2 commute. This theorem shows that it cannot matter which norm we take (provided one exists at all). We see that the analytic arguments of Appendices I and II are not really very relevant. Not only are they contained in the more general arguments in the text, but the differences in their details cannot bring in anything new.

APPENDIX IV

We summarize very briefly and without any comments the main results from the theory of Banach algebras which are needed in the text and other appendices. References are to Ref. 10 in the form "a.b." ≡ Sec. a Paragraph b, and we also give his terminology, which does not always agree with that of other authors.

Definition IV.1 A *Banach algebra* is a complete normed algebra, i.e., an algebra which is a Banach space and in which the norm satisfies

$$||xy|| \leq ||x||\,||y||.$$

Examples of Banach algebras: matrix rings, both finite- and infinite-dimensional, in the latter case with the restriction, say,

$$||a|| = \max_p \sum_q |a_{pq}|^2 < \infty.$$

The algebra of continuous complex-valued functions on a compact space with pointwise multiplication and the norm

$$||f|| = \max_x |f(x)|.$$

The algebra $L(H)$ of all bounded linear operators on a Hilbert space H, with the norm

$$||B|| = \sup_{||x||=1} ||Bx|| \qquad [x \in H, B \in L(H)].$$

Definition IV.2: an *algebra with involution* is an algebra over the complex field in which there is an operation * with the properties

$$(kx + k'y)^* = \bar{k}x^* + \bar{k}'y^*$$
$$x^{**} = x$$
$$(xy)^* = y^*x^*$$

where x, y are in the algebra, k, k' are complex numbers, and the bar denotes complex conjugation.

Definition IV.3: a *Hilbert algebra* is a Banach algebra with involution which is also a Hilbert space and which satisfies the further conditions:

(1) The two norms coincide
(2) $(xy, z) = (y, x^*z)$, where (x, y) is the scalar product in the Hilbert space
(3) If $x \neq 0$, then also $x^*x \neq 0$.

The important example of a Hilbert algebra is the algebra of (possibly infinite-dimensional) matrices a_{ij} for which

$$||a|| = \sum_{ij} |a_{ij}^2|$$

and in which the scalar product is given by

$$(a, b) = \sum_{ij} a_{ij}\bar{b}_{ij}.$$

We shall call this algebra $\mathfrak{C}$.

Theorem IV.4: Every Hilbert algebra is isomorphic to the orthogonal direct sum of algebras $\mathfrak{C}$ (possibly-finite-dimensional). Proof: see Ref. 10, 25.5.

Definition IV.5: an algebra is *semisimple* if the intersection of all its (left-, right-, two-sided) ideals contains only the zero element.

Theorem IV.6 (Gel'fand–Neumark theorem): Let B be a commutative Banach algebra with identity, having an involution which apart from the usual algebraic conditions (definition IV.2) satisfies

$$||x^*x|| = ||x^*||\,||x||.$$

One can introduce a topology on the space M of all maximal ideals of B in which M is compact; then if $C(M)$ is the algebra of all continuous complex-valued functions on M with the definitions of the operations given in the example above, then $C(M)$ and B are symmetrically and isometrically isomorphic (see Ref. 10, 16.2)

Definition IV.7: A Banach algebra with involution having an identity e is said to be *completely symmetric* if for any element x, the element $(e + x^*x)$ always has an inverse (Ref. 10: 14; 20.4; 23).

A wide variety of conditions for complete symmetry are given in Sec. 23 of Ref. 10; in particular, B is completely symmetric if it satisfies the conditions of the Gel'fand–Neumark theorem or if it is a symmetric algebra of operators in a Hilbert space. A commutative Banach algebra is completely symmetric if and only if the characters satisfy $a^*(x) = \bar{a}(x)$.

Threshold Regge Poles for Coupled Channels* †

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(Received 22 October 1964)

The threshold Regge poles are investigated in a variety of many-channel problems. The cases considered are a simple j-independent interaction between two spin-zero channels, the tensor force problem for two spin-$\frac{1}{2}$ particles and a truncated interaction between a particle and a bound system of two particles.

I. INTRODUCTION

IT is well known that if one wishes to construct a scattering amplitude via a "one-pole" approximation in the complex angular momentum[1-4] plane then the approximate partial wave amplitude would behave near threshold as $k^{2\alpha(0)+1}$ where $\alpha(0)$ is the position where this pole leaves the real axis. Nor is any other finite sum of poles going to give the proper k^{2l+1} dependence. This problem has been resolved[5-8] by considering an infinite number of poles.

The extension of the analytic continuation of the partial wave amplitude into the complex j-plane to the cases of more than one channel has been discussed by many authors.[9-13] However, the threshold dependence of a many channel problem has heretofore received little attention. It is to this problem that we shall devote our interest.

We shall rely solely on potential theory in the following. In the second section we introduce the formalism to be used by means of a simple example of two coupled spin-zero channels, interacting via a j-independent potential.

In Sec. III we consider the tensor force problem. An expression for the Jost function is found using the regular wavefunction with the proper subtraction terms so that no unphysical assumptions on the tensor force are necessary. Using this expression, we are able to demonstrate the existence of the threshold poles.

A three-body problem is considered in Sec. IV. We take two particles in a bound s-state and allow them to be excited via the incident particle only to a p-wave state with no ionization possible. Assuming that the particle–particle interaction is a superposition of Yukawa potentials, we are able to write down the explicit j-dependence of the potential. A similarity transformation is introduced which removes the j-dependence of the potential. With the aid of this transformation we are able to see that the transformed Jost function has a simple fixed pole at $j = -\frac{1}{2}$, that the determinant has no poles, and that the transformed S-matrix has no fixed poles.

II. TWO COUPLED SPIN-ZERO CHANNELS

In order to illustrate the method of proof that we shall use to establish the existence of the threshold trajectories in the various cases we will consider, let us work with the simple problem of two coupled, two body, spin-zero channels. While appearing a bit academic, this problem has the advantage that it is the simplest one to require a matrix formulation. Hence the method of proof will be essentially the same as that which will be employed in the following more interesting problems. As a further simplification we assume that the potential is strictly local. The Schrödinger equation is

$$-\psi''(r) + (\lambda^2 - \tfrac{1}{4})r^{-2}\psi(r) + V(r)\psi(r) = K^2\psi(r), \tag{2.1}$$

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where

$$V(r) = \begin{bmatrix} V_{11}(r) & V_{12}(r) \\ V_{21}(r) & V_{22}(r) \end{bmatrix} \tag{2.2}$$

and

$$K^2 = \begin{bmatrix} k_\alpha^2 & 0 \\ 0 & k_\beta^2 \end{bmatrix}, \qquad k_\alpha^2 = k_\beta^2 + \Delta^2. \tag{2.3}$$

In Eq. (2.1), $\lambda^2 = (l + \frac{1}{2})^2$ is a scalar and $\psi(r)$ is a square-matrix solution, each column of which is a vector solution of (2.1), the columns differing by the boundary conditions. Thus when we define a matrix solution $F(\lambda, K; r)$ such that

$$\lim_{r\to\infty} F(\lambda, K; r)\, e^{iKr} = 1, \tag{2.4}$$

then the first column would behave at infinity as

$$\begin{pmatrix} e^{-ik_\alpha r} \\ 0 \end{pmatrix}$$

and the second column as

$$\begin{pmatrix} 0 \\ e^{-ik_\beta r} \end{pmatrix}.$$

$F(\lambda, K; r)$ satisfies the following integral equation:

$$F(\lambda, K; r) = F_0(\lambda, K; r) - \int_r^\infty dr' G_\lambda(K; r, r') V(r') F(\lambda, K; r'), \tag{2.5}$$

where

$$F_0(\lambda, K; r) = \exp\left[-\tfrac{1}{2}i\pi(\lambda + \tfrac{1}{2})\right](\tfrac{1}{2}\pi r)^{\frac{1}{2}} \times \begin{pmatrix} k_\alpha^{\frac{1}{2}} H_\lambda^{(2)}(k_\alpha r) & 0 \\ 0 & k_\beta^{\frac{1}{2}} H_\lambda^{(2)}(k_\beta r) \end{pmatrix}, \tag{2.6}$$

$$G_\lambda(K; r, r') = \begin{pmatrix} g_\lambda(k_\alpha; r, r') & 0 \\ 0 & g_\lambda(k_\beta; r, r') \end{pmatrix}, \tag{2.7}$$

and

$$g_\lambda(k; r, r') = \frac{\pi}{2} \frac{(rr')^{\frac{1}{2}}}{\sin \pi\lambda} [J_\lambda(kr) J_{-\lambda}(kr') - J_\lambda(kr') J_{-\lambda}(kr)]. \tag{2.8}$$

We have used J_λ as the regular Bessel function and $H_\lambda^{(2)}$ as the Hankel function of the second kind. We may also define a regular solution $\varphi(\lambda, K; r)$ to (2.1) by the boundary condition

$$\lim r^{-\lambda-\frac{1}{2}} \varphi(\lambda, K; r) = (\tfrac{1}{2}\pi)^{\frac{1}{2}} 2^{-\lambda} / \Gamma(1 + \lambda). \tag{2.9}$$

$\varphi(\lambda, K; r)$ then satisfies the integral equation

$$\varphi(\lambda, K; r) = \varphi_0(\lambda, K; r) + \int_0^r dr' G_\lambda(K; r, r') V(r') \varphi(\lambda, K; r'), \tag{2.10}$$

where

$$\varphi_0(\lambda, K; r) = (\tfrac{1}{2}\pi r)^{\frac{1}{2}} \begin{pmatrix} k_\alpha^{-\lambda} J_\lambda(k_\alpha r) & 0 \\ 0 & k_\beta^{-\lambda} J_\lambda(k_\beta r) \end{pmatrix}. \tag{2.11}$$

The proof of the convergence of the iterative solutions to (2.10) and (2.5) follow similarly as in the single-channel case.[5] We observe from Eq. (2.4) that $F(\lambda, K; r)$ and $F(\lambda, -K; r)$ are independent solutions to (2.1). Hence we may write

$$\varphi(\lambda, K; r) = (1/2i)[F(\lambda, -K; r) K^{-1} \tilde{F}(\lambda, K) - F(\lambda, K; r) K^{-1} \tilde{F}(\lambda, -K)], \tag{2.12}$$

$$F(\lambda, K) = W[\varphi(\lambda, K; r), F(\lambda, K; r)] = \tilde{\varphi}' F - \tilde{\varphi} F'. \tag{2.13}$$

The boundary condition (2.4) together with (2.2) shows

$$2i^{-1} \varphi(\lambda, K; r) F^{-1}(\lambda, -K) \cong [e^{-iKr} - e^{iKr} K^{-1} \tilde{F}(\lambda, K) \tilde{F}^{-1}(\lambda, -K)]; \tag{2.14}$$

hence

$$S(\lambda, K) = \exp\left[\tfrac{1}{2}i\pi(\lambda + \tfrac{1}{2})\right] K^{-1} \tilde{F}(\lambda, K) \tilde{F}^{-1}(\lambda, -K), \tag{2.15}$$

and we see that

$$W[\varphi(\lambda, K; r), \varphi(\lambda, K; r)] = 0.$$

Using (2.13) and the boundary condition (2.4) we find

$$F(\lambda, -K) K^{-1} \tilde{F}(\lambda, K) = F(\lambda, K) K^{-1} \tilde{F}(\lambda, -K). \tag{2.16}$$

Thus we may write

$$S(\lambda, K) = \exp\left[\tfrac{1}{2}i\pi(\lambda + \tfrac{1}{2})\right] F^{-1}(\lambda, -K) F(\lambda, K) K^{-1}, \tag{2.17}$$

where we have established the symmetry of the S matrix. The choice of the phase of S is fixed by requiring

$$S(\lambda, K) \underset{k\to\infty}{\longrightarrow} 1$$

for arbitrary λ.

Inserting the integral equations (2.5) and (2.10) into (2.13) and using the scalar Wronskians of the Bessel and Hankel functions[14] we find

[14] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, New York, 1958).

$$f(\lambda, K) \equiv \exp\left[-i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]K^{\frac{1}{2}-\lambda}F(\lambda, K)$$
$$= 1 - i\exp\left[i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]K^{\lambda-\frac{1}{2}}$$
$$\times\int_0^\infty dr\varphi_0(\lambda, K; r)V(r)F(\lambda, K; r). \quad (2.18)$$

It was noted earlier that we may write

$$F(\lambda, K; r) = \sum_{n=0}^{\infty} F^{(n)}(\lambda, K; r), \quad (2.19)$$

where

$$F^{(0)}(\lambda, K; r) = F_0(\lambda, K, r),$$
$$F^{(n)}(\lambda, K; r) = (-)^n$$
$$\times\int^\infty dr' G_\lambda(K; r, r')V(r')F^{(n-1)}(\lambda, K, r'). \quad (2.20)$$

Applying (2.19) we have

$$f(\lambda, K) = 1 - i\exp\left[i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]K^{\lambda-\frac{1}{2}}$$
$$\times\sum_{n=0}^{\infty}\int_0^\infty dr\varphi_0(\lambda, K, r)V(r)F^{(n)}(\lambda, K; r)$$
$$= 1 - i\exp\left[i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]K^{\lambda-\frac{1}{2}}$$
$$\times\int_0^\infty dr\varphi_0(\lambda, K; r)V(r)F_0(\lambda, K; r)$$
$$+ i\exp\left[i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]K^{\frac{1}{2}-\lambda}$$
$$\times\int_0^\infty dr\varphi_0(\lambda, K; r)V(r)G_\lambda(K; r, r')V(r')F_0(\lambda, K; r')$$
$$+ \cdots \quad (2.21)$$

or

$$f_{\mu\nu}(\lambda, K) = \delta_{\mu\nu} - i\exp\left[i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]k_\mu^{\lambda-\frac{1}{2}}$$
$$\times\left\{\int_0^\infty dr\varphi_{0_\mu}(\lambda, K; r)V_{\mu\nu}(r)F_{0_\nu}(\lambda, K; r) - \int_0^\infty dr\right.$$
$$\times\int_r^\infty dr'\varphi_{0_\mu}(\lambda, K; r)\sum_\epsilon V_{\mu\epsilon}(r)G_{\lambda_\epsilon}(K; r, r')V_{\epsilon\nu}(r')$$
$$\left.\times F_{0_\nu}(\lambda, K; r') + \cdots\right\}. \quad (2.21a)$$

Since we are interested in the threshold dependence we shall expand $f_{\mu\nu}$ near $k_\alpha = 0$ and $k_\beta \to i\Delta$ is a constant. We shall also use

$$H_\lambda^{(2)}(kr)J_\lambda(kr') \underset{\substack{k\cong 0\\ \lambda\cong 0}}{\simeq} \frac{1}{i\pi\lambda}\left(\frac{r'}{r}\right)^\lambda\left[e^{i\pi\lambda}\left(\frac{kr}{2}\right)^{2\lambda}\frac{\Gamma(1-\lambda)}{\Gamma(1+\lambda)} - 1\right] \quad (2.22)$$

and

$$g_\lambda(k; r, r') \underset{\substack{k\cong 0\\ \lambda\cong 0}}{\simeq} (rr')^{\frac{1}{2}}\frac{1}{2\lambda}\left[\left(\frac{r'}{r}\right)^\lambda - \left(\frac{r}{r'}\right)^\lambda\right]. \quad (2.23)$$

Equation (2.23) shows that in any order all of the k-dependence in (2.21a) will come from the terms $\varphi_{0_\mu}(\lambda, K; r)$ and $F_{0_\nu}(\lambda, K; r)$.

The Regge poles are determined by the zeros of the determinant of $F(\lambda, -K)$.[12,15] Thus we look at

$$\det F(\lambda, k) = F(\lambda, K)_{\alpha\alpha}F(\lambda, K)_{\beta\beta}$$
$$- F(\lambda, K)_{\alpha\beta}F(\lambda, K)_{\beta\alpha}. \quad (2.24)$$

Inserting (2.21a) into (2.24) and then examining it near $k_\alpha = 0$, $\lambda = 0$ we find

$$\det f(\lambda, K) = \left\{1 - \frac{1}{\lambda}[k_\alpha^{2\lambda}c(\lambda) - c(0)]\right\}f_{\beta\beta}(0, i\Delta), \quad (2.25)$$

where

$$C(\lambda) = \int_0^\infty dr V_{\alpha\alpha}(r)e^{i\pi\lambda}\frac{\Gamma(1-\lambda)}{\Gamma(1+\lambda)} + \cdots + \frac{1}{f_{\beta\beta}}$$
$$\times\left[\left(\frac{\pi}{2}\right)^2\int_0^\infty dr\int_0^\infty dr' rr' V_{\alpha\beta}(r)V_{\beta\alpha}(r')(i\Delta)^{\frac{1}{2}-\lambda}\right.$$
$$\times\exp\left[-i\frac{\pi}{2}(\lambda+\tfrac{1}{2})\right]H_\lambda^{(2)}(i\Delta r')J_\lambda(i\Delta r)$$
$$\left.\times\frac{1}{i\pi}\left(\frac{r}{r'}\right)^\lambda e^{i\pi\lambda}\left(\frac{r'}{r}\right)^{2\lambda}\frac{\Gamma(1-\lambda)}{\Gamma(1+\lambda)} + \cdots\right].$$

In a similar manner we find for $k_\beta \simeq 0$, $\lambda \simeq 0$

$$\det f(\lambda, -K) = \left\{1 - \frac{1}{\lambda}[C'(\lambda)k_\beta^{2\lambda} - C'(0)]\right\}f_{\alpha\alpha}(\Delta). \quad (2.26)$$

For either (2.25) or (2.26) we have

$$\det f(\lambda, -K) = \left[1 - \frac{1}{\lambda}C(0)\right][1 - k^{2\lambda}e^{-i\pi\lambda}D(\lambda)] = 0, \quad (2.27)$$

where

$$D(\lambda) \equiv C(\lambda)[C(0) - \lambda]^{-1}; \qquad D(0) = 1,$$

and we have divided by the factor $f_{\nu\nu}$. The Regge poles are thus determined by

$$1 - k^{2\lambda}e^{-i\pi\lambda}D(\lambda) = 0 \quad \text{for} \quad E \to 0^+ \quad (2.28)$$
$$1 - |k|^{2\lambda}D(\lambda) = 0 \quad \text{for} \quad E \to 0^-. \quad (2.28a)$$

[15] R. G. Newton, J. Math. Phys. 1, 319 (1960).

These being just the equations Desai and Newton[6] have solved, we may write down their solutions for $E \to 0^+$

$$\lambda^{(n)} = \frac{2n\pi}{\log E/E_0} e^{i\varphi}, \quad \tan\varphi = \frac{1}{\pi}\log\frac{E}{E_0}, \qquad n = \pm 1, \pm 2, \cdots \ll \frac{\log E/E_0}{2\pi} \tag{2.29}$$

and for $E \to 0^-$

$$\lambda^{(n)} = \frac{\pm 2n\pi}{|\log -E/E_0|} + i\frac{(2\pi n)^2 a}{|\log -E/E_0|}, \qquad n = 1, 2, \cdots \ll \frac{|\log -E/E_0|}{2\pi}. \tag{22.9a}$$

We thus come to the conclusion that as the first channel opens up (i.e., $k_\alpha \simeq 0$) an infinite number of poles approaches the point $\lambda = 0$ or $l = -\frac{1}{2}$. If we then increase the energy until the second channel opens up (i.e., $k_\beta \simeq 0$) we have another set of poles approaching the point $\lambda = 0$.

III. TENSOR FORCE

In this section we shall consider the scattering of two spin-$\frac{1}{2}$ particles interacting with a spin–spin force and a tensor force;[13] that is,

$$V(r) = V_c(r) + V_\sigma(r)\vec{\sigma}_1\cdot\vec{\sigma}_2 + V_t(r)S_{12}, \tag{3.1}$$

where

$$S_{12} = 3\vec{\sigma}_1\cdot\hat{r}\vec{\sigma}_2\cdot\hat{r} - \vec{\sigma}_1\cdot\vec{\sigma}_2. \tag{3.2}$$

The tensor-force term leads to a set of coupled radial Schrödinger equations for the triplet case with parity $(-)^{j+1}$. For the triplet case with parity $(-)^j$ and the singlet case the equations are uncoupled and hence basically the same as the spin-zero case. In matrix notation the coupled equations are

$$-d^2\psi(r)/dr^2 + C(j)r^{-2}\psi(r) + V^{(j)}(r)\psi(r) = k^2\psi(r), \tag{3.3}$$

where

$$V(r) = \frac{1}{2j+1}\begin{bmatrix}(2j+1)V_d(r) - 2(j-1)V_t(r) & 6[j(j+1)]^{\frac{1}{2}}V_t(t) \\ 6[j(j+1)]^{\frac{1}{2}}V_t(r) & (2j+1)V_d(r) - 2(j+2)V_t(r)\end{bmatrix} \tag{3.4}$$

with

$$V_d(r) = V_c(r) + V_\sigma(r).$$

The centrifugal term $C(j)$ is given by

$$C(j) = \begin{bmatrix} j(j-1) & 0 \\ 0 & (j+1)(j+2)\end{bmatrix}. \tag{3.5}$$

As before we may define an irregular matrix solution

$$F(j, k; r) = F_0(j, k; r) - \int_r^\infty dr' G(j, k; r, r')V(r')F(j, k; r'), \tag{3.6}$$

where

$$F_0(j, k; r) = e^{-\frac{1}{2}i\pi j}(\tfrac{1}{2}\pi kr)^{\frac{1}{2}}\begin{bmatrix}H^{(2)}_{j-\frac{1}{2}}(kr) & 0 \\ 0 & -H^{(2)}_{j+\frac{1}{2}}(kr)\end{bmatrix} \tag{3.7}$$

and

$$G(j; k; r, r') = \begin{bmatrix} g_{j-\frac{1}{2}}(k; r, r') & 0 \\ 0 & g_{j+\frac{1}{2}}(k; r, r')\end{bmatrix}. \tag{3.8}$$

The terms g_j are defined in (2.8). Looking at the potential term (3.4) we can see that we can expect trouble with an iterative solution to (4.8) when j approaches the point $-\frac{1}{2}$. This point has been fully discussed by Desai and Newton.[6] We shall merely summarize their arguments.

We note that the matrix

$$U_j = \begin{pmatrix}(j+1)^{\frac{1}{2}} & j^{\frac{1}{2}} \\ j^{\frac{1}{2}} & -(j+1)^{\frac{1}{2}}\end{pmatrix} \quad U_j^{-1} = (2j+1)^{-1}U_j \tag{3.9}$$

diagonalizes the potential $V^{(j)}$ under a similarity transformation of the form

$$V' = U_jV^{(j)}U_j^{-1} = \begin{pmatrix}V_d + 2V_t & 0 \\ 0 & V_d - 4V_t\end{pmatrix}. \tag{3.10}$$

Thus the procedure is to define the wavefunctions as in (3.6), a regular wavefunction and a Jost function. These functions are then transformed as in (3.10) and we see that they acquire, at worst, simple poles. Further, it can be shown that there is no pole in the determinant of eth Jost function. However, we need not concern ourselves with the point $j = -\frac{1}{2}$; for we will find that in looking at the threshold poles we are interested in the points $j = \frac{1}{2}, -\frac{3}{2}$.

Let us now consider the problem of defining a regular wavefunction. If we were to go ahead and define it in analogy to (2.10), then we would be forced to make some strong assumptions about the

tensor force in order that the integrals converge at $r = 0$. This can easily be seen by examining the (2,1) element of the matrix $G_t(k; r, r')V(r')\varphi_0(r')$. It contains a term of the form

$$V_t(r')g_{j+\frac{1}{2}}(k; r, r')J_{j-\frac{1}{2}}(kr')$$

which blows up as $1/r$ as $r \to 0$. To avoid this difficulty, we write

$$\varphi(j, k; r)$$
$$= \varphi_0(j, k; r)\left[1 + 6[j(j+1)]^{\frac{1}{2}}k^{-2}\int_1^r dr' \frac{1}{r'} V_t(r')P\right]$$
$$+ \int_0^r dr' \{G(j, k; r, r')V^t(r')\varphi(j, k; r')$$
$$- 6[j(j+1)]^{\frac{1}{2}}k^{-2}(1/r')\varphi_0(j, k; r')V_t(r')P\}, \quad (3.11)$$

where

$$\varphi_0(j, k; r) = \left(\frac{\pi kr}{2}\right)^{\frac{1}{2}}k^{-i}\begin{pmatrix} J_{j-\frac{1}{2}}(kr) & 0 \\ 0 & J_{j+\frac{1}{2}}(kr)\end{pmatrix} \quad (3.12)$$

and

$$P = \begin{pmatrix} 0 & 0 \\ 1 & 0\end{pmatrix}. \quad (3.13)$$

We may now define the Jost function

$$F(j, k) = W[\varphi(j, k; r), F(j, k; r)]$$
$$= \tilde{\varphi}'(j, k; r)F(j, k; r) - \tilde{\varphi}(j, k; r)F'(j, k; r) \quad (3.14)$$

so that

$$\varphi(j, k; r) = (1/2ik)[F(j, -k; r)\tilde{F}(j, k)$$
$$- F(j, k; r)\tilde{F}(j, -k)] \quad (3.15)$$

and

$$S(j, k) = \exp i\pi(j+1)F^{-1}(j, -k)F(j, k). \quad (3.16)$$

In the usual case we would, in order to evaluate $F(j, k)$, take (3.14), substitute the integral equations for $\varphi(j, k; r)$ and $F(j, k; r)$ and, using the fact that the Wronskian is independent of r, evaluate it at the origin. However in this, the tensor force case, that procedure leads to a great deal of difficulty due to the presence of the subtraction term in the integral equation for $\varphi(j, k; r)$.

Hence we will resort to the trick of using

$$V_t'(r) \equiv r^\sigma V_t(r), \qquad \sigma > 1. \quad (3.17)$$

Thus we are able to write

$$\varphi(j, k; r) = \varphi_0(j, k; r)R(j)$$
$$+ \int_0^r dr' G(j, k; r, r')V'^{(t)}(r')\varphi(j, k; r') \quad (3.11a)$$

where

$$R(j) = 1 - 6[j(j+1)]^{\frac{1}{2}}\int_0^1 dr \frac{1}{r} V_t'(r)P. \quad (3.18)$$

When we are finished we shall let $\sigma \to 0$. Now we put (3.11a) into (3.14) and evaluate it as $r \to \infty$. We find

$$f(j, k) \equiv i \exp(\tfrac{1}{2}i\pi j)k^{j-1}F(j, k)$$
$$= \tilde{R}(j) - i \exp(\tfrac{1}{2}i\pi j)k^{j-1}$$
$$\times \int_0^\infty \tilde{\varphi}(j, k; r)V'^t(r)F_0(j, k; r). \quad (3.19)$$

However, it is obvious, if we look at the first Born term, that we cannot let $\sigma \to 0$ at this point; we must still arrange the subtraction terms. Thus

$$f(j, k) = 1 + 6[j(j+1)]^{\frac{1}{2}}k^{-2}$$
$$\times \int_1^\infty dr \frac{1}{r} V_t(r)\tilde{P} - i \exp(\tfrac{1}{2}i\pi j)k^{j-1}\left\{\int_0^\infty dr\varphi_0(j, k; r)\right.$$
$$\times V^{(t)}(r)F_0(j, k; r) + 6i[j(j+1)]^{\frac{1}{2}} \exp(-\tfrac{1}{2}i\pi j)k^{-1-i}$$
$$\times \frac{1}{r} V_t(r)\tilde{P} + 6i \exp(-\tfrac{1}{2}i\pi j)k^{-1-i}[j(j+1)]^{\frac{1}{2}}\int_0^\infty dr$$
$$\left.\times \int_1^r dr' \frac{1}{r'} V_t(r')\tilde{P}\varphi_0(j, k; r)V^{(t)}(r)F_0(j, k; r) + \cdots\right\}, \quad (3.20)$$

where we have used the following iterative solution for $\varphi(j, k; r)$:

$$\varphi(j, k; r$$
$$= \varphi_0(j, k; r)\left[1 + 6[j(j+1)]^{\frac{1}{2}}k^{-2}\int_1^r dr' \frac{1}{r'} V_t(r')P\right]$$
$$+ \int_0^r dr' G(j, k; r, r')V^{(t)}(r')[\varphi_0(j, k; r') - \varphi_0(j, k; r)$$
$$\times 6[j(j+1)]^{\frac{1}{2}}k^{-2}(1/r')V_t(r')P] + \cdots. \quad (3.21)$$

Now (3.20) and (3.21) contain the proper subtractions to ensure convergence. Therefore we have allowed $\sigma \to 0$ and removed the primes on the potential terms.

It is now a straightforward matter to evaluate the determinant of $F(j, k)$. Using Eqs. (2.22) and (2.23) we find for

$$j \cong \tfrac{1}{2}, \qquad \lambda = j - \tfrac{1}{2}, \qquad k \cong 0,$$
$$\det f(\lambda, k) = \left\{1 - \frac{1}{\lambda}[k^{2\lambda}C(\lambda, j) - C(0, j)]\right\}G(j), \quad (3.22)$$

where $C(0, j)$ is a continuous bounded function of j near the point $j = \frac{1}{2}$. (See Appendix A for an ex-

pression for C.) Also for $j \cong -\frac{3}{2}$, $\nu = j + \frac{3}{2}$ and $k \cong 0$ we have

$$\det f(\nu, k) = [1 - \nu^{-1}[k^{2\nu}C'(\nu, j) - C'(0, j)]]G'(j). \tag{3.23}$$

Obviously (3.22) and (3.23) admit to the solutions (2.29) and (2.29a). We have thus established that there are two sets of threshold trajectories which appear as $k \to 0$. One set approaches the point $j = \frac{1}{2}$ and the other $j = -\frac{3}{2}$. In addition to these two terms there is the case of the parity $(-)^j$. This state also has threshold poles approaching the point $j = -\frac{1}{2}$. We have been working in a single j-plane; this plane may be thought of as two separate l-planes separated by two units. The question as to which amplitudes these poles contribute is not at all clear at the present time.

IV. GENERALIZED INTERACTION

In this section we shall consider a more general problem of two channels where we have two spin-0 particles in the initial state which may either elastically scatter or produce two particles, one with spin-1 and the other with spin-0 in the final state. We shall concern ourselves only with a parity conserving interaction. Hence, this problem immediately separates into two parts: (a) the initial and final intrinsic parities are the same, and (b) the initial and final intrinsic parities are different. Under part (a), the problem divides, depending on whether the orbital angular momentum $l = j$ or $l = j \pm 1$. The first case is just the example worked out in the second section. The second case is just a specialization of the tensor force problem we worked in the third section. In part (b) the separation is a bit trickier. In the elastic channel the states of orbital angular momentum $l = j$, hence of parity $(-)^j$, are coupled to the states in the inelastic or "production" channel of $l = j \pm 1$, but by parity conservation, not to the states of $l = j$ in the inelastic channel. The states of $l = j$ in the inelastic channel are completely uncoupled and can be ignored. For the problem when the initial parity is $(-)^j$, we shall use a model of a truncated three-body problem.

Let us consider three spin-zero particles: particle No. 1 is an incident particle; particle No. 2 is a bound particle, and particle No. 3 is a fixed "core." We truncate this problem by stipulating that the bound system of particles No. 2 and No. 3 has only one s- and one p-wave bound state and that there can be no ionization. Using the formalism for the three-body problem found in Ref. 16 we write down the following Schrödinger equation which is essentially eq. (2.10) of Ref. 16

$$-\psi''(r) + (\Lambda^2 - \tfrac{1}{4})r^{-2}\psi(r) + V(r)\psi(r) = K^2\psi(r) \tag{4.1}$$

where

$$\Lambda^2 = \begin{bmatrix} \lambda^2 & 0 & 0 \\ 0 & \nu^2 & 0 \\ 0 & 0 & \mu^2 \end{bmatrix},$$

$$\lambda = j + \tfrac{1}{2}, \tag{4.2}$$

$$\nu = j - \tfrac{1}{2}, \tag{4.3}$$

$$\mu = j + \tfrac{3}{2}, \tag{4.4}$$

and

$$K^2 = \begin{bmatrix} k_\alpha^2 & 0 & 0 \\ 0 & k_\beta^2 & 0 \\ 0 & 0 & k_\beta^2 \end{bmatrix}. \tag{4.6}$$

We have thus reduced the three-body problem to a simpler two-body formalism. In order to illustrate the meaning of (4.1) let us write down the elements of the matrix V in terms of

$$W_{l_1,l_2;l_1',l_2'}(j; E_2, E_2'; r) = \int_0^\infty dr_2 \psi_{l_2}^*(E_2 r_2) W_{l_1,l_2;l_1',l_2'}(j'; r, r_2)\psi_{l_2'}(E_2' r_2) \tag{4.7}$$

and

$$W_{l_1,l_2;l_1',l_2'}(j; r_1, r_2) = \int d\Omega_1\, d\Omega_2 Y_{jl_1l_2}^{M*}(\hat{r}_1, \hat{r}_2) Y_{jl_1'l_2'}^{M}(\hat{r}_1, \hat{r}_2) V_{12}(\mathbf{r}_1 - \mathbf{r}_2), \tag{4.8}$$

where l_1 is the angular momentum of the incident particle no. 1; V_1 is the interaction between particle No. 1 and the core; l_2 is angular momentum of the bound particle, which can take the values 0, 1; $E_2 = G_0$, G_1 are the binding energies in the s- and p-wave states, respectively, and anything else is as defined in Ref. 16. It will be shown that this potential is symmetric providing we choose the bound-state wavefunctions $\psi_{l_2}(E_2, r_2)$ to be real.

$$V_{11} = V_1 + W_{j,0;j,0}(j; G_0, G_0; r), \tag{4.9}$$

$$V_{12} = V_{21} = W_{j,0;j-1,1}(j; G_0, G_1; r), \tag{4.10}$$

$$V_{13} = V_{31} = W_{j,0;j+1,1}(j; G_0, G_1; r), \tag{4.11}$$

$$V_{22} = V_1 + W_{j-1,1;j-1,1}(j; G_1, G_1; r), \tag{4.12}$$

[16] R. G. Newton, Nuovo Cimento 29, 400 (1963).

$$V_{32} = V_{23} = W_{j-1,1;j+1,1}(j; G_1, G_1; r), \tag{4.13}$$

$$V_{33} = V_1 + W_{j+1,1;j+1,1}(j; G_1, G_1; r). \tag{4.14}$$

We can proceed in the usual manner to write down the regular and irregular wavefunctions and the Jost function:

$$F(\Lambda, K; r) = F_0(\Lambda, K; r) - \int_r^\infty dr' G(\Lambda, K; r, r') V(r') F(\Lambda, K; r'), \tag{4.15}$$

$$\lim_{r\to\infty} e^{iKr} F(\lambda, K; r) = 1, \tag{4.16}$$

$$F_0(\Lambda, K; r) = (\tfrac{1}{2}\pi r)^{\frac{1}{2}} \begin{bmatrix} e^{-\frac{1}{2}i\pi(\lambda+\frac{1}{2})} k_\alpha^{\frac{1}{2}} H_\lambda^{(2)}(k_\alpha r) & 0 & 0 \\ 0 & e^{-\frac{1}{2}i\pi(\nu+\frac{1}{2})} k_\beta^{\frac{1}{2}} H_\nu^{(2)}(k_\beta r) & 0 \\ 0 & 0 & e^{-\frac{1}{2}i\pi(\mu+\frac{1}{2})} k_\beta^{\frac{1}{2}} H_\mu^{(2)}(k_\beta r) \end{bmatrix}, \tag{4.17}$$

$$G(\Lambda, K; r, r') = \begin{bmatrix} g_\lambda(k_\alpha; r, r') & 0 & 0 \\ 0 & g_\nu(k_\beta; r, r') & 0 \\ 0 & 0 & g_\mu(k_\beta; r, r') \end{bmatrix}, \tag{4.18}$$

$$\phi(\Lambda, K; r) = \phi_0(\Lambda, K; r) + \int_0^r dr' G(\Lambda, K; r, r') \phi(\Lambda, K, r'), \tag{4.19}$$

$$\phi_0(\Lambda, K; r) = \left(\frac{\pi r}{2}\right)^{\frac{1}{2}} \begin{bmatrix} k_\alpha^{-\lambda} J_\lambda(k_\alpha r) & 0 & 0 \\ 0 & k_\beta^{-\nu} J_\nu(k_\beta r) & 0 \\ 0 & 0 & k_\beta^{-\mu} J_\mu(k_\beta r) \end{bmatrix}. \tag{4.20}$$

It may be thought that we should include some subtraction terms in (4.19). This however is not necessary as we will discuss later.

Using exactly the same methods we used in Sec. II, we may define

$$F(\Lambda, K) = W[\phi(\Lambda, K; r), F(\Lambda, K; r)]. \tag{4.21}$$

Hence

$$f(\Lambda, K) = iK^{\Lambda-\frac{1}{2}} \exp[\tfrac{1}{2}i\pi(\Lambda + \tfrac{1}{2})] F(\Lambda, K) = 1 - iK^{\Lambda-\frac{1}{2}} \exp[\tfrac{1}{2}i\pi(\Lambda + \tfrac{1}{2})] \times \int_0^\infty dr \phi_0(\Lambda, K; r) V(r) F(\Lambda, K; r), \tag{4.22}$$

where

$$e^{\frac{1}{2}i\pi(\Lambda+\frac{1}{2})} = \begin{bmatrix} e^{\frac{1}{2}i\pi(\lambda+\frac{1}{2})} & 0 & 0 \\ 0 & e^{\frac{1}{2}i\pi(\nu+\frac{1}{2})} & 0 \\ 0 & 0 & e^{\frac{1}{2}i\pi(\mu+\frac{1}{2})} \end{bmatrix} \tag{4.23}$$

and

$$K^{\Lambda-\frac{1}{2}} = \begin{bmatrix} k_\alpha^{\lambda-\frac{1}{2}} & 0 & 0 \\ 0 & k_\beta^{\nu-\frac{1}{2}} & 0 \\ 0 & 0 & k_\beta^{\mu-\frac{1}{2}} \end{bmatrix}. \tag{4.24}$$

Again it follows

$$\phi(\Lambda, K; r) = (1/2i)[F(\Lambda, -K; r) K^{-1} \tilde{F}(\Lambda, K) - F(\Lambda, K; r) K^{-1} \tilde{F}(\Lambda, -K)] \tag{4.25}$$

and thus

$$S(\Lambda, K) = f^{-1}(\Lambda, -K) f(\Lambda, K). \tag{4.26}$$

Let us now turn to the problem of evaluating the j-dependence of the potential matrix. We make the simplifying assumption that $V_{12}(|\mathbf{r}_1 - \mathbf{r}_2|)$ is a superposition of Yukawas; hence

$$V_{12}(|\mathbf{r}_1 - \mathbf{r}_2|) = \int du \rho(u) e^{-u|\mathbf{r}_1 - \mathbf{r}_2|} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = -4\pi \int du \rho(u) G(iu; \mathbf{r}_1, \mathbf{r}_2), \tag{4.27}$$

where G is the usual free two-particle Green's function. Thus[16]

$$V_{12}(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{-2i}{(r_1 r_2)^{\frac{1}{2}}} \sum_{lm} (-)^l Y_l^m(\hat{r}_1) Y_l^{m*}(\hat{r}_2) \int du \times \rho(u) J_{l+\frac{1}{2}}(iur_<) H_{l+\frac{1}{2}}^{(2)}(iur_>). \tag{4.28}$$

Inserting this in Eqs. (4.7) and (4.8) and using Eq. (4.34) in Rose[17] we find

$$W_{l_1,l_2;l_1',l_2'}(j; E_2, E_2'; r) = \frac{-2i}{4\pi} \sum_l (2l+1) \sum_{\substack{m m_1 m_2 \\ m_1' m_2'}} \times C_{l_1 l_2}(j, M; m_1, m_2) C_{l_1' l_2'}(j, M; m_1', m_2') \times C_{l l_1'}(l_1, m_1; m, m_1') C_{l l_2}(l_2', m_2'; m, m_2) \times C_{l, l_1'}(l_1, 0; 0, 0) C_{l, l_2}(l_2', 0; 0, 0) \times \left[\frac{(2l_2+1)(2l_1'+1)}{(2l_2'+1)(2l_1+1)}\right]^{\frac{1}{2}} A(l; l_2, E_2, l_2', E_2'; r), \tag{4.29}$$

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

where

$$A(l;\, l_2, E_2, l_2', E_2';\, r) = \int du\rho(u)u \times \left[r^{-\frac{1}{2}} J_{l+\frac{1}{2}}(iur) \int_{r_2>r} dr_2 r_2^{-\frac{1}{2}} H^{(2)}_{l+\frac{1}{2}}(-iur_2)\psi_{l_2}(r_2)\psi_{l_2'}(r_2) + r^{-\frac{1}{2}} H^{(2)}_{l+\frac{1}{2}}(-iur) \int_{r_2<r} dr_2 r_2^{-\frac{1}{2}} J_{l+\frac{1}{2}}(iur_2)\psi_{l_2}(r_2)\psi_{l_2'}(r_2) \right]. \tag{4.30}$$

Since E_2 is fixed when l_2 is given, we drop E_2 in the notation for A. Using Eq. (6.6b) in Rose[17] we find

$$W_{l_1,l_2;l_1',l_2'}(j; E_2, E_2';\, r) = (-)^{l_1+l_1'}[(2l_2+1)(2l_1'+1)]^{\frac{1}{2}} \times \sum_l W(l_1, l_2, l_1', l_2'; j, l)(2l+1)C_{ll_1'}(l_1, 0; 0, 0) \times C_{ll_2}(l_2', 0; 0, 0)B(l; l_2, l_2'; r), \tag{4.31}$$

where

$$B(l; l_2, l_2'; r) = -(2i/4\pi)A(l; l_2, l_2'; r) \tag{4.32}$$

and $W(l_1, l_2, l_1', l_2'; j, l)$ is a Racah coefficient. It is easily seen from (4.31), (4.30) and the symmetry relations for the Clebsch–Gordan and Racah coefficients that the potential matrix V is symmetric.

Using (4.31) and the tables in Rose[17] and Edmonds[18] we explicitly evaluate the j-dependence of the potential V.

$$V_{11} = V_1(r) + B(0; 0, 0; r) \equiv U_1(r), \tag{4.9a}$$

$$V_{12} = [3j/(2j+1)]^{\frac{1}{2}} B(1; 0, 1; r), \tag{4.10a}$$

$$V_{13} = -\left[\frac{3(j+1)}{2j+1}\right]^{\frac{1}{2}} B(1; 0, 1; r), \tag{4.11a}$$

$$V_{22} = V_1(r) + B(0; 1, 1; r) + \frac{j-1}{2j+1} B(2; 1, 1; r) \equiv U_2(r) + \frac{j-1}{2j+1} B(2; 1, 1; r), \tag{4.12a}$$

$$V_{23} = -3\left[\frac{j(j+1)}{2j+1}\right]^{\frac{1}{2}} B(2; 1, 1; r), \tag{4.13a}$$

$$V_{33} = V_1(r) + B(0; 1, 1; r) + \frac{j+2}{2j+1} B(2; 1, 1; r) \equiv U_2(r) + \frac{j+2}{2j+1} B(2; 1, 1; r). \tag{4.14a}$$

Thus the potential matrix V is of the form

$$V = \begin{bmatrix} U_1 & \left[\frac{3j}{2j+1}\right]^{\frac{1}{2}} B(1; 0, 1) & -\left[\frac{3(j+1)}{2j+1}\right]^{\frac{1}{2}} B(1; 0, 1) \\ \left[\frac{j}{2j+1}\right]^{\frac{1}{2}} B(1; 0, 1) & U_2 + \frac{j-1}{2j+1} B(2; 1, 1) & -3\frac{[j(j+1)]^{\frac{1}{2}}}{2j+1} B(2; 1, 1) \\ -\left[\frac{3(j+1)}{2j+1}\right]^{\frac{1}{2}} B(1; 0, 1) & -3\frac{[j(j+1)]^{\frac{1}{2}}}{2j+1} B(2; 1, 1) & U_2 + \frac{j+2}{2j+1} B(2; 1, 1) \end{bmatrix}. \tag{4.33}$$

As in the case of the tensor force we are faced with the possibility of an essential singularity in the S-matrix at $j = -\frac{1}{2}$ unless we can find some r-independent transformation that will remove the $1/(2j+1)$ -dependence. It might be noted that if one identifies U_2 and $B(2; 1, 1)$ with V_d and V_t of the previous section, we have a submatrix whose form is exactly that of the tensor force. Hence we would expect that our results would be the same as that case in the limit in which $B(1; 0, 1) \to 0$. That this is not true is seen from the fact that (4.33) contains four independent functions of r; $U_1(r)$, $U_2(r)$, $B(1; 0, 1; r)$, $B(2; 1, 1; r)$. Hence it will be impossible to diagonalize V with an r-independent matrix. An alternate method is to note that two of the eigenvalues of V involve square roots of $B(r)$. Thus our transformation will be entirely different from the transformation used in the tensor force case. This situation is somewhat analogous to what happens in the tensor force problem when one adds $L\cdot S$ coupling.

The problem of the behavior of the regular wavefunction near $r = 0$ is not present. This comes from the fact that (4.32) may be shown to have the proper r-dependence near the origin[16] so that no subtractions are needed, provided the weight function $\rho(u)$ behaves reasonably as $u \to \infty$.

We shall, in this section, subject all the formalism to the similarity transformation $AMA^{-1} = \bar{M}$ where

$$A = \begin{bmatrix} (2j+1)^{-\frac{1}{2}} & 0 & 0 \\ 0 & j^{\frac{1}{2}} & (j+1)^{\frac{1}{2}} \\ 0 & -j^{\frac{1}{2}}(2j+1)^{-1} & (j+1)^{\frac{1}{2}}(2j+1)^{-1} \end{bmatrix} \tag{4.34}$$

[18] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

and

$$A^{-1} = \begin{bmatrix} (2j+1)^{\frac{1}{2}} & 0 & 0 \\ 0 & \frac{1}{2}j^{-\frac{1}{2}} & -\frac{1}{2}(2j+1)j^{-\frac{1}{2}} \\ 0 & \frac{1}{2}(j+1)^{-\frac{1}{2}} & \frac{1}{2}(2j+1)(j+1)^{-\frac{1}{2}} \end{bmatrix}. \tag{4.35}$$

Hence

$$\bar{V} = AVA^{-1} = \begin{bmatrix} U_1 & 0 & -\sqrt{3}B(1;0,1) \\ -\sqrt{3}B(1;0,1) & U_2 - B(2;1,1) & 3B(2;1,1) \\ -\sqrt{3}B(1;0,1) & 0 & U_2 + B(2;1,1) \end{bmatrix}, \tag{4.36}$$

$$\bar{\Lambda}^2 = \begin{bmatrix} (j+\frac{1}{2})^2 & 0 & 0 \\ 0 & j^2+j+\frac{5}{4} & (2j+1)^2 \\ 0 & 1 & j^2+j+\frac{5}{4} \end{bmatrix}, \tag{4.37}$$

$$\bar{K}^2 = \begin{bmatrix} k_\alpha^2 & 0 & 0 \\ 0 & k_\beta^2 & 0 \\ 0 & 0 & k_\beta^2 \end{bmatrix}. \tag{4.38}$$

Since the transformed differential equation and boundary condition have no poles, Eqs. (4.36), (4.37), (4.38), (4.22), and (4.23) imply that there are no poles as a function of j in $\bar{F}(\Lambda, K, r)$. The fact that $\bar{G}(\Lambda, K; r, r')$ has no poles is easily verified by direct calculation with the use of the recurrence relations for the Bessel functions[14] and the equation

$$\bar{G}(\Lambda, K; r, r) = \begin{bmatrix} g_\lambda(k_\alpha; r, r') & 0 & 0 \\ 0 & \frac{1}{2}[g_\mu(k_\beta; r, r') + g_\nu(k_\beta; r, r')] & \frac{1}{2}(2j+1)[g_\mu(k_\beta; r, r') - g_\nu(k_\beta, r, r')] \\ 0 & \frac{1}{2}(2j+1)^{-1}[g_\mu(k_\beta; r, r') - g_\nu(k_\beta; r, r')] & \frac{1}{2}[g_\mu(k_\beta; r, r') + g_\nu(k_\beta; r, r')] \end{bmatrix}. \tag{4.39}$$

There is, however, a simple pole in $\bar{\phi}(\Lambda, K; r)$ since

$$\bar{\phi}(\Lambda, K; r) = \begin{bmatrix} \phi_{0\lambda}(k_\alpha r) & 0 & 0 \\ 0 & \frac{1}{2}[\phi_{0\mu}(k_\beta r) + \phi_{0\nu}(k_\beta r)] & \frac{1}{2}(2j+1)[\phi_{0\mu}(k_\beta r) - \phi_{0\nu}(k_\beta r)] \\ 0 & \frac{1}{2}(2j+1)^{-1}[\,]_{0\mu}(k_\beta r) - \phi_{0\nu}(k_\beta r)] & \frac{1}{2}[\phi_{0\mu}(k_\beta r) + \phi_{0\nu}(k_\beta r)] \end{bmatrix}, \tag{4.40}$$

where

$$\phi_{0\sigma}(kr) = (\tfrac{1}{2}\pi r)^{\frac{1}{2}}k^{-\sigma}J_\sigma(kr), \qquad \sigma = \mu, \nu, \lambda.$$

The Regge trajectories are determined by the zeros of $\det f(\Lambda, K)$. Since we expect that the threshold poles for $k_\alpha \cong 0$ will end at $\lambda = 0$, we must see if this determinant has a pole at $j = -\frac{1}{2}$. It will be easier to consider

$$\bar{G}\bar{F}(\Lambda, K) \equiv \bar{F}_1(\Lambda, K) = i\bar{G}K^{\frac{1}{2}-\bar{\Lambda}} \exp\,[-\tfrac{1}{2}i\pi(\bar{\Lambda} + \tfrac{1}{2})]\bar{F}(\Lambda, K),$$

where

$$G = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k_\beta^2 \end{bmatrix}. \tag{4.41}$$

Obviously the determinants differ only by

$$\det \bar{G}\bar{K}^{(\frac{1}{2}-\Lambda)} \exp\,[\tfrac{1}{2}i\pi(\Lambda + \tfrac{1}{2})] = \det GK \exp\,[-\tfrac{1}{2}i\pi(\bar{\Lambda} + \tfrac{1}{2})]$$

which has no poles as function of j.

From (4.20), the recurrence relations for the Bessel functions and the fact $\mu = \nu + 2$, we find

$$\bar{F}_1(\Lambda, K) = i\bar{G}K^{\frac{1}{2}-\bar{\Lambda}} \exp\,[-\tfrac{1}{2}i\pi(\bar{\Lambda} + \tfrac{1}{2})] + G' \int_0^\infty dr\bar{\phi}_0(\Lambda, K, r)\bar{V}(r)\bar{F}(\Lambda, K; r) \tag{4.42}$$

where

$$G'K^{\frac{1}{2}-\bar{\Lambda}} \exp\,[-\tfrac{1}{2}i\pi(\bar{\Lambda} + \tfrac{1}{2})] = \begin{bmatrix} k_\alpha^\lambda & 0 & 0 \\ 0 & 0 & \dfrac{2j+1}{2}\,k_\beta^{\frac{1}{2}-\nu}e^{-\frac{1}{2}i\pi(\mu+\frac{1}{2})} \\ 0 & \dfrac{1}{2(2j+1)}\,k_\beta^{\frac{1}{2}-\nu}e^{-\frac{1}{2}i\pi(\mu+\frac{1}{2})} & 0 \end{bmatrix} \tag{4.43}$$

and

$$G'\phi_0'(\Lambda, K; r) = (\tfrac{1}{2}\pi r)^{\frac{1}{2}}\begin{bmatrix} k_\alpha^{-\lambda}J_\lambda(k_\alpha r) & 0 & 0 \\ 0 & \tfrac{1}{2}(2j+1)k_\beta^{-\nu}J_{\nu+1}(k_\beta r) & \tfrac{1}{2}(2j+1)k_\beta^{-\nu}J'_{\nu+1}(k_\beta r) \\ 0 & \tfrac{1}{2}(2j+1)^{-1}k_\beta^{-\nu}J'_{\nu+1}(k_\beta r) & \tfrac{1}{2}(2j+1)k_\beta^{-\nu}J_{\nu+1}(k_\beta r) \end{bmatrix}. \quad (4.44)$$

Using Eqs. (4.42), (4.43), and (4.44) it follows that we may write

$$\bar{F}_1(\Lambda, K) = (2j+1)^{-1}BM + CD + BD' + (2j+1)E_1 + (2j+1)^2E_2 + \cdots, \quad (4.45)$$

where

$$B = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad (4.46)$$

$$B^2 = 0, \quad (4.46a)$$

$$C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (4.47)$$

$$BC = CB = 0, \quad (4.47a)$$

and the matrices M, D, and D' are independent of j.

Equation (4.45) immediately implies that det $\bar{F}_1(\Lambda, K)$ has at worst a simple pole at $j = -\frac{1}{2}$. By explicit evaluation, using the first Born term for $F(\Lambda, K; r)$ we may see that det $F(\Lambda, K) \neq 0$ as $j \to -\frac{1}{2}$. These two statements and Eq. (4.45) show that $\bar{F}_1^{-1}(\Lambda, K)$ also has at worst a simple pole at $j = -\frac{1}{2}$. Hence we write

$$\bar{F}_1^{-1}(\Lambda, K) = (2j+1)^{-1}N_0 + N_1 + (2j+1)N_2 + (2j+1)^2N_3 + \cdots, \quad (4.48)$$

$$\bar{F}_1^{-1}(\Lambda, K)\bar{F}_1(\Lambda, K) = \bar{F}_1(\Lambda, K)\bar{F}_1^{-1}(\Lambda, K) = 1. \quad (4.49)$$

Equations (4.48), (4.49), and (4.45) imply

$$E_1N_0 + CD'N_1 + BD'N_1 + BMN_2 = 1. \quad (4.50)$$

Multiplying from left by B we find

$$BE_1N_0 = B. \quad (4.51)$$

The important consequence of (4.51) is that $N_0 \neq 0$. Thus $\bar{F}_1^{-1}$ has *exactly* a simple pole. The fact that both $\bar{F}_1^{-1}$ and $\bar{F}_1$ have simple poles shows that det $\bar{F}_1$ has no pole at $j = -\frac{1}{2}$.

We also have

$$\bar{F}_1^{-1}\bar{F}_1 = (2j+1)^{-2}N_0BM + (2j+1)^{-1} \times (N_0CD' + N_0BD'' + N_1BM) + \cdots = 1. \quad (4.52)$$

Equation (4.52) implies that N_1 and N_0 are left multiples of B:

$$N_0 = N_0'B, \quad (4.53)$$

$$N_1 = N_1'B. \quad (4.54)$$

We recall that

$$\bar{S}(\Lambda, K) = \bar{F}_1^{-1}(\Lambda, -K)e^{\frac{1}{2}i\pi(\bar{\Lambda}+\frac{1}{2})}\bar{F}_1(\Lambda, K), \quad (4.55)$$

where

$$\exp[\tfrac{1}{2}i\pi(\bar{\Lambda}+\tfrac{1}{2})] = \begin{bmatrix} e^{\frac{1}{2}i\pi(\lambda+\frac{1}{2})} & 0 & 0 \\ 0 & 0 & (2j+1)e^{\frac{1}{2}i\pi(\mu+\frac{1}{2})} \\ 0 & \dfrac{1}{2j+1}e^{\frac{1}{2}i\pi(\nu+\frac{1}{2})} & 0 \end{bmatrix}$$

$$= \exp\{[\tfrac{1}{2}i\pi(\nu+\tfrac{1}{2})]/2j+1\ B + M. \quad (4.56)$$

Hence Eqs. (4.55), (4.54), and (4.56) imply that there is no pole at $j = -\frac{1}{2}$ in $\bar{S}$.

We shall now look at det $F(\Lambda, K)$ as $k_\alpha, k_\beta \to 0$ with $\lambda, \nu, \mu \cong 0$. The procedure is the following: first we substitute the iterative solution for $F(\Lambda, K, r)$ in the Jost function; then we evaluate the determinant of the Jost function, and then we use Eqs. (2.22) and (2.23) for evaluating the limit $k_\beta \to 0$, $\nu \to 0$. We find

$$k_\alpha \cong 0 \qquad \lambda \cong 0$$

$$\det F = \{1 - \lambda^{-1}[k_\alpha^{2\lambda}C(\lambda) - C(0)]\}G(k_\beta, \mu, \nu), \quad (4.57)$$

$$k_\beta \cong 0 \qquad \nu \cong 0$$

$$\det F = \{1 - \nu^{-1}[k_\beta^{2\nu}C'(\nu) - C'(0)]\}G'(k_\alpha, \lambda, \mu), \quad (4.58)$$

$$k_\beta \cong 0 \qquad \mu \cong 0$$

$$\det F = \{1 = \mu^{-1}[k_\beta^{2\mu}C''(\mu) - C''(0)]\}G''(k_\beta, \lambda, \nu). \quad (4.59)$$

(An expression for C' is given in Appendix B.) With the help of Eqs. (4.3), (4.4), and (4.5) we see that as the spin-0 or "α" channel opens, we have an infinite number of poles of the form given in (2.29) approaching the point of $j = -\frac{1}{2}$. As the

spin-1 or "β" channel opens up we have two sets of poles as given in (2.29). One set approaches $j = \frac{1}{2}$ and the other $j = -\frac{3}{2}$.

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APPENDIX A

The expression for C defined in Sec. III is given below.

$$C(\lambda) = \frac{1}{2j+1} e^{i\pi\lambda} \frac{\Gamma(1-\lambda)}{\Gamma(1+\lambda)} \Big\{ \int_0^\infty dr \Big(\frac{r}{2}\Big)^{2\lambda+1} [(2j+1)V_d(r) - 2(j-1)V_t(r)] - \frac{1}{f_{\beta\beta}} \frac{36j(j+1)}{\pi^2(2j+1)} \Big[\int_0^\infty dr$$
$$\cdot \int_0^r dr' V_t(r) V_t(r') r r' \Big(\frac{r'}{r}\Big)^\lambda \Big(\frac{r}{2}\Big)^{2\lambda} \phi_{0\nu}(kr) f_{0\nu}(kr) + \int_1^\infty dr \frac{1}{r} V_t(r) \int_0^\infty dr \Big(\frac{r}{2}\Big)^\nu r^{-\lambda} \Gamma(1+\Gamma) V_t(r) \Big] + \frac{1}{(2j+1) f_{\beta\beta}}$$
$$\cdot \int_0^\infty dr \int_0^r dr' \Big(\frac{r}{2}\Big)^{\lambda+1} \Big(\frac{r'}{2}\Big)^{\lambda+1} [(2j+1)V_d(r') - 2(j-1)V_t(r')][(2j+1)V_d(r) - 2(j-1)V_t(r)] + \cdots \Big\},$$

$$f_{\beta\beta} = -\frac{i e^{\frac{1}{2}i\pi i} k^{j-1}}{2j+1} \int_0^\infty dr \phi_{0\nu}(kr)[(2j+1)V_d(r) - 2(j+2)V_t(r)]F_{0\nu}(kr) + \cdots .$$

APPENDIX B

The expression for C' defined in Sec. IV is given below.

$$C'(\nu) = \frac{1}{2} \int_0^\infty dr\, r \Big[\frac{3j}{2j+1}\Big]^{\frac{1}{2}} B(1;0,1;r) \int dr'\, r' \Big[\frac{3j}{2j+1}\Big]^{\frac{1}{2}} B(1;0,1;r') \Big(\frac{r}{r'}\Big)^\nu \Big(\frac{r'}{2}\Big)^{2\nu} e^{i\pi\nu} \frac{\Gamma(1-\nu)}{\Gamma(1+\nu)} H_\lambda(\Delta r') J_\lambda(\Delta r)$$
$$- \frac{1}{2 f_{\mu\mu}} \int dr\, r \Big[\frac{3j}{2j+1}\Big]^{\frac{1}{2}} B(1;0,1;r) \int dr'\, r' \Big[\frac{3(j+1)}{2j+1}\Big]^{\frac{1}{2}} B(2;1,1;r') \int dr''' \Big[\frac{3(j+1)}{2j+1}\Big]^{\frac{1}{2}} B(1;0,1;r''')$$
$$\cdot \Big(\frac{r}{r'}\Big)^\nu \Big(\frac{r'}{2}\Big)^{2\nu} \frac{\Gamma(1-\nu)}{\Gamma(1+\nu)} H_\lambda(\Delta r) J_\lambda(\Delta r''') + e^{i\pi\nu} \int dr\, r \Big[U_2(r) + \frac{j-1}{2j+1} B(2;1,1;r)\Big] \Big(\frac{r}{2}\Big)^{2\nu} \frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}$$
$$\cdot \Big\{ f_{\lambda\lambda} + \frac{1}{f_{\mu\mu}} \int dr\, r \Big[\frac{3(j+1)}{2j+1}\Big]^{\frac{1}{2}} B(1;1,0;r) \int dr'\, r' \Big[\frac{3(j+1)}{2j+1}\Big]^{\frac{1}{2}} B(1;0,1;r') H_\lambda(\Delta r') J_\lambda(\Delta r) \Big\}$$
$$- \frac{f_{\lambda\lambda}}{f_{\mu\mu}} \int dr\, r \frac{[3j(j+1)]^{\frac{1}{2}}}{2j+1} B(2;1,1;r) \int dr'\, r' \frac{[3j(j+1)]^{\frac{1}{2}}}{2j+1} B(2;1,1;r') \frac{\Gamma(1-\nu)}{\Gamma(1+\nu)} \Big(\frac{r'}{r}\Big)^\nu \Big(\frac{r'}{2}\Big)^{2\nu} + \cdots ,$$

$$f_{\mu\mu} = 1 - i \int dr\, r \Big[U_2(r) + \frac{j+2}{2j+1} B(2;1,1;r)\Big] \frac{1}{i \sin \pi\mu\, \Gamma(1-\mu)\Gamma(1+\mu)} + \cdots ,$$

$$f_{\lambda\lambda} = 1 - i \int dr\, r U_1(r) H_\lambda(\Delta r) J_\lambda(\Delta r).$$

On the Bound-State Wavefunctions of a Nonlocal Solvable Potential

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The Schrödinger equation is solved in the momentum representation with a nonlocal factorable potential, with at most two point eigenvalues. When the potential is a bilinear form in the Bessel transforms of Yukawa functions, we prove that it is impossible to have two bound states whose asymptotic behavior is determined by the binding energy.

1. INTRODUCTION

IN order to investigate the nucleon–nucleus scattering in an independent-particle scheme,[1] we are interested in constructing a complete set of suitably orthonormalized single-particle states. Owing to the possibility of freely fixing the zero-order-approximation (no-correlation model) we have tried to define them as the eigenstates of the Hamiltonian

$$H = H_0 + V, \tag{1.1}$$

where H_0 is the kinetic energy and V a nonlocal factorable potential of the type[2]

$$\langle pJ|\ V\ |p'J'\rangle = -\delta_{JJ'} \sum_n G_n g_{nJ}(p) g_{nJ}(p') \tag{1.2}$$

here J stands for the set $\{Jlm_J\}$, n the principal quantum number and G_n are positive parameters. Such a potential is useful because the corresponding Schrödinger equation is easily solvable for both the discrete and the continuous spectra.

In the presence of degeneracy (i.e., several n corresponding to the same J) it can be shown[2] that the number of bound states is at most equal to the number of positive G_n.

2. ASYMPTOTIC BEHAVIOR OF THE BOUND-STATE EIGENFUNCTIONS

The asymptotic behavior of the eigenfunctions $U(r)$ belonging to the discrete spectrum of the Hamiltonian (1.1) will depend, in general, both on the binding energy and the nonlocality range of the potential.

In our shell-model approach, the potential (1.2) plays the role of a Hartree–Fock self-consistent single-particle potential.[3] While on general grounds this is expected to be nonlocal, in the usual spectroscopic calculations a local one is chosen. Hence we impose the condition that the asymptotic behavior of our bound solutions is the same as that for a local potential.

The radial Schrödinger equation for a bound s state in a local central potential is

$$U'' - [q^2 + V(r)]U = 0, \tag{2.1}$$

where $q = (-2ME/\hbar^2)^{\frac{1}{2}}$, E being the binding energy.

It is well known that the asymptotic behavior of its solutions cannot be derived, in general, from the equation obtained by substituting in Eq. (2.1) the value of $V(r)$ at large distances.

Nevertheless it can be stated[4] that, when the condition

$$\int_{r_0}^{\infty} V^2(r)\, dr < \infty \tag{2.2}$$

is satisfied, the solution of (2.1) which goes to zero at infinity is of the type

$$U(r) \propto e^{-q\tau(r)}, \tag{2.3}$$

with

$$\tau(r) = r + \frac{1}{2}\int_{r_0}^{r} V(t)\, dt. \tag{2.4}$$

Among the potentials usually adopted in spectroscopic calculations, the harmonic oscillator does not satisfy (2.2). It is well known that the harmonic oscillator wavefunctions, as used in nuclear spectroscopy, when introduced in reaction amplitude calculations, give results which disagree with experiments. This is due to the fact that their amplitude decreases too rapidly with increasing energy and so they give too small values for the reduced widths.[5]

Thus, since we want to construct a "good" basis

[1] A. Agodi, F. Catara, and M. Di Toro (to be published).
[2] G. C. Ghirardi and A. Rimini, J. Math. Phys. 5 (1964) 722.
[3] The self-consistency hypothesis is usually introduced in spectroscopic calculations whenever one considers phenomenological values for the single-particle energies [see, e.g., N. Vinh-Mau, thesis, Université de Paris, 1963; V. Gillet, thesis, Université de Paris, 1962, J. Sawicki Phys. Rev. 126 2231 (1962).
[4] G. Ascoli, Boll. Unione Mat. Ital. 8, 3 (1953).
[5] A. M. Lane, Rev. Mod. Phys. 32 (1960) 519. Using, e.g., eigenfunctions of a Saxon–Woods well, the cross-section values are in better agreement with experimental results.

for both spectroscopic and reaction calculations, we want to consider "realistic" potentials, i.e., such that the condition (2.2) is satisfied and so the bound eigenfunctions behave asymptotically as in Eq. (2.3).

Note also that, since their value for $r > R$ (where R is a suitably fixed range) is negligible, when we consider large r-values, Eq. (2.4) becomes

$$\tau(r) = r + h, \tag{2.5}$$

h being an R-dependent constant. Therefore the asymptotic behavior of the bound-state wavefunctions of such potentials is

$$U(r) \propto e^{-qr}. \tag{2.6}$$

From these remarks we are led to impose that the bound eigenfunctions of the nonlocal potential (1.2) have an asymptotic behavior governed, as in Eq. (2.6), by the binding energy.

3. GENERAL SOLUTION

With our choice (1.2) of the potential, the radial Schrödinger equation in the momentum representation becomes (leaving the J label as understood)

$$(\alpha_{n'}^2 + p^2)\psi_{n'}(p) = 2M \sum_n G_n g_n(p) \cdot \int g_n(p')\psi_{n'}(p')p'^2\, dp' \tag{3.1}$$

with

$$\alpha_n^2/2M = -E_n. \tag{3.2}$$

The solutions of the integral equation (3.1) are[6]

$$\psi_{n'}(p) = \sum_n N_n^{(n')} g_n(p)/(\alpha_{n'}^2 + p^2) \tag{3.3}$$

with the conditions

$$2MG_{n'} \int \frac{g_{n'}(p') \sum_n N_n^{(n'')} g_n(p')}{\alpha_{n''}^2 + p'^2} p'^2\, dp' = N_{n'}^{(n'')},$$

i.e.,

$$\sum_n \left(\delta_{nn'} - 2MG_{n'} \int \frac{g_{n'}(p')g_n(p')}{\alpha_{n''}^2 + p'^2} p'^2 dp'\right) N_n^{(n'')} = 0, \tag{3.4}$$

where $N_n^{(n'')}$ are normalization constants.

4. TWOFOLD S DEGENERACY

We have chosen for the functions $g(p)$[7,8]

$$g_n(p) = 1/(C_n^2 + p^2). \tag{4.1}$$

Substituting Eq. (4.1) in to Eq. (3.3), we obtain the explict expression of the solutions:

$$\psi_n = \frac{1}{\alpha_n^2 + p^2} \sum_{n'} \frac{N_{n'}^{(n)}}{C_{n'}^2 + p^2} \tag{4.2}$$

(in our case $n, n', n'' = 1, 2$).

In Eq. (4.2) we have to determine the constants α_n, $N_n^{(n')}$, G_n and the range parameters of the interaction C_n.

We take the parameters α_n as determined from experiment.[9] The system (3.4) plus normalization conditions uniquely determine the $N_n^{(n')}$.

The secular equations associated to (3.4) give the "strengths" G_n for each pair of C_n.

We will show, for any C_n, the nonexistence of solutions which satisfy Eq. (2.6).

With

$$x = 1/G_1; \qquad y = 1/G_2, \tag{4.3}$$

the secular equations become

$$\begin{aligned}(x - a_1)(y - b_1) - d_1^2 &= 0,\\ (x - a_2)(y - b_2) - d_2^2 &= 0,\end{aligned} \tag{4.4}$$

where

$$a_1 = \frac{\pi M}{2C_1(C_1 + \alpha_1)^2}, \qquad a_2 = \frac{\pi M}{2C_1(C_1 + \alpha_2)^2},$$

$$b_1 = \frac{\pi M}{2C_2(C_2 + \alpha_1)^2}, \qquad b_2 = \frac{\pi M}{2C_2(C_2 + \alpha_2)^2},$$

$$d_1 = \frac{-\pi M}{(C_1 + C_2)(C_1 + \alpha_1)(C_2 + \alpha_1)},$$

$$d_2 = \frac{-\pi M}{(C_1 + C_2)(C_1 + \alpha_2)(C_2 + \alpha_2)}.$$

With $\alpha_1 > \alpha_2$ and putting

$$\begin{aligned}x' &= x - a_1,\\ y' &= y - b_1,\end{aligned} \tag{4.5}$$

the system (4.4) takes the form

$$\begin{aligned}Bx'^2 - Ax' + d_1^2 &= 0,\\ y' &= A - Bx',\end{aligned} \tag{4.6}$$

where

$$\begin{aligned}x' + a_1 &> 0,\\ y' + b_1 &> 0,\end{aligned} \tag{4.7}$$

because x, y are positive quantities.

[6] E. T. Whittaker and G. M. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England, 1935), p. 227.

[7] Y. Yamaguchi, Phys. Rev. 95, 1628 (1954).

[8] Note that in the s case this represents the Bessel transform of a Yukawa function.

[9] In fact, this will not be essential for our purposes.

In Eq. (4.6) we have

$$A = (d_1^2 - d_2^2 + x_0' y_0')/x_0', \qquad B = y_0'/x_0' > 0, \tag{4.8}$$

where

$$x_0' = a_2 - a_1 > 0, \qquad y_0' = b_2 - b_1 > 0. \tag{4.9}$$

In order that the conditions (4.7) are satisfied, it is necessary that

$$(A + b_1)/B > -a_1 \tag{4.10}$$

Let us consider now the first of the equations (4.6). From the reality of its solutions we get

$$\Delta = A^2 - 4B\, d_1^2 \geq 0. \tag{4.11}$$

Our condition on the asymptotic behavior of the wavefunction in the configuration space imposes some restriction to the range of allowed C_n values.

The Bessel transforms of the solutions (4.2) are

$$\psi_{E_1,\frac{1}{2}}(r) \propto (e^{-\alpha_1 r} - e^{-C_1 r} - e^{-C_2 r})/r, \qquad \psi_{E_2,\frac{1}{2}}(r) \propto (e^{-\alpha_2 r} - e^{-C_1 r} - e^{-C_2 r})/r \tag{4.12}$$

According to what is stated in Sec. 2, the asymptotic behavior of the functions (4.12) should be governed by the terms involving the energies and so we get

$$C_1, C_2 > \alpha_1, \alpha_2. \tag{4.13}$$

The inequalities (4.10) and (4.11) are never consistent with the conditions (4.13) (see Appendix), hence the problem does not admit solutions satisfying Eq. (2.6).

Concluding we note the impossibility of using this potential in a shell-model approach to the unified treatment of nuclear structure and reactions.

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APPENDIX

Replacing the quantities involved in Eq. (4.10) by their analytic expressions, we get in units α_2

$$(C_2 - C_1)(C_1 + C_2)^2[2C_1C_2 + (\alpha_1 + 1)(C_1 + C_2) + 2\alpha_1] - 8C_1C_2(C_1 + 1)(C_2 + 1)(C_1 + C_2 + \alpha_1 + 1) > 0, \tag{A1}$$

whence

$$C_2 > C_1. \tag{A2}$$

On the other hand, Eq. (4.11) is satisfied when either

$$x_0' y_0' \geq (d_1 + d_2)^2 \tag{A3}$$

or

$$x_0' y_0' \leq (d_1 - d_2)^2. \tag{A4}$$

The explicit expression of Eq. (A3) is

$$F(\alpha_1) = (C_1 + C_2)^2[(C_1 + \alpha_1)^2 - (C_1 + 1)^2] \cdot [(C_2 + \alpha_1)^2 - (C_2 + 1)^2] - 4C_1C_2[(C_1 + 1)(C_2 + 1) + (C_1 + \alpha_1)(C_2 + \alpha_1)]^2 \geq 0, \tag{A5}$$

with

$$C_2 > C_1 > \alpha_1 > 1. \tag{A6}$$

Note that $F(\alpha_1 = 1) < 0$.

It can be shown that

$$dF(\alpha_1)/d\alpha_1 < 0 \quad \text{for} \quad 1 \leq \alpha_1 \leq C_1.$$

Hence $F(\alpha_1)$ is always negative (in the considered interval) and Eq. (A5) is never satisfied.

In the same way let us rewrite (A4):

$$(C_1 + C_2)^2[(C_1 + \alpha_1)^2 - (C_1 + 1)^2] \cdot [(C_2 + \alpha_1)^2 - (C_2 + 1)^2] - 4C_1C_2[(C_1 + 1)(C_2 + 1) - (C_1 + \alpha_1)(C_2 + \alpha_1)]^2 \leq 0. \tag{A7}$$

By easy algebraic calculations it becomes

$$(\alpha_1 + 1) + 2(C_1 + C_2) \leq 0, \tag{A8}$$

which obviously is never satisfied.

On a Set of Coupled Second-Order Differential Equations*

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An alternative method for solving a set of coupled second-order differential equations, which often appears in theoretical treatments of many-body problems, is proposed. This method makes use of both mathematical relations derived in matrix theory and physical properties of the potentials provided by the set of equations to be solved.

I. INTRODUCTION

A COUPLED set of second-order differential equations often appears in the theoretical treatment of many-body problems. For example, the compound-state formation in resonance scattering experiments may be described mathematically by a set of coupled second-order differential equations. The commonly adopted method for solving such a set of equations is the well-known iteration procedure. In this paper, we propose an alternative approach which makes use of both mathematical relations derived in matrix theory and physical properties of the potentials provided by the set of equations to be solved.

This method, in the present form, is useful for diagonal potentials having a singularity not higher than the second order within a finite range of the concerned variable and for coupling potentials which tend to zero faster than certain positive powers of the variable at the origin. The actual values of the power depend on the characteristic values of the singularity of the diagonal potentials.

The exact problem of concern in this paper is formulated in the matrix representation in the next section. The resultant equation is then solved in Sec. III. We choose bound-state boundary conditions for the solution (extension to other boundary conditions is straightforward). For such a case we encounter interesting eigenvalue problems appropriate for virtual states having physically well-defined lifetimes, such as compound-nuclear states or autoionization states. Finally in Appendix A we include, for completeness, the procedures found by Gantmacher[1] for calculating the matrix elements appearing in the solution for the set of coupled second-order differential equations.

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[1] F. R. Gantmacher, *The Theory of Matrices* (Chelsea Publishing Company, New York, 1959), Vol. II, pp. 148–153. (translated from Russian).

II. FORMULATION OF THE PROBLEM

We consider a set of n coupled second-order differential equations

$$\left\{\frac{d^2}{dx^2}+\frac{2}{x}\frac{d}{dx}-\frac{l_i(l_i+1)}{x^2}+\mu[E-V_i(x)]\right\}\psi_i(x)=\sum_{j\neq i}^{n}\mu V_{ij}(x)\psi_j(x), \qquad (2.1)$$

where n and the l's are positive integers, μ and E are constants, $x = r/r_0$ is a dimensionless continuous variable and the V's are functions of x to be referred to as potentials. We consider Eq. (2.1) for two general cases, namely the short-range potential case and the long-range potential case.

We assume there exists a value of r_0 such that the variable x is conveniently divided into two regions for the potentials:

(i) In the internal region $0 \leq x \leq 1$, we assume, for both short- and long-range potential cases, that the diagonal potentials take the form

$$V_i(x) = \alpha_i/x^2 - \beta_i/x + V_i^{(0)}(x), \qquad (2.2)$$

where the α's and the β's are constants and the $V_i^{(0)}$'s are analytic at all points within this region. For the coupling potentials, we require the functionals $V_{ij}(x)x^{\gamma_j-\gamma_i}$ to be analytic at all points within this region, where

$$\gamma_i = \{(l_i+\tfrac{1}{2})^2+\mu\alpha_i\}^{\frac{1}{2}}-\tfrac{1}{2}. \qquad (2.3)$$

(ii) In the external region $x \geq 1$, we assume for the short-range potential case that the $V_i^{(0)}$ [in Eq. (2.2)] and the V_{ij}'s are zero, and for the long-range potential case that all the potentials in Eq. (2.1) may be replaced by their corresponding asymptotic forms.

The basic idea of our approach is to arrange the set of n coupled equations (2.1) into a matrix differential equation[2]

[2] The Schrödinger eigenvalue problem has been treated in terms of matrix differential equation by O. Hellman, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 32, Nos. 4, 10 (1960).

$$d\Phi/dx = \mathbf{A}(x)\Phi \tag{2.4}$$

by introducing the columnar matrix

$$\Phi = \begin{pmatrix} d\phi/dx \\ \phi \end{pmatrix} \tag{2.5}$$

and the square matrix

$$\mathbf{A}(x) = \begin{bmatrix} \mathbf{0} & \mathbf{A}_{21} \\ \mathbf{I} & \mathbf{0} \end{bmatrix}, \tag{2.6}$$

with

$$\phi = \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_n \end{bmatrix}, \qquad \varphi_i = x\psi_i(x), \tag{2.7}$$

$$\mathbf{A}_{21}(x) = \begin{bmatrix} \mu V_{11} & \mu V_{12} & \cdots & \mu V_{1n} \\ \mu V_{21} & \mu V_{22} & \cdots & \mu V_{2n} \\ \vdots & \vdots & & \vdots \\ \mu V_{n1} & \mu V_{n2} & \cdots & \mu V_{nn} \end{bmatrix}, \tag{2.8}$$

$$V_{ii}(x) = \frac{\gamma_i(\gamma_i+1)}{\mu x^2} - \frac{\beta_i}{x} + (V_i^{(0)}(x) - E), \tag{2.9}$$

where **0** and **I** are null and unit matrices, respectively. This arrangement reduces the order of differentiation. Thus we are led to consider a matrix differential equation of the first order.

We solve the matrix differential equation according to the division of the potential in the two regions subject to the appropriate bound-state boundary conditions,

$$\Phi(x=0) = \begin{pmatrix} \mathbf{C} \\ \mathbf{0} \end{pmatrix}, \qquad \Phi(x \to \infty) = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \tag{2.10}$$

where **C** is a real constant matrix[3]

$$\mathbf{C} = \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_n \end{bmatrix}. \tag{2.11}$$

We then require these solutions in the two regions to satisfy the continuity conditions at $x = 1$

$$\Phi_{\mathrm{I}} = \Phi_{\mathrm{II}} \begin{cases} d\phi_{\mathrm{I}}/dx \overset{x=1}{=} d\phi_{\mathrm{II}}/dx, & \text{(2.12a)} \\ \phi_{\mathrm{I}} \overset{x=1}{=} \phi_{\mathrm{II}}, & \text{(2.12b)} \end{cases}$$

where the subscripts I and II label the internal region $0 \leq x \leq 1$ and the external region $x \geq 1$, respectively. The continuity equation (2.12b) together with the normalization relations for the ψ's (i.e., the φ's) determine uniquely all the unknown constants. The continuity equation (2.12a) provides solutions for eigenvalues.

[3] This is a sufficient boundary condition at orgin since $\varphi_i(x) = x\psi_i(x)$ and $\psi_i(x=0) = c_i$.

III. SOLUTION OF COUPLED SECOND-ORDER DIFFERENTIAL EQUATIONS

A. Internal Region

The matrix differential equation

$$d\Phi/dx = \mathbf{A}(x)\Phi \tag{3.1}$$

is not in a convenient form since matrix $\mathbf{A}(x)$ has an irregular singularity at point $x = 0$. We notice that this irregularity may be removed by a transformation so that the new representation has only a regular singularity at point $x = 0$.

To accomplish this transformation, we construct a nonsingular matrix $\mathbf{B}(x)$:

$$\mathbf{B}(x) = \begin{bmatrix} \mathbf{0} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix}, \tag{3.2}$$

with

$$\mathbf{B}_{12}(x) = \mathbf{B}_{21}(x) = \begin{bmatrix} x^{-(\gamma_1+1)} & & & 0 \\ & x^{-(\gamma_2+1)} & & \\ & & \ddots & \\ 0 & & & x^{-(\gamma_n+1)} \end{bmatrix}, \tag{3.3}$$

$$B_{22}(x) = \begin{bmatrix} \dfrac{\kappa_1 x - \gamma_1 - 1}{x^{\gamma_1+2}} & & & 0 \\ & \dfrac{\kappa_2 x - \gamma_2 - 1}{x^{\gamma_2+2}} & & \\ & & \ddots & \\ 0 & & & \dfrac{\kappa_n x - \gamma_n - 1}{x^{\gamma_n+2}} \end{bmatrix}, \tag{3.4}$$

$$\kappa_i = \mu\beta_i/2(\gamma_i+1) \tag{3.5}$$

and make the transformation

$$\Psi = \mathbf{B}(x)\Phi. \tag{3.6}$$

We obtain from Eq. (3.1)

$$d\Psi/dx = \{\mathbf{D}/x + \mathbf{P}(x)\}\Psi, \tag{3.7}$$

with

$$\mathbf{D} = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_{22} \end{bmatrix} \qquad \mathbf{P}(x) = \begin{bmatrix} \mathbf{P}_{11} & \mathbf{I} \\ \mathbf{P}_{21} & \mathbf{P}_{22} \end{bmatrix}, \tag{3.8}$$

where

$$\mathbf{D}_{22} = \begin{bmatrix} -2(\gamma_1+1) & & & 0 \\ & -2(\gamma_2+1) & & \\ & & \ddots & \\ 0 & & & -2(\gamma_n+1) \end{bmatrix}, \quad (3.9) \text{ and } \mathbf{P}_{22} = -\mathbf{P}_{11} = \begin{bmatrix} \kappa_1 & & & 0 \\ & \kappa_2 & & \\ & & \ddots & \\ 0 & & & \kappa_n \end{bmatrix}, \quad (3.10)$$

$$\mathbf{P}_{21} = \begin{bmatrix} \mu(V_1^{(0)} - E) - \kappa_1^2 & \mu V_{12}x^{\gamma_2-\gamma_1} & \cdots & \mu V_{1n}x^{\gamma_n-\gamma_1} \\ \mu V_{21}x^{\gamma_1-\gamma_2} & \mu(V_2^{(0)} - E) - \kappa_2^2 & \cdots & \mu V_{2n}x^{\gamma_n-\gamma_2} \\ \vdots & \vdots & & \vdots \\ \mu V_{n1}x^{\gamma_1-\gamma_n} & \mu V_{n2}x^{\gamma_2-\gamma_n} & \cdots & \mu(V_n^{(0)} - E) - \kappa_n^2 \end{bmatrix}. \quad (3.11)$$

Since the $V_i^{(0)}$'s and the $V_{ij}x^{\gamma_j-\gamma_i}$'s are analytic within the region $0 \leq x \leq 1$, matrix $\mathbf{P}(x)$ possesses in this region an absolutely convergent power-series expansion.

$$\mathbf{P}(x) = \sum_{i=0}^{\infty} \mathbf{P}_i x^i. \quad (3.12)$$

The general solution of Eq. (3.7) is[1] (Appendix A)

$$\Psi = \mathbf{G}(x)x^{\mathbf{M}}x^{\mathbf{W}}\Psi_0, \quad (3.13)$$

with

$$\mathbf{G}(x) = \mathbf{I} + \sum_{i=1}^{\infty} \mathbf{G}_i x^i \equiv \begin{bmatrix} \mathbf{G}_{11}(x) & \mathbf{G}_{12}(x) \\ \mathbf{G}_{21}(x) & \mathbf{G}_{22}(x) \end{bmatrix}, \quad (3.14)$$

$$\mathbf{M} = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{M}_{22} \end{bmatrix}, \quad \mathbf{M}_{22} = \begin{bmatrix} -m_1 & & & 0 \\ & -m_2 & & \\ & & \ddots & \\ 0 & & & -m_n \end{bmatrix}, \quad (3.15)$$

$$\mathbf{W} = \begin{bmatrix} 0 & \mathbf{W}_{12} \\ 0 & \mathbf{W}_{22} \end{bmatrix}, \quad (3.16)$$

where $m_i = [\text{Re } (2(\gamma_i + 1))]$ is the integral part of the number Re $[2(\gamma_i + 1)]$ and Ψ_0 is an arbitrary column matrix to be determined by the boundary conditions. The blocks $\mathbf{W}_{12}$ and $\mathbf{W}_{22}$ of matrix $\mathbf{W}$ are related to $\mathbf{D}$ and given in Appendix B. It will be shown that the desired solution, satisfying the appropriate boundary condition at $x = 0$, does not require the knowledge of $\mathbf{W}_{12}$ and $\mathbf{W}_{22}$. The determination of the elements for the set of coefficient matrices $\{\mathbf{G}_i\}$ appearing in the absolutely convergent series (3.14) are given in detail in Appendix A.

Now the solution in the internal region can be written down from Eq. (3.6)

$$\Phi_I = \mathbf{B}^{-1}\Psi = \mathbf{B}^{-1}(x)\mathbf{G}(x)x^{\mathbf{M}}x^{\mathbf{W}}\Psi_0, \quad (3.17)$$

with

$$\mathbf{B}^{-1}(x) = \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{21}^{-1} \\ \mathbf{B}_{12}^{-1} & 0 \end{bmatrix}, \quad (3.18)$$

where

$$\mathbf{B}_{11}(x) = \begin{bmatrix} x^{\gamma_1}(1 + \gamma_1 - \kappa_1 x) & & & 0 \\ & x^{\gamma_2}(1 + \gamma_2 - \kappa_2 x) & & \\ & & \ddots & \\ 0 & & & x^{\gamma_n}(1 + \gamma_n - \kappa_n x) \end{bmatrix}, \quad (3.19)$$

$$\mathbf{B}_{21}^{-1} = \mathbf{B}_{12}^{-1} = \begin{bmatrix} x^{\gamma_1+1} & & & 0 \\ & x^{\gamma_2+1} & & \\ & & \ddots & \\ 0 & & & x^{\gamma_n+1} \end{bmatrix}. \quad (3.20)$$

We require Φ_I to be regular at the origin [i.e., Eq. (2.10)]. Since $\mathbf{B}^{-1}(x)\mathbf{G}(x)$ in Eq. (3.17) is well-behaved at $x = 0$, we must choose Ψ_0 carefully so that $x^{\mathbf{M}}x^{\mathbf{W}}\Psi_0$ is also regular at the origin. It can be shown that

$$x^{\mathbf{M}}x^{\mathbf{W}}\Psi_0 = \begin{bmatrix} 1 & 0 \\ 0 & x^{\mathbf{M}_{22}} \end{bmatrix}\begin{bmatrix} 1 & \mathbf{F} \\ 0 & x^{\mathbf{W}_{22}} \end{bmatrix}\Psi_0 = \begin{bmatrix} 1 & \mathbf{F} \\ 0 & x^{\mathbf{M}_{22}}x^{\mathbf{W}_{22}} \end{bmatrix}\Psi_0, \quad (3.21)$$

where $\mathbf{F}$ is a series in terms of $\ln x$. The obvious choice of Ψ_0 is

$$\Psi_0 = \begin{bmatrix} \mathbf{C}' \\ 0 \end{bmatrix} \quad \text{with} \quad \mathbf{C}' = \begin{bmatrix} C_1' \\ C_2' \\ \vdots \\ C_n' \end{bmatrix}. \quad (3.22)$$

The solution in the internal region is then

$$\Phi_I = \begin{bmatrix} \{\mathbf{B}_{11}(x)\mathbf{G}_{11}(x) + \mathbf{B}_{21}^{-1}(x)\mathbf{G}_{21}(x)\}\mathbf{C}' \\ \mathbf{B}_{12}^{-1}(x)\mathbf{G}_{11}(x)\mathbf{C}' \end{bmatrix}. \quad (3.33)$$

It is worthwhile to note that $x^{\mathbf{M}}x^{\mathbf{W}}$ is never really needed in the actual calculation.

B. External Region

a. *Short-Range Potential*

We now consider the solution for $x \geq 1$ for the short-range potential case. For such a case, the set of coupled differential equations [Eq. (2.1)], in the external region $x \geq 1$, becomes uncoupled. It is, then, more convenient to start from the individual uncoupled equation

$$\left\{\frac{d^2}{dx^2} - \frac{\gamma_i(\gamma_i + 1)}{x^2} + \frac{\beta_i}{x} + \mu E\right\}\varphi_i^{(II)}(x) = 0, \quad i = 1, 2, \cdots, n. \quad (3.24)$$

The solution of Eq. (3.24) for negative E, satisfying the bound-state boundary conditions, is[4]

$$\varphi_i^{(II)}(x) = W_{\tau_i,\gamma_i+\frac{1}{2}}((\beta_i/\tau_i)x), \quad (3.25)$$

with

$$\tau_i = \beta_i/(2[\mu\,|E|]^{\frac{1}{2}}), \quad (3.26)$$

where the Whittaker function $W_{\zeta\eta}(z)$ has the integral representation

$$W_{\zeta\eta}(z) = \frac{z^{\zeta}e^{-z/2}}{\Gamma(\eta - \zeta - \frac{1}{2})} \times \int_0^\infty e^{-t}(1 + t/z)^{\eta+\zeta-\frac{1}{2}}t^{\eta-\zeta-\frac{1}{2}}\,dt. \quad (3.27)$$

The constant for $\varphi_i^{(II)}(x)$ in Eq. (3.25) is chosen, without loss of generality, to be unity.

Making use of the differential property of the Whittaker function,[4] we obtain

$$\frac{d\varphi_i^{II}}{dx} = \frac{1}{x}\left\{\frac{\tau_i^2 - \beta_i x}{2\tau_i}W_{\tau_i,\gamma_i-\frac{1}{2}}\left(\frac{\beta_i}{\tau_i}x\right) - (\gamma_i - \tau_i)(\gamma_i + \tau_i - 1)W_{\tau_i-1,\gamma_i-\frac{1}{2}}\left(\frac{\beta_i}{\tau_i}x\right)\right\}. \quad (3.28)$$

Thus the solution in the external region is

$$\Phi_{II} = \begin{bmatrix} d\phi_{II}/dx \\ \phi_{II} \end{bmatrix} \quad (3.29)$$

where the elements in columns $d\Phi_{II}/dx$ and Φ_{II} are given by Eqs. (3.28) and (3.25), respectively.

Now we require the continuity conditions to be satisfied at $x = 1$, we obtain from Eqs. (3.23) and (3.29)

$$\{\mathbf{B}_{11}(x)\mathbf{G}_{11}(x) + \mathbf{B}_{12}^{-1}(x)\mathbf{G}_{21}(x)\}\mathbf{C}' \overset{x=1}{=} d\phi_{II}(x)/dx, \quad (3.30a)$$

$$\mathbf{B}_{12}^{-1}(x)\mathbf{G}_{11}(x)\mathbf{C}' \overset{x=1}{=} \phi_{II}(x). \quad (3.30b)$$

The continuity equation of the wavefunctions at $x = 1$ [Eq. (3.30b)], determines all the C_i''s, hence the C_i's in Eq. (2.11). By normalizing the φ_i's, i.e.,

$$\varphi_i(x) = C_i'\{C_i\varphi_i^{(I)}(x) + \varphi_i^{(II)}(x)\}, \quad (3.31)$$

we determine all the C_i''s. Thus all the unknown constants are determined uniquely.

The continuity equations of the derivatives of the wavefunctions at $x = 1$ [Eq. (3.30a)] provides solutions for the eigenvalue appropriate for virtual states. It should be noted that virtual states are not eigenstates of the time translational operator; they formally do not satisfy the bound-state boundary conditions.[5] We can, nevertheless, show that the lifetime of such states is physically well-defined. Thus, for virtual states having a sufficiently long lifetime to be observable experimentally, we are permitted to impose the bound-state boundary conditions on them.[6]

b. *Long-Range Potential*

There is no unique formula derivable for treating long-range potential cases in the external region. Each case must be treated according to its appropriate asymptotic expression of the potential. For this reason we consider an example.

We consider the set of coupled equations arising

[4] E. T. Whittaker, Bull. Am. Math. Soc. **10**, 125 (1904); L. J. Slater, *Confluent Hypergeometric Functions* (Cambridge University Press, New York, 1960).

[5] M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964), Chap. 8.

[6] H. Feshbach, Ann. Phys. (N. Y.) **19**, 287 (1962); J. C. Y. Chen, J. Chem. Phys. **40**, 3507, 3513 (1964).

from electron scattering by hydrogen atoms.[7] We confine our consideration to the compound-state formation in the elastic scattering just below the $2s$–$2p$ threshold. For simplicity, we will treat the problem within $2s$–$2p$ close-coupling approximation and neglect exchange effects. Under these conditions, the appropriate system matrix $\mathbf{A}$ defined in Eq. (2.4) takes the form (in atomic units)

$$\mathbf{A}(x) = \begin{bmatrix} 0 & 0 & 2r_0^2(V_{2s} - k^2/2) - 2r_0/x & 2r_0^2 V_{2s2p} \\ 0 & 0 & 2r_0^2 V_{2p2s} & 2r_0^2(V_{2p} - k^2/2) - 2r_0/x + 2/x^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \tag{3.32}$$

where

$$r_0^2 V_{2s} = r_0^2\left\{\frac{1}{r} - \left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{8}\right)e^{-r}\right\} \underset{r\to\infty}{\to} \frac{r_0}{x},$$

$$r_0^2 V_{2p} = r_0^2\left\{\frac{1}{r} - \left(\frac{1}{r} + \frac{3}{4} + \frac{r}{4} + \frac{r^2}{24}\right)e^{-r} + 12\left[\frac{1}{r^3} - \left(\frac{1}{r^3} + \frac{1}{r^2} + \frac{1}{2r} + \frac{1}{6} + \frac{r}{24} + \frac{r^2}{144}\right)e^{-r}\right]\right\} \to \frac{r_0}{x}, \tag{3.33}$$

$$r_0^2 V_{2s2p} = r_0^2 V_{2p2s} = 3r_0^2\left\{\frac{1}{r^2} - \left(\frac{1}{r^2} + \frac{1}{r} + \frac{1}{2} + \frac{r}{6} + \frac{r^2}{24}\right)e^{-r}\right\} \underset{r\to\infty}{\to} \frac{3}{x^2},$$

and $k = i(2|E|)^{\frac{1}{2}}$ is the wavenumber of the electron.

Substitution of the asymptotic expression for the potentials yield for $\mathbf{A}(x)$ matrix

$$\mathbf{A}(x) = \begin{bmatrix} 0 & 0 & -r_0^2k^2 & 6/x^2 \\ 0 & 0 & 6/x^2 & 2/x^2 - r_0^2k^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{3.34}$$

To solve the matrix differential equation (2.4) in the external region $x \geq 1$ with $\mathbf{A}(x)$ given by Eq. (3.34), we introduce the transformation

$$\Psi = \mathbf{T}\Phi, \tag{3.35}$$

with

$$\mathbf{T} = \begin{bmatrix} \frac{a+1}{2a} & -\frac{3}{a} & 0 & 0 \\ \frac{a-1}{2a} & \frac{3}{a} & 0 & 0 \\ 0 & 0 & \frac{a+1}{2a} & -\frac{3}{a} \\ 0 & 0 & \frac{a-1}{2a} & \frac{3}{a} \end{bmatrix} \qquad \Phi = \begin{bmatrix} \partial\varphi_{2s}/\partial x \\ \partial\varphi_{2p}/\partial x \\ \varphi_{2s} \\ \varphi_{2p} \end{bmatrix}, \tag{3.36}$$

[7] T. -Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962), p. 184.

where $a = (37)^{\frac{1}{2}}$, and obtain the decoupuled equation

$$\frac{d}{dx}\Psi = \begin{bmatrix} 0 & 0 & \frac{1-a}{x^2} - r_0^2k^2 & 0 \\ 0 & 0 & 0 & \frac{1+a}{x^2} - r_0^2k^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}\Psi. \tag{3.37}$$

Hence we are led to solve the following two equations

$$\left\{\frac{d^2}{dx^2} - \frac{1-a}{x^2} + r_0^2k^2\right\}f_1 = 0, \tag{3.38}$$

$$\left\{\frac{d^2}{dx^2} - \frac{1+a}{x^2} + r_0^2k^2\right\}f_2 = 0 \tag{3.39}$$

for bound-state solution. The solution of Eq. (3.38) for imaginary k is

$$f_1 = x^{\frac{1}{2}}H_{i\nu}^{(1)}(ir_0\,|k|\,x), \qquad \nu = (a - 5/4)^{\frac{1}{2}}, \tag{3.40}$$

where $H_{i\nu}^{(1)}(iz)$ is the Hankel function of the first kind. For our special case, with pure imaginary order and argument, the Hankel function has the integral representation

$$H_{i\nu}^{(1)}(iz) = \frac{2e^{\pi\nu/2}}{i\pi}\int_0^\infty \exp\left[-z\cosh(t)\right] \times \cos(\nu t)\,dt. \tag{3.41}$$

For Eq. (3.39) there is no bound-state solution, hence we take $f_2 = 0$.

The solution in the external region then is

$$\Phi_{II} = \mathbf{T}^{-1}\Psi = \begin{bmatrix} df_1/dx \\ \frac{1}{6}(1-a)\,df_1/dx \\ f_1 \\ \frac{1}{6}(1-a)f_1 \end{bmatrix}. \tag{3.42}$$

Proceeding as described before with the continuity requirement,[8] we can again determine the constants and solve the eigenvalue problem.

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APPENDIX A

The solution of matrix differential equation

$$d\Psi/dx = \{\mathbf{D}/x + \mathbf{P}(x)\}\Psi \tag{A1}$$

with

$$\mathbf{P}(x) = \sum_{t=0}^{\infty} \mathbf{P}_t x^t, \tag{A2}$$

which converges absolutely for every x within a finite interval $0 \leq x \leq x_0$ has been studied by Gantmacher.[1] We are here interested in the case where $\mathbf{D}$ is diagonal whose characteristic values $\lambda_1, \lambda_2, \cdots, \lambda_\nu$ satisfy the inequalities

$$\mathrm{Re}\,(\lambda_1) \geq \mathrm{Re}\,(\lambda_2) \cdots \geq \mathrm{Re}\,(\lambda_\nu), \tag{A3}$$

where ν is the order of the matrices in Eq. (A1).

The approach is to seek a transformation $\mathbf{G}(x)$ which is analytic within the interval $0 \leq x \leq x_0$, having the boundary condition $\mathbf{G}(x = 0) = \mathbf{I}$, i.e., $\mathbf{G}(x)$ possesses an absolutely convergent power series

$$\mathbf{G}(x) = \mathbf{I} + \mathbf{G}_1 x + \mathbf{G}_2 x^2 + \cdots. \tag{A4}$$

The transformed function Υ satisfies

$$d\upsilon/dx = \{\mathbf{D}/x + \mathbf{Q}(x)\}\upsilon \tag{A5}$$

with

$$\Psi = \mathbf{G}(x)\upsilon, \tag{A6}$$

where the matrix $\mathbf{Q}(x)$ also possesses an absolutely convergent power series in the internal $0 \leq x \leq x_0$

$$\mathbf{Q}(x) = \sum_{t=0}^{\infty} \mathbf{Q}_t x^t. \tag{A7}$$

Other than the requirements (A4), (A5), and (A7), matrices $\mathbf{G}(x)$ and $\mathbf{Q}(x)$ are quite arbitrary.

[8] It should be noted that the potentials given in Eqs. (3.33) satisfy the conditions for the internal region $0 \leq x \leq 1$ discussed in Sec. II. Thus, the internal-region solution given by Eq. (3.23) is valid for this problem.

From Eq. (A1) with the help of Eqs. (A5) and (A6), we find

$$d\mathbf{G}/dx + x^{-1}[\mathbf{G}, \mathbf{D}] = (\mathbf{P}(x)\mathbf{G}(x) - \mathbf{G}(x)\mathbf{Q}(x)) \tag{A8}$$

where $[A, B]$ is the commutator of A and B defined by $[A, B] = AB - BA$. Substituting the series expressions for $\mathbf{P}$, $\mathbf{G}$, and $\mathbf{Q}$ from Eqs. (A2), (A4) and (A7) into Eq. (A8) and equating the coefficients of the equal powers of x on the two sides, we obtain an infinite set of matrix equations for the unknown coefficients

$$[\mathbf{G}_t, \mathbf{D}] + t\mathbf{G}_t = \sum_{s=0}^{t-1} \{\mathbf{P}_s \mathbf{G}_{t-s-1} - \mathbf{G}_{t-s-1}\mathbf{Q}_s\}, \qquad t \geq 1. \tag{A9}$$

Introducing, for the elements of matrices in Eq. (A9), the notation

$$\mathbf{G}_t = (g_{ij}^{(t)}), \quad \mathbf{P}_t = (p_{ij}^{(t)}), \quad \mathbf{Q}_t = (q_{ij}^{(t)}), \tag{A10}$$

we are able to write

$$(t - \lambda_i + \lambda_j) g_{ij}^{(t)} = \sum_{s=0}^{t-1} \sum_{k=1}^{\nu} \{p_{ik}^{(s)} g_{kj}^{(t-s-1)} - g_{ik}^{(t-s-1)} q_{kj}^{(s)}\}, \qquad t \geq 1. \tag{A11}$$

As long as the conditions stated in Eqs. (A4), (A5), and (A7) are simultaneously satisfied, the elements of matrices $\mathbf{G}(x)$ and $\mathbf{Q}(x)$ may be chosen quite arbitrarily for the convenience of calculating one from the other. Starting from $\mathbf{G}_1$ and $\mathbf{Q}_0$, we make the choice

$$\begin{aligned} q_{ij}^{(0)} &= 0 \quad \text{if} \quad \lambda_i - \lambda_j \neq 1, \\ g_{ij}^{(1)} &= 0 \quad \text{if} \quad \lambda_i - \lambda_j = 1. \end{aligned} \tag{A12a}$$

Then, from Eq. (A11), the rest elements can be determined uniquely (remembering $g_{ij}^{(0)} = \delta_{ij}$)

$$\begin{aligned} q_{ij}^{(0)} &= p_{ij}^{(0)} \quad \text{if} \quad \lambda_i - \lambda_j = 1, \\ g_{ij}^{(1)} &= p_{ij}^{(0)}/(1 - \lambda_i + \lambda_j) \quad \text{if} \quad \lambda_i - \lambda_j \neq 1. \end{aligned} \tag{A12b}$$

After $\mathbf{G}_1$ and $\mathbf{Q}_0$ are calculated from (A12), we may proceed to determine all the matrices $\mathbf{G}_2\mathbf{Q}_1$; $\mathbf{G}_3\mathbf{Q}_2$; $\cdots$ in succession from the formulas

$$q_{ij}^{(t-1)} = 0,$$

$$g_{ij}^{(t)} = [p_{ij}^{(t-1)} + f_t(p, g, q)]/(t - \lambda_i + \lambda_j), \quad \text{if} \quad t \neq \lambda_i - \lambda_j, \tag{A13a}$$

$$g_{ij}^{(t)} = 0, \quad q_{ij}^{(t-1)} = p_{ij}^{(t-1)} + f_t(p, g, q), \quad \text{if} \quad t = \lambda_i - \lambda_j, \tag{A13b}$$

where

$$f_t(p, g, q) = \sum_{s=0}^{t-2} \sum_{k=1}^{r} \{p_{ik}^{(s)} g_{kj}^{(t-s-1)} - g_{ik}^{(t-s-1)} q_{kj}^{(s)}\}. \tag{A14}$$

It is clear from Eqs. (A12) and (A13) that, among all the elements $q_{ij}^{(t)}$ of the whole set of matrices $\{\mathbf{Q}_t\}$, their can be, for each given pair of subscripts (i', j'), at most one $q_{i'j'}^{(t)}$, different from zero. If such a different-from-zero element exists, it is located in matrix $\mathbf{Q}_{t'}$ with $t' = \lambda_{i'} - \lambda_{j'} - 1$. It is also clear, with the help of Eq. (A3), that all elements $q_{ij}^{(t)}$ of the matrix $\mathbf{Q}_t$ are zero for $i > j$. Hence matrix $\mathbf{Q}$ is of the form

$$\mathbf{Q}(x) = \sum_{t=0}^{\infty} \mathbf{Q}_t x^t = \begin{bmatrix} 0 & q_{12}^{(\lambda_1-\lambda_2-1)} x^{\lambda_1-\lambda_2-1} & q_{13}^{(\lambda_1-\lambda_3-1)} x^{\lambda_1-\lambda_3-1} & \cdots & q_{1r}^{(\lambda_1-\lambda_r-1)} x^{\lambda_1-\lambda_r-1} \\ 0 & 0 & q_{23}^{(\lambda_2-\lambda_3-1)} x^{\lambda_2-\lambda_3-1} & \cdots & q_{2r}^{(\lambda_2-\lambda_r-1)} x^{\lambda_2-\lambda_r-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, \tag{A15}$$

where $q_{ij}^{(\lambda_i-\lambda_j-1)}$ differs from zero only when $\lambda_i - \lambda_j$ is a positive interger.

By defining

$$\lambda_i - \lambda_j = [\mathrm{Re}\,(\lambda_i)] - [\mathrm{Re}\,(\lambda_j)] \equiv m_i - m_j, \tag{A16}$$

where m_i is the integral part of the number Re (λ_i), similarly for m_j, we may rewrite matrix $\mathbf{Q}(x)$ from Eq. (A15) in the form

$$\mathbf{Q}(x) = x^{\mathbf{M}}(\mathbf{U}/x)x^{-\mathbf{M}} \tag{A17}$$

with

$$\mathbf{M} = \begin{bmatrix} m_1 & & & 0 \\ & m_2 & & \\ & & \ddots & \\ 0 & & & m_r \end{bmatrix}, \tag{A18}$$

$$\mathbf{U} = \begin{bmatrix} 0 & q_{12}^{(m_1-m_2-1)} & q_{13}^{(m_1-m_3-1)} & \cdots & q_{1r}^{(m_1-m_r-1)} \\ 0 & 0 & q_{23}^{(m_2-m_3-1)} & \cdots & q_{2r}^{(m_2-m_r-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, \tag{A19}$$

With $\mathbf{Q}(x)$ expressed in the form (A17), we can determine Υ from (A5).

Substitution of $\mathbf{Q}(x)$ from (A17) into (A5) yields

$$\frac{d}{dx}\Upsilon = \left\{\frac{\mathbf{D}}{x} + x^{\mathbf{M}}\frac{\mathbf{U}}{x}x^{-\mathbf{M}}\right\}\Upsilon. \tag{A20}$$

It is not difficult to see that the appropriate expression for Υ is

$$\Upsilon = x^{\mathbf{M}}x^{\mathbf{U}+\mathbf{D}-\mathbf{M}}. \tag{A21}$$

The general solution for the matrix differential equation (A1) is then

$$\Psi = \mathbf{G}(x)x^{\mathbf{M}}x^{\mathbf{U}+\mathbf{D}-\mathbf{M}}\Psi_0,$$

where Ψ_0 is an arbitrary constant column matrix.

APPENDIX B.

The blocks $\mathbf{W}_{12}$ and $\mathbf{W}_{22}$ are

$$\mathbf{W}_{12} = \begin{bmatrix} \omega_{1,n+1}^{(2\gamma_1+1)} x^{2\gamma_1+1} & \omega_{1,n+2}^{(2\gamma_2+1)} x^{2\gamma_2+1} & \cdots & \omega_{1,2n}^{(2\gamma_n+1)} x^{2\gamma_n+1} \\ \omega_{2,n+1}^{(2\gamma_1+1)} x^{2\gamma_1+1} & \omega_{2,n+2}^{(2\gamma_2+1)} x^{2\gamma_2+1} & \cdots & \omega_{2,2n}^{(2\gamma_n+1)} x^{2\gamma_n+1} \\ \vdots & \vdots & & \vdots \\ \omega_{n,n+1}^{(2\gamma_1+1)} x^{2\gamma_1+1} & \omega_{n,n+2}^{(2\gamma_2+1)} x^{2\gamma_2+1} & \cdots & \omega_{n,2n}^{(2\gamma_n+1)} x^{2\gamma_n+1} \end{bmatrix},$$

$$\mathbf{W}_{22} = \begin{bmatrix} \delta_1 & \omega_{n+1,n+2}^{(2\gamma_2-2\gamma_1-1)} x^{2\gamma_2-2\gamma_1-1} & \cdots & \omega_{n+1,2n}^{(2\gamma_n-2\gamma_1-1)} x^{2\gamma_n-2\gamma_1-1} \\ 0 & \delta_2 & \cdots & \omega_{n+2,2n}^{(2\gamma_n-2\gamma_2-1)} x^{2\gamma_n-2\gamma_2-1} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \delta_n \end{bmatrix},$$

where $\delta_i = m_i - 2(\gamma_i + 1)$ and the elements $\omega_{i,n+j}^{(2\gamma_j+1)}$ or $\omega_{n+i,n+j}^{(2\gamma_j-2\gamma_i-1)}$ differ from zero when $2\gamma_j$ or $2\gamma_j - 2\gamma_i$ is a positive integer, respectively. Thus, in the case where the γ's of matrix $\mathbf{D}$ are not even divisors of an integer, matrix $\mathbf{W}$ becomes a null matrix.

Singular Logarithmic Potentials in Coordinate Space*

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In previous works we have studied the problem of the determination of the Jost function for singular repulsive potentials behaving near the origin like inverse powers. The key was to define "new Jost solutions" which, still being asymptotically ingoing (or outgoing) waves, tend to constant (Jost functions) near the origin. It was shown from the perturbation expansion in coordinate space of these "new Jost solutions" that we can construct the Jost functions by connecting the radial coordinate r and the order of the perturbation expansion p. More precisely, if we introduce an $r(p)$ dependence, the Jost function is the limit of convergent sequences provided $r(p)$ goes to zero less rapidly than a given limiting dependence $r_L(p)$. In this paper, working in coordinate space, the same method is extended for two other families of singular potentials: firstly, we consider the case in which the most singular part of the potentials behaves like $G^2(\log r^{-1})^\beta r^{-2n}$, ($n \geq 1$, β arbitrary) near the origin; secondly, we study exponentially singular repulsive potentials of finite range. It is found that the more singular is supposed to be the potential, the higher becomes the available limiting dependence.

I. INTRODUCTION

PREVIOUSLY,[1-3] we have studied singular potentials behaving like powers near the origin and such that the most singular term is repulsive, approaching G^2r^{-2n} asymptotically, as $r \to 0$. In all cases the starting point was the same. We want to factorize in an exact manner the most singular part of the solutions near the origin. Then we define "new Jost solutions" which are still asymptotically ingoing (or outgoing) waves and tend to be constant (Jost functions) near the origin. In Refs. 1 and 2, the problem was studied with the help of the Laplace transform. In Ref. 1 ($n = 1$) the factorization procedure was sufficient to solve the problem of explicitly constructing the Jost function, while in Ref. 2 it was in addition necessary to consider the Jost function as the limit of convergent sequences.

In Ref. 3 the problem was studied directly in coordinate space and reduced to the following form. The Jost function is the convergent limit $f(k, r)_{r\to 0} = f(k, 0)$, defined as

$$f(k, 0) = \lim_{r\to 0}\left[\lim_{p\to\infty}\sum_{q=0}^{p} f_q(k, r)\right],$$

where $f_q(k, r)$ is the qth order term of the perturbation which, considered by itself, is divergent (for $n > 1$) in the limit $r \to 0$. But this was shown to be simply due to the failure of the ordinary perturbative expansion since it was explicitly proved that the Jost function actually exists. It was shown, however, that, if we introduce an $r(p)$ dependence, we can connect the two limits $r \to 0$ and $p \to \infty$ in such a way that

$$f(k, 0) = \lim_{p\to\infty}\sum_{q=0}^{p} f_q(k, r(p))$$

$$\text{if} \quad r(p) \geq r_L(p) = p^{\epsilon-1/(n-1)}.$$

Recently[4-9] other families of singular potentials

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[1] H. Cornille, Nuovo Cimento **33**, 434 (1964).

[2] H. Cornille and E. Predazzi, "Singular Potentials with Short Range," CERN preprint 9125/Th. 441—a brief report of this work has been given in Phys. Letters **10**, 149 (1964).

[3] H. Cornille, "Singular Potentials in Coordinate Space," CERN preprint 9608/Th. 479.

[4] (a) B. A. Arbuzov, A. T. Filippov, and O. A. Khrustalev Phys. Letters **8**, 205 (1964). (b) We note that for $\beta = 1$, $\epsilon = 1$, the corresponding result (17) for the "regular" part of the solution is not the same as given in Ref. 4, Eq. (14). But from the exact whole solution given in Ref. 4, Eq. (3), it is easy to see that the behavior (17) given in the present paper is the correct one.

[5] L. Bertocchi, S. Fubini, and G. Furlan, Nuovo Cimento **32**, 745 (1964).

[6] F. Calogero and M. Cassandro, "Asymptotic Nature of the Perturbation Expansion for the Scattering Parameters due to a Potential which Behaves at the Origin as $gr^{-2}\log(R/r)$" (preprint).

[7] T. T. Wu, "Scattering by the Singular Potential $-gr^{-4}\cdot\log r$" (preprint).

[8] H. M. Aly, Riazuddin, and A. M. Zimerman, "Singular Logarithmic Potentials and Peratization;" Scattering by Singular Logarithmic Potentials;" "Highly Singular Potential and Peratization" (preprints).

[9] A rather general formalism has been developed by K. Meetz [Nuovo Cimento **34**, 690 (1964)] using the definition of the Jost function proposed by A. Pais and T. T. Wu [Phys. Rev. **134**, B1303 (1964)]. The paper by Meetz does not, however, cover the problem treated here.

(logarithmics and exponentials) have been investigated. The study of singular logarithmic potentials in coordinate space appears interesting also in order to test the so called "Peratization" technique[7,8]. In fact, singular repulsive potentials are studied mainly since the mathematical difficulties encountered in this game seem rather similar to those arising from the study of unrenormalizable field theories. In both cases we are led to expansions nonanalytic with respect to the coupling constant. In particular, the existence of singularities of logarithmic type seems to arise in connection with quantum electrodynamics problems. One of the most important problem is then to give a correct interpretation to the limiting process used. We recall now what has been said in Ref. 3 about the procedure of convergence [$r(p) \to 0$, as $p \to \infty$, $r(p) \geq r_L(p)$] used in coordinate space for the pertubation expansion of the new Jost solutions. This procedure means, roughly speaking, that if we consider an approximation up to a certain order p of the perturbation expansion, we must take into account, at most, only the part of the interaction which is outside a limiting radius $r_L(p)$. When p grows up, this radius decreases but it strictly reduces to zero only when p is infinite.

It is the aim of this paper to extend the results given in Ref. 3 for potentials approaching G^2r^{-2n} asymptotically, as $r \to 0$, in coordinate space, to other families of singular potentials by using the same method of convergence by connecting the order of pertubation and the radial coordinate limiting procedure.

In Sec. II we briefly recall the main features of the method in coordinate space. In Sec. III we study the behavior of the solutions of the Schrödinger equation near the origin for families of singular potentials where the most singular part near the origin behaves asymptotically as $G^2(\log 1/r)^{\beta}r^{-2n}$ ($n \geq 1$) as $r \to 0$, $r^{-2n}\exp(\gamma/r^{\eta})(\gamma, \eta > 0)$ as $r \to 0$. In Secs. IV and V we show how we can obtain the Jost function for the logarithmic case and in Sec. VI we briefly consider the case of exponentially singular potentials of finite range.

II. FORMULATION OF THE PROBLEM IN COORDINATE SPACE

We consider the Schrödinger equation

$$(d^2/dr^2 + k^2)u = V(r)u. \tag{1}$$

In previous works[1-3] we have studied the problem of the determination of the Jost function for repulsive potentials singular like inverse powers near the origin and such that the most singular term is asymptotically equal to G^2r^{-2n} ($n \geq 1$, $G^2 > 0$ for $n > 1$) as $r \to 0$. In all cases the starting point was the same: we consider a Jost solution $R(k, r)$ of (1) which is an asymptotically ingoing wave [$R(k, r)_{r\to\infty} \backsim e^{-ikr}$]. Near the origin we have

$$R(k, r) \underset{r\to 0}{\sim} Y_{\text{sing}}(r)\ \text{const}_1 + Y_{\text{reg}}(r)\ \text{const}_2. \tag{2}$$

(Everything could be repeated here and in the following if we had considered the asymptotically outgoing wave.)

We define a new Jost solution by putting

$$R(k, r) = Z(r)F(k, r) \underset{r\to\infty}{\sim} e^{-ikr}. \tag{3}$$

In (3) we want to impose on $Z(r) = \exp(\int_\infty^r \psi(r')dr')$ the following conditions:

$$\text{(i)}\quad Z(r) \underset{r\to 0}{\sim} Y_{\text{sing}}(r) \quad \text{or} \quad F(k, r) \underset{r\to 0}{\sim} \text{const}_1,$$

$$\text{(ii)}\quad Z(r) \underset{r\to\infty}{\sim} 1 \quad \text{or} \quad F(k, r) \underset{r\to\infty}{\sim} e^{-ikr}.$$

Then the S matrix is given by

$$S(k) = F(k, 0)/F(-k, 0). \tag{4}$$

From (1) and (3) we have for $f(k, r) = F(k, r)e^{ikr}$, the Volterra integral equation

$$f(k, r) = 1 + \frac{1}{2ik}\int_r^\infty (e^{2ik(r-r')} - 1) \times [-2\psi(r')\, d/dr' + W(r')]f(k, r')\, dr', \tag{5}$$

where

$$W = V - \psi^2 - \psi',$$

where ψ' is defined as $d\psi/dr$.

In Refs. 1 and 2 we have studied (5) with the use of Laplace transform. For $n = 1$, the factorization (3) of the most singular part of (1) was sufficient[1] in order to obtain a finite expansion for the Jost function. For $n > 1$, a more elaborate treatment[2] was necessary; the main features being that firstly the Jost function can be considered as the limit of convergent sequences and secondly that we can connect the limiting procedure $r \to 0$ and the integration path in the inverse Laplace transform. In Refs. 3, Eq. (5) was studied directly in coordinate space and for the family of potentials considered, singular like inverse powers near the origin, it has been shown from the iteration of (5) in the case $n > 1$ that the following properties hold:

$$\text{(a)}\quad f(k, 0) = 1 + \lim_{r\to 0}\left(\sum_1^\infty f_a(k, r)\right), \tag{6}$$

(b) $\lim_{r\to 0} f_a(k, r)$ is divergent, (7)

(c) $f(k, 0) = 1 + \lim_{p\to\infty} \sum_1^p f_a(k, r(p))$

if $r(p) \geq \text{const } p^{\epsilon - 1/(n-1)}$. (8)

It is the aim of this paper to show that the results of Ref. 3, obtained in coordinate space, can be extended to other families of singular potentials, mainly when logarithmic terms are present.

We note that with respect to the two conditions imposed to $Z(r)$, the first one is the most important. But this condition $Z(r) \sim_{r\to 0} Y_{\text{sing}}(r)$ requires that we know the exact behavior of the solutions of (1) near the origin for each family of potentials considered. We also recall that in Refs. 1–3 for potentials singular like powers near the origin, we have chosen

$$\psi(r) = e^{-\lambda r} \sum_i \frac{a_i}{r^{\gamma_i}} \qquad (\lambda > 0). \tag{9}$$

The factor $\exp(-\lambda r)$ was taken in order to satisfy condition (ii), but we remark that the exponential form is not the only one which ensures that $Z(r) \to_{r\to\infty} 1$. In (9) the choice $\sum_i a_i/r^{\gamma_i}$ is more important, and in fact not arbitrary, the reason being that for potentials singular like powers near the origin, the "regular" and the "singular" part of the solutions of (1) near the origin are of the form

$$\exp\left(\sum_i \frac{b_i}{r^{\gamma_i}} + C \log r\right) \quad \text{with} \quad \gamma_i > 0.$$

III. BEHAVIOR OF THE SOLUTION NEAR THE ORIGIN

A. Outline of the Method

We want to determine the "regular" and the "singular" part of the solutions u of (1) near the origin for particular choices of potentials. We define

$$u(r) = \left(\exp \int_a^r \bar{\psi}(r')\, dr'\right) v(r) \qquad (a \text{ small and} > 0), \tag{10}$$

and we ask that $v(r) \to$ const as $r \to 0$. From (1) we get

$$(d^2/dr^2 + 2\bar{\psi}\, d/dr - W + k^2)v = 0, \tag{11}$$

$$W = -\bar{\psi}^2 - d\bar{\psi}/dr + V \equiv W(\bar{\psi}).$$

If we solve entirely the Riccati equation $W = 0$, we solve the problem for $k = 0$. But here we want to take on the same footing both cases $k = 0$ and $k \neq 0$. Then it is sufficient to extract only the most singular part of W in such a way that the remaining $v(r) \to_{r\to 0}$ const. What is important is to take at least all singular terms of u which are factorized in the behavior of u near the origin. We now explain the method.

(a) For potentials more singular than r^{-2} near the origin, we put $\bar{\psi} = \sum_{i=1}^m \bar{\psi}_i(r)$ and define the sequences

$$W_1 = W(\bar{\psi}_1)$$
$$\vdots \qquad \vdots$$
$$W_i = W\Big(\sum_{j=1}^{i} \bar{\psi}_j\Big).$$

Firstly we choose $\bar{\psi}_1$ such that $\bar{\psi}^2$ removes the most singular term of the potential, V_1. We consider always the case where the most singular term is repulsive, and behaves as $G^2 V_1(r)$ as $r \to 0$, and we have two solutions for $\bar{\psi}_1$ corresponding to $\pm G V_1^{\frac{1}{2}}$. Secondly we choose $\bar{\psi}_2$ such that $2\bar{\psi}_1\bar{\psi}_2$ removes the most singular term of W_1 and so on. All these terms $\bar{\psi}_i(r)$ give singularities for u near the origin [when inserted in (10)] if

$$\lim_{r\to 0} \int_a^r \bar{\psi}_i(r')\, dr' \to \pm\infty. \tag{12}$$

We stop the procedure $\bar{\psi}_m$ if the next term $\bar{\psi}_{m+1}$ is such that

$$\lim_{r\to 0} \int_a^r \bar{\psi}_{m+1}(r')\, dr' \to \begin{cases} \text{const} \\ 0 \end{cases}. \tag{13}$$

This means that if we include this supplementary term in $\bar{\psi}$ we merely change the constant to which $v(r)$ approaches for $r \to 0$. Now, of course, this method works only if u has a finite number of factorized singularities near the origin. But later we give examples where an infinity of singularities occurs. In this case, it is more convenient to group together many singular terms of the potentials and choose again $\bar{\psi}_1$ as to remove the most singular part of the potential.

(b) For potentials singular as r^{-2} near the origin we have only one term $\bar{\psi}_1 = \text{const}/r$, (see Ref. 1).

(c) For potentials less singular than r^{-2} near the origin, firstly if $V(r) \sim r^{-\lambda}$ $(\lambda < 2)$, we are in the usual case of "regular" potentials. Secondly if $V(r) \sim_{r\to 0} G^2 (\log 1a/r)^{\beta} r^{-2}$ $(\beta < 0)$, we are in a delicate case because $\bar{\psi}_1$ is more singular than $\bar{\psi}_1^2$ and we must modify the prescriptions of (a); we can also make a change of variables in order to reduce to the case (a).

Note that the prescriptions (a) and (b) applied to potentials having a singular power behavior near the origin, give rise to the procedure used for studying the cases considered in Refs. 1–3.

B. Logarithmic Case with a Centrifugal-Like Term

$$V(r) \underset{r\to 0}{\sim} \frac{G^2}{r^2}[\log(1/r)]^\beta + \frac{l(l+1)}{r^2}. \tag{14}$$

(i) If $\beta > 0$ we use the method outlined before in this section [in Sec. III A (a)] and we get for $N - \frac{1}{2} < \beta^{-1} < N + \frac{1}{2}$ $(N = 0, 1, 2, \cdots)$

$$\bar{\psi}_\epsilon = \frac{\epsilon G}{r}[\log(1/r)]^{\beta/2}\sum_{i=0}^{N}\frac{a_i}{[\log(1/r)]^{i\beta}} + \frac{1}{2r} + \frac{\beta}{4r\log(1/r)};$$

$$\epsilon = \pm 1, \qquad a_0 = 1, \qquad a_i = \frac{(l+\frac{1}{2})^{2i}}{G^{2i}}c_i,$$

$$c_1 = \tfrac{1}{2}, \qquad c_i = (-1)^{i-1}\frac{(2j-3)!!}{2^j j!};$$

$$u_\epsilon(r) \underset{r\to 0}{\sim} Y_\epsilon(r) = r^{\frac{1}{2}}[\log(1/r)]^{-\beta/4} \times \exp\left[-\epsilon G\sum_{i=0}^{N}\frac{a_i[\log(1/r)]^{1+\beta(\frac{1}{2}-i)}}{1+\beta(\tfrac{1}{2}-j)}\right];$$

$$W(\bar{\psi}_\epsilon) \sim O([r^2\log(1/r)]^{-1}); \tag{15}$$

for $\beta^{-1} = N - \frac{1}{2}$ $(N = 1, 2, \cdots)$

$$Y_\epsilon(r) = r^{\frac{1}{2}}[\log(1/r)]^{-\beta/4-\epsilon G a_N} \times \exp\left[-\epsilon G\sum_{i=0}^{N-1}\frac{a_i[\log(1/r)]^{1+\beta(\frac{1}{2}-i)}}{1+\beta(\tfrac{1}{2}-j)}\right]. \tag{16}$$

Thus, when $\beta \to 0$, the number of essential singularities increases (as N increases), and from (15) it is easy to see that, at the limit $\beta = 0$, all these essential singularities cancel and the series sums up to give the expected power behavior

$$\exp\left\{\left[\frac{1}{2} + \epsilon G\left(1 + \frac{(l+\frac{1}{2})^2}{G^2}\right)^{\frac{1}{2}}\right](\log r)\right\}.$$

We can test (15) in the case $\beta = 1$ when the exact solution for $k = 0$ is known[4]:

$$Y_\epsilon(r) \simeq r^{\frac{1}{2}}[\log(1/r)]^{-\frac{1}{4}} \times \exp\left[-\epsilon G\frac{2}{3}\left(\log\frac{1}{r}\right)^{\frac{3}{2}} - \frac{\epsilon}{G}(l+\tfrac{1}{2})^2\left(\log\frac{1}{r}\right)^{\frac{1}{2}}\right]. \tag{17}$$

(ii) For $\beta = -\eta < 0$, we consider (1) for $k = 0$ and make the change of variable $x^{-1} = \log(1/r)$. We put $u = x^{-1}e^{-1/2x}g(x)$ and we get

$$\left[\frac{d^2}{dx^2} - \frac{G^2}{x^{4-\eta}} - \frac{(l+\frac{1}{2})^2}{x^4}\right]g(x) = 0\,. \tag{18}$$

To (18) we apply the procedure sketched in Sec. III A (a) for potentials more singular than x^{-2}. Coming back to the r variable we get finally $u_\epsilon(r) \underset{r\to 0}{\sim} Y_\epsilon(r)$ for

$$\eta > 1\,, \qquad Y_\epsilon(r) = r^{\epsilon(l+\frac{1}{2})+\frac{1}{2}};$$

for

$$N < \eta^{-1} < N + 1 \qquad (N = 1, 2, \cdots),$$

$$\bar{\psi}_\epsilon = [\epsilon(l+\tfrac{1}{2}) + \tfrac{1}{2}]/r + \frac{[\epsilon(l+\frac{1}{2})]}{r}\sum_{i=1}^{N} b_i[\log(1/r)]^{-i\eta},$$

$$\epsilon = \pm 1, \quad b_1 = \frac{1}{2}\left(\frac{G}{l+\frac{1}{2}}\right)^2, \quad b_i = \left(\frac{G}{l+\frac{1}{2}}\right)^{2i}c_i;$$

$$Y_\epsilon(r) = r^{\frac{1}{2}+\epsilon(l+\frac{1}{2})} \times \exp\left[-\epsilon(l+\tfrac{1}{2})\sum_{i=1}^{N}\frac{b_i}{1-j\eta}\left(\log\frac{1}{r}\right)^{1-i\eta}\right]$$

$$W(\bar{\psi}_\epsilon) \simeq O[r^{-2}(\log 1/r)^{-1-\eta}] \tag{19}$$

[c_i being the same as in (15)]; for $\eta^{-1} = N$ $(N = 1, 2, \cdots)$, $\bar{\psi}_\epsilon$ is still given by (19) and

$$Y_\epsilon(r) = \frac{r^{\frac{1}{2}+\epsilon(l+\frac{1}{2})}}{(\log 1/r)^{\epsilon(l+\frac{1}{2})b_N}} \times \exp\left[-\epsilon(l+\tfrac{1}{2})\sum_{i=1}^{N-1}\frac{b_i}{1-j\eta}\left(\log\frac{1}{r}\right)^{1-i\eta}\right] \tag{20}$$

(where the sum in the exponential is empty if $N = 1$).

Thus only when $\beta < -1$ one has that $Y_\epsilon(r)$ is the same as in the regular case ($V \underset{r\to 0}{\sim} r^{-\gamma}$, $\gamma < 2$).

Here also when $|\beta| \to 0$, the number of essential singularities increases and at the limit $|\beta| = 0$ we find from (19) the correct power behavior.

We want to remark that by a rearrangement of the potential we can obtain very quickly the solutions in both the cases $\beta > 0$ and $\beta < 0$. For $\beta > 0$ we write

$$V = \frac{G^2}{r^2}\left(\log\frac{1}{r}\right)^\beta\left[1 + \left(\frac{l+\frac{1}{2}}{G}\right)^2\left(\log\frac{1}{r}\right)^{-\beta}\right] - \frac{1}{4r^2}.$$

Then at a first stage we obtain

$$\bar{\psi}_\epsilon = \frac{\epsilon G}{r}\left(\log\frac{1}{r}\right)^{\beta/2}\left[1 + \left(\frac{l+\frac{1}{2}}{G}\right)^2\left(\log\frac{1}{r}\right)^{-\beta}\right]^{\frac{1}{2}} + \frac{\beta}{4r}\left(\log\frac{1}{r}\right)^{-1} + \frac{1}{2r}.$$

We then expand the square root in the first term of $\bar{\psi}_\epsilon$ by retaining all the terms satisfying (12) and we stop at the first term which satisfies (13).

So doing we obtain (15) and (16). For $\beta = -\eta < 0$ we write

$$V = \frac{G^2(l+\frac{1}{2})^2}{r^2}\left[1 + \left(\frac{G}{l+\frac{1}{2}}\right)^2\left(\log\frac{1}{r}\right)^{-\eta}\right] - \frac{1}{(4r^2)}.$$

We have directly

$$\bar{\psi}_\epsilon = \frac{\epsilon(l+\frac{1}{2})}{r}\left[1 + \left(\frac{G}{l+\frac{1}{2}}\right)^2\left(\log\frac{1}{r}\right)^{-\eta}\right]^{\frac{1}{2}} + \frac{1}{2r}.$$

Here also we expand the square root keeping only terms satisfying (12) and in this way we have directly (19) and (20).

Now we want to compare the properties of the solutions with respect to r and G corresponding to two different behaviors of the potential, which near the origin behave respectively as

$$V \sim G^2 r^{-2(1+\gamma)} + \frac{l(l+1)}{r^2} \qquad (\gamma \lesseqgtr 0, \quad \gamma = 0)$$

and

$$V \sim \frac{G^2}{r^2}\left(\log\frac{1}{r}\right)^\beta + \frac{l(l+1)}{r^2}, \qquad (\beta \lesseqgtr 0).$$

In the case of power behavior, r^{-2} (or $\gamma = 0$) is the transition case between solutions which have a power behavior ($\gamma \leq 0$) and solutions which have essential singularities of the exponential type $\exp[\pm G/(\gamma r^\gamma)]$ ($\gamma > 0$). But between these two classes: power [or exponential of $(\log r)^1$] and exponential of powers, other classes of singularities can occur, for instance, exponentials of $(\log r)^\xi$ ($\xi \neq 1$). In the logarithmic potentials case, $\beta = -1$ is the critical value between pure power behavior ($\beta > -1$) of the solution near the origin $r^{\frac{1}{2}+\epsilon(l+\frac{1}{2})}$ and other singularities as exponentials and logarithms ($\beta < -1$). For $\beta = -1$ one has

$$Y_\epsilon(r) = r^{\frac{1}{2}+\epsilon(l+\frac{1}{2})}(\log 1/r)^{\frac{1}{2}\epsilon G^2/(l+\frac{1}{2})}.$$

But $\beta = 0$ is another critical value if we compare the most singular part $\bar{Y}_\epsilon(r)$ of $Y_\epsilon(r)$ coming from the centrifugal potential and the leading remaining singularity of $V(r)$

$\beta > 0$:

$$\bar{Y}_\epsilon(r) \sim \exp\left[\frac{1}{2}\log r - \frac{\epsilon G}{1+\frac{1}{2}\beta}\left(\log\frac{1}{r}\right)^{1+\frac{1}{2}\beta}\right];$$

$-1 < \beta = -\eta < 0$:

$$\bar{Y}_\epsilon(r) \sim \exp\left[(\epsilon(l+\tfrac{1}{2})+\tfrac{1}{2})\log r - \frac{\epsilon}{2}\frac{G^2}{(l+\frac{1}{2})(1-\eta)}\left(\log\frac{1}{r}\right)^{1-\eta}\right].$$

Thus in the first case ($\beta > 0$) the dominant term comes always from the potential whereas in the second case ($-1 < \beta < 0$) the dominant singularity comes from the centrifugal term. Consequently, to these different radial coordinate behavior of the solutions will correspond different properties with respect to G^2. We consider the attractive case $G^2 < 0$. For $\beta > 0$ we are in the same situation as in the power behavior case $\gamma > 0$. We have the same difficulties in order to distinguish between the "regular" and the "singular" solution because the solutions (15) are both oscillating when $r \to 0$. This occurs because of the presence of $(G^2)^{\frac{1}{2}}$ in these solutions. On the contrary, for $-1 < \beta < 0$, because only G^2 occurs in (19) and (20), or equivalently because the centrifugal barrier gives the dominant contribution, one can consider $G^2 \to -G^2$ in (19) and (20) and we have no difficulties in order to define the "regular" and the "singular" solution for the attractive case $G^2 < 0$ and $l \neq 0$. For $l = 0$, $-1 < \beta < 0$, under $G^2 \to -G^2$, the two corresponding solutions are still real (no oscillating terms) and $Y_\epsilon \to 0$ in both cases $\epsilon = \pm 1$. But for instance $Y_1(r)/r \to 0$ and $Y_{-1}(r)/r \to \infty$.

C. Logarithmic Case with a Power Term More Singular than the Centrifugal One

Firstly we consider the case of a purely logarithmic term plus centrifugal barrier

$$V(r) = G^2 r^{-2n}\left(\log\frac{1}{r}\right)^\beta + \frac{l(l+1)}{r^2} \qquad (n \text{ arbitrary} > 1). \tag{21}$$

We apply the method given in Sec. III A (a), and we find

$$\bar{\psi}_\epsilon = \frac{\epsilon G}{r^n}\left(\log\frac{1}{r}\right)^{\beta/2} + \frac{\beta}{4r\log(1/r)} + n/(2r),$$

$$Y_\epsilon(r) = r^{\frac{1}{2}n}\left(\log\frac{1}{r}\right)^{-\beta/4}\exp\left[\epsilon G\int_{\text{const}}^r dr'\,\frac{(\log 1/r')^{\beta/2}}{(r')^n}\right],$$

$$W(\bar{\psi}) \sim O(1/r^2). \tag{22}$$

We see that the centrifugal potential never modifies the behavior of the solution near the origin, contrary to what we possibly had in the $n = 1$ case, as previously discussed.

Now we consider a more general potential

$$V(r) = \frac{G^2}{r^{2n}}\left[\left(\log\frac{1}{r}\right)^\beta + Ar^\delta h(r)\right] + \frac{l(l+1)}{r^2}, \tag{23}$$

where $\eta > 1$, β arbitrary, $\delta \geq 0$, $|h(r)| < \text{const}$, $|h'(r)| < \text{const}$, $h(0) = 1$, $A > 0$ if $\delta = 0$, $2n - \delta > 2$. In the case $\delta > 0$ we find, if we apply the prescriptions given in Sec. III A (a), that there is always a finite number of singularities so that we

can find a term $\bar{\psi}_m$ such that the next term satisfies (13). On the contrary in the case $\delta = 0$ where the two most singular terms have the same power and differ only by a logarithmic term, we find an infinity of singularities. Then we do not apply strictly the method given in Sec. III A (a) but we rather consider as a whole the part of the potential in (23) which does not include the centrifugal term and we find

$$\bar{\psi}_\epsilon(r) = \frac{\epsilon G}{r^n}\left[\left(\log\frac{1}{r}\right)^\beta + Ar^\delta h(r)\right]^{\frac{1}{2}} + \frac{\beta}{4r\log(1/r)} + \frac{n}{2r},$$

$$Y_\epsilon(r) \sim \frac{r^{\frac{1}{2}n}}{(\log 1/r)^{\beta/4}} \cdot \exp\left[\epsilon G\int_a^r r'^{-n}\left\{\left(\log\frac{1}{r'}\right)^\beta + Ar'^\delta h(r')\right\}^{\frac{1}{2}} dr'\right] \quad (a \text{ small and} > r),$$

$$W(\bar{\psi}) \sim O(r^{-2}). \tag{24}$$

Firstly we consider the case $\delta > 0$. Now we can expand the square root in the first term of $\bar{\psi}$ which gives

$$\epsilon G\left(\log\frac{1}{r}\right)^{\beta/2}\sum_j c_j r^{j\delta-n}\left[Ah(r)\left(\log\frac{1}{r}\right)^{-\beta}\right]^j$$

[where c_j are defined by (15)]. We see that the degree of singularity of the power $r^{j\delta-n}$ decreases with increasing j and there exists always a jth term of the kind $r^{-\epsilon_1}(\log 1/r)^{-\epsilon_2}$ (with $\epsilon_1 < 1$) or $r^{-1}(\log 1/r)^{-\epsilon_3}$ ($\epsilon_3 > 1$) which satisfies (13).

Secondly, in the case $\delta = 0$, it is easy to see that an expansion of the square root does not change the power r^{-n} and then all the corresponding terms are singular.

It should be mentioned that of course to any of the potentials previously considered, we can add any quantity which does not affect the behavior of the solution near the origin or, to be more precise, any term for which Eq. (13) is satisfied. For instance a potential which is less singular than the centrifugal term obviously is allowed as can be seen from (15), (19), and (22). The same remark will apply to the following case.

D. Exponentially Singular Behavior

In fact the logarithmic case is not the only one which gives the possibility of having an infinity of singularities. More generally, this can also be the case when two singular potentials of the same family differ only by singularities of a weaker kind. We will see that this is also the case for two exponentially singular potentials with different power factors. We are interested only in the behavior of the solutions near the origin.

Firstly we consider the case of a single exponential term,

$$V = G^2 r^{-2n}\exp(\eta/r^\gamma) + A/r^{-m} + l(l+1)/r^2 \quad (n > 0,\ \eta > 0,\ \gamma > 0,\ m > 0). \tag{25}$$

We get

$$\bar{\psi}_\epsilon = \frac{\epsilon G}{r^n}\exp\frac{\eta}{2r^\gamma} + \frac{\eta\gamma}{4r^{1+\gamma}} + \frac{n}{2r},$$

$$Y_\epsilon \backsimeq r^{n/2}\exp\left[-\frac{\eta}{4r^\gamma} + \int_{\text{const}}^r \frac{\epsilon G}{r'^n}\exp\left(\frac{\eta}{2r'^\gamma}\right)dr'\right],$$

$$W(\bar{\psi}_\epsilon) \sim O(r^{-m_0}). \tag{26}$$

where m_0 is the larger number between m and $2+\gamma$.

Secondly we consider the more general case

$$V = \frac{G^2}{r^{2n}}\left[\exp\frac{\eta}{r^\gamma} + Ar^\mu\exp\frac{\eta\delta}{r^\beta}\right] + \frac{l(l+1)}{r^2} \tag{27}$$

$(\gamma > 0,\ \eta > 0,\ \delta > 0,\ 0 \le \beta \le \gamma,\ \mu \ge 0;$ if $\beta = \gamma$ then $\delta \le 1)$.

We get

$$\bar{\psi}_\epsilon = (\epsilon G/r^n)\exp[\eta/(2r^\gamma)] \cdot[1 + Ar^\mu\exp\{-\eta r^{-\gamma}(1-\delta r^{\gamma-\beta})\}]^{\frac{1}{2}} + \frac{nr}{2} + \frac{\eta\gamma}{4r^{\gamma+1}}. \tag{28}$$

In the case $\beta < \gamma$ we see that, from the expansion of the square root in $\bar{\psi}_1$, only the first term gives a singularity [i.e., such that Eq. (12) is satisfied]. Then in this case we can take for $\bar{\psi}$ the expression given in (26) and the singularities near the origin are like in (26).

In the case $\beta = \gamma$, $\delta < 1$, we have to take into account only a finite number of terms of the expansion of the square root of $\bar{\psi}_1$. More explicitly we have terms like

$$\frac{\epsilon G}{r^n}\sum_0^m c_j(Ar^\mu)^j\exp[(\eta/r^\gamma)\{\tfrac{1}{2} - j\eta(1-\delta)\}].$$

We can therefore always find an integer m such that the next term corresponding to $m+1$ satisfies (13).

In the case $\beta = \gamma$, $\delta = 1$, the two most singular terms of the potential are of the same exponential kind and differ only by the power they have as factor. It is easy to see that all the terms of the expansion of the square root in $\bar{\psi}$ give a singularity

such that in this case we have an infinity of singularities.

Finally we have in all cases for potentials (25) or (27)

$$Y_\epsilon(r) \sim r^{\frac{1}{4}n} \exp\left[-\eta\gamma/(4r^\gamma) + \int_a^r \frac{\epsilon G}{r'^n} \exp\left(\frac{\eta}{2r'^\gamma}\right) \cdot\{1 + Ar'^\mu \exp\left[-\eta r'^{-\gamma}(1 - \delta r'^{\gamma-\beta})\right]\}^{\frac{1}{2}} dr'\right].$$

It is clear that, for very general cases as for instance (24) and (29), it will be impossible, except for very special cases, to give a finite expression in terms of elementary functions for $Y_\epsilon(r)$. This, however, as it will become clear later on, is not a very important problem. All what is relevant to our purposes is that we have been able to extract behavior of the "regular" and "singular" solutions near the origin.

IV. CONSTRUCTION OF THE SINGULAR FACTOR IN THE LOGARITHMIC CASE

We recall the conditions for $Z(r) = \exp\left[\int_\infty^r \psi(r')dr'\right]$

(i) $$Z(r) \underset{r\to 0}{\sim} CY_{\text{sing}}(r),$$

(ii) $$Z(r) \underset{r\to\infty}{\to} 1,$$

where C is a constant independent of k. In order to satisfy simultaneously these two conditions, we write formally $\psi = e^{-\lambda r}\phi$ and we impose that

$$\lim_{r\to 0} \int_{\text{const}}^r \psi(r')\, dr'$$

gives the same singularities as $\int_{\text{const}}^r \bar{\psi}(r')dr'$ studied in Sec. III. Equivalently, we put $e^{-\lambda r}\phi(r) \sim \bar{\psi}(r)$. This equivalence relation simply means that

$$\lim_{r\to 0} \int_{\text{const}}^r [e^{-\lambda r'}\phi(r') - \bar{\psi}(r')]\, dr' = \text{const}.$$

Practically we determine $\phi(r)$ as a sum of terms

$$\phi(r) = \sum_{i=1}^m \phi_i(r) \sim e^{\lambda r}\bar{\psi}(r)$$

and we stop at m when $\phi_{m+1}(r)$ satisfies (13). This is always possible for singularities coming from logarithms and powers.

Firstly we consider the potential (14) with an exponential decreasing factor in order to avoid the difficulties of asymptotic behavior of the solutions of (1) when $r \to \infty$

$$V(r) = \frac{G^2}{r^2}\left(\log\frac{1}{r}\right)^\beta e^{-\mu r} + \frac{l(l+1)}{r^2}. \qquad (14')$$

We note that the presence of $\exp(-\mu r)$ does not affect the behavior of the solutions near the origin and we take in this case $\psi(r) = \exp(-\frac{1}{2}\mu r)\bar{\psi}_{\epsilon=-1}(r)$, where $\bar{\psi}_{\epsilon=-1}$ is defined, according to the corresponding values of β by (15), (16), (19), and (20).

Now we consider the more general case (23) in which the noncentrifugal term goes to zero more rapidly than r^{-2} for $r \to \infty$ (going to zero as a power of higher degree than 2).

If we suppose that n is such that $N + 1 < n < N + 2$ (N integer), we can take

$$\phi = \bar{\psi}_{\epsilon=-1}(r)\left(\sum_{j=0}^N \frac{(\lambda r)^j}{j!}\right),$$

where $\bar{\psi}_{\epsilon=-1}$ is given by (24). We get

$$\psi = \phi e^{-\lambda r} \underset{r\to 0}{\sim} \bar{\psi}_{\epsilon=-1}(r) + r^{N+1}\bar{\psi}_{\epsilon=-1}(r)(1 + O(r)).$$

Thus, in these logarithmic cases, we can always find $Z(r)$ satisfying conditions (1) and (2).

V. DETERMINATION OF THE JOST FUNCTION IN THE LOGARITHMIC CASE

We recall that the "old" Jost solution $R(k, r)$ behaves near the origin according to (2). Then, the "new" Jost solution defined by (3), with the condition $Z(r) \to_{r\to 0} Y_{\text{sing}}(r)$, behaves near the orgin like

$$F(k, r) \underset{r\to 0}{\sim} \left(\text{const}_1 + \frac{Y_{\text{reg}}(r)}{Y_{\text{sing}}(r)}\,\text{const}_2\right) \underset{r\to 0}{\to} \text{const}_1. \qquad (30)$$

We consider now the integral equation (5) for the function $f(k, r)$ in the case of potentials (14') and (23) [which includes the case of the potential (21)]. In these case $\psi(r)$ has been determined in the preceding section. We iterate formally the integral equation (5)

$$f(k, r) = 1 + \sum_1^\infty f_q(k, r). \qquad (31)$$

The Jost function is defined by

$$f(k, 0) - 1 = \lim_{r\to 0}\left(\sum_1^\infty f_q(k, r)\right). \qquad (32)$$

For the families of potentials considered we want to construct explicitly the Jost function from (31) and (32). To this aim we study the qth term $f_q(k, r)$ of the perturbation expansion and also the behavior of the whole function $f(k, r)$ [Eq. (31)] near the origin.

(1) Firstly we note that near the origin the integral equation (5) is equivalent to the differential equation (11) for $f(k, r)e^{ikr}$. Then it is easy to show that

near the origin

$$f(k, r) \sim \text{const}_1 + \text{const}_2 \bar{f}(r, G),$$

where $\bar{f}(r, G) \to 0$ as $r \to 0$.

For potentials like (14′) with $\beta < 0$, $|\beta| < 1$ we find from (19)

$$\bar{f}(r, G) \sim r^{2l+1} \exp\left[-\frac{G^2}{l+\frac{1}{2}} \frac{(\log 1/r)^{1-|\beta|}}{1-|\beta|} \cdot(1 + O(r))\right]. \quad (33)$$

For potentials like (14′) with $\beta = -1$, from (20) we have

$$\bar{f}(r; G) \underset{r\to 0}{\sim} r^{2l+1}(\log 1/r)^{-G^2/(l+\frac{1}{2})}. \quad (34)$$

For potentials like (14′) with $\beta > 0$ we find from (15) and (16)

$$\bar{f}(r, G) \underset{r\to 0}{\sim} \exp\left[-2G \frac{(\log 1/r)^{1+\frac{1}{2}\beta}}{1+\frac{1}{2}\beta}(1 + O(r))\right]. \quad (35)$$

In all these cases $\bar{f}(r, G) \to 0$ as $r \to 0$ for $G^2 > 0$ or $G > 0$ and $f(k, r) \to \text{const}_1$, so that the limit in (32) exists. This result reflects only the fact that (30) is satisfied and that we have taken the correct singular factor Z which factorizes the singular part of $R(k, r)$.

We note now the big difference between the cases $\beta > 0$ and $\beta < 0$. In the first case ($\beta > 0$), if we change $G \to -G$ or $G^2 \to -G^2$, the corresponding $\bar{f}(r, G)$ [and consequently $f(r, k)$] are either infinite or oscillating. This illustrates the nonanalyticity with respect to G at $G = 0$. On the contrary, in the case $\beta < 0$, with the same change $G \to -G$ or $G^2 \to -G^2$, the corresponding $\bar{f}(r, G)$ still goes to zero. In this case, $G = 0$ is not a singular point with respect to the coupling strength.

As far as these properties of $\bar{f}(r, G)$ are concerned, if we consider potentials with behavior near the origin like power $V \simeq G^2 r^{-2n}$, a similar situation to $\beta > 0$ arises for $n > 1$[2,3] and a similar situation to $\beta < 0$ ($|\beta| \leq 1$) occurs for $n = 1$[1,3]. In fact these analogies will go farther when we will consider the perturbation expansion (31) of $f(k, r)$.

For potentials like (23) we find from (24)

$$\bar{f}(r, G) \underset{r\to 0}{\sim} \exp\left\{\left[-2G \int_r^{\text{const}} r'^{-n}\left[\left(\log \frac{1}{r'}\right)^{\beta} + Ar'^{\delta}h(r')\right]^{\frac{1}{2}} dr'\right](1 + O(r'))\right\}. \quad (36)$$

In this case also $\bar{f}(r, G) \to_{r\to 0} 0$ and we have similar properties as in the case (14′) $\beta > 0$ if we consider the change $G \to -G$ or $G^2 \to -G^2$.

(2) Secondly we consider each qth iteration and we find: for potentials (14′) with $\beta < 0$ ($|\beta| \leq 1$)

$$\lim_{r\to 0} f_q(k, r) \to \text{const}.$$

Thus in this case each iteration of (31) gives a finite contribution to the sum and

$$f(k, 0) = 1 + \sum_1^{\infty} f_q(k, 0).$$

In this case the factorization Z of the most singular part of R is sufficient in order to solve the problem we are faced with of constructing the Jost function. This is similar to what found for the potential $V = Ge^{-\mu r}r^{-2}$,[1,3] and is a consequence of the analyticity with respect to G previously noted.

For potentials (14′) with $\beta > 0$ or (23), we get

$$\lim_{r\to 0} f_q(k, r) \to \infty.$$

Thus in these cases of potentials more singular than the centrifugal barrier we are in the same situation as in Ref. 3 for potentials which behave as $\sim G^2 r^{-2n}$ ($n > 1$) as $r \to 0$

(a) $\lim_{r\to 0}\left[\lim_{p\to\infty} \sum_1^p f_q(k, r)\right]$ is finite,

(b) $\lim_{p\to\infty}\left[\sum_1^p (\lim_{r\to 0} f_q(k, r))\right]$ is divergent.

Here we try to solve the problem by the method used in Ref. 3. We connect the order p of the perturbative expansion ($p \to \infty$) and the radial coordinate r in order to have the following relation when $r(p) \to 0$ as $p \to \infty$.

$$\lim_{p\to\infty}\left[\sum_1^p f_q(k, r(p))\right] = f(k, 0) - 1 \text{ if } r(p) \geq r_L(p); \quad (37)$$

or, equivalently to (37), we define

$$R(p, r, k) = \sum_{p+1}^{\infty} f_q(k, r),$$

and we impose

$$\lim_{p\to\infty} R(p, r(p), k) \to 0, \qquad r(p) \geq r_L(p). \quad (38)$$

The problem is thus reduced to find, if possible, limiting dependences $r_L(p)$ such that (38) is satisfied. As in Ref. 3, we have only to investigate the singular part of the perturbation expansion (37) of $f(k, r)$.

In the case of potentials (14′) (with $\beta > 0$) it

is shown in the Appendix that we have for small r and large p

$$|R(p, r, k)| \leq \sum_{p+1}^{\infty} \left[\frac{2G(\log 1/r)^{1+\frac{1}{2}\beta}}{1+\frac{1}{2}\beta} + \text{const} \right]^q \frac{q(\text{const})^q}{q!}. \quad (39)$$

From (39) and with the help of the Stirling formula

$$q! \underset{q\to\infty}{\sim} q^q e^{-q}(2\pi q)^{\frac{1}{2}}$$

it is easy to see that

$$\lim_{p\to\infty} R(p, r(p), k) \to 0 \quad \text{if} \quad r(p) \geq 1/(\exp[\text{const}\, p^{1/(\beta/2+1)-\epsilon}]) \quad (40)$$

where ϵ is arbitrarily small and positive and the constant is positive.

In the case of potentials (21) we get in the appendix for r small and large p

$$|R(p, r, k)| < \sum_{p+1}^{\infty} \left[\frac{\text{const}}{r^{n-1}} \left(\log \frac{1}{r}\right)^{\beta/2} + \text{const} \right]^q \frac{q(\text{const})^q}{q!} \quad (41)$$

with all constants positive. We find in this case

$$\lim_{p\to\infty} R(p, r(p), k) \to 0 \text{ if } r(p) \geq \text{const}/(p^{1/(n-1)-\epsilon}) \quad (42)$$

(ϵ small and > 0). [Note that (42) is not the most refined limiting dependence but the difference is not significant.] Thus we have the same limiting dependence as in the power case[3] $V \underset{r\to 0}{\sim} G^2 r^{-2n}$ $(n > 1)$.

We rewrite now the potential (23)

$$V(r) = (G^2/r^{2n})[(\log 1/r)^\beta + Ar^\delta h(r)] + l(l+1)/r^2 \quad (23)$$

with the same restrictions about n, δ, A, h as in Sec. III; one of these restrictions being for instance that when $r \to \infty$ the noncentrifugal part of the potential decreases more rapidly than $1/r^{2+\epsilon}$, $(\epsilon > 0)$.

If $\delta > 0$ or if $\delta = 0$ with $\beta > 0$, we get for R the bound (41) and consequently the, same limiting dependence (42) obtained above for potentials (21).

If $\delta = 0$ and $\beta < 0$, then the leading term of the potential is a power like term G^2A/r^{2n}, $(A > 0)$ and we get

$$|R(p, r, k)| < \sum_{p+1}^{\infty} \left[\frac{\text{const}}{r^{n-1}} + \text{const} \right]^q \frac{q(\text{const})^q}{q!}$$

with all constants positive. In this case we still have the limiting dependence $(p^{1/(n-1)-\epsilon})$.

VI. DETERMINATION OF THE JOST FUNCTION IN THE EXPONENTIAL CASE

For simplicity we study only the $l = 0$ wave with an exponential potential of finite range

$$V(r) = \left[\frac{G^2}{r^{2n}} \exp\left(\frac{\eta}{r^\gamma}\right) + \frac{A}{r^m} \right] \theta(r_0 - r), \quad (\eta, \gamma, m > 0). \quad (25')$$

We consider a solution $R(k, r)$ of (1) such that $R(k, r) = e^{ikr}$ for $r \geq r_0$. We still define a new Jost solution $F(k, r)$ for $r \leq r_0$ with the relation

$$R(k, r) = F(k, r) \exp \int_{r_0}^{r} \bar{\psi}_{-1}(r')\, dr' \quad (r \leq r_0). \quad (43)$$

We take in (43) $\bar{\psi}_{-1}$ given by (26) because the centrifugal term does not modify the behavior of R near the origin.

We put $F(k, r)e^{ikr} = f(k, r)$ as previously and near the origin we have

$$f(k, r) \sim \text{const}_1 + \bar{f}(r, G)\, \text{const}_2,$$

where from (26)

$$\bar{f}(r, G) \underset{r\to 0}{\sim} \exp\left\{ -2G \int_r^{\text{const}} r'^{-n} \exp\left(\frac{\eta}{2r'^\gamma}\right) dr' \right\}. \quad (44)$$

The corresponding integral equation for $f(k, r)$ is now

$$f(k, r) = 1 + \frac{1}{2ik} \int_r^{r_0} (e^{2ik(r-r')} - 1) \cdot \left(-2\bar{\psi}(r') \frac{d}{dr'} + W(r') \right) f(k, r')\, dr'. \quad (45)$$

We iterate

$$f(k, r) = 1 + \sum_q f_q(k, r)$$

and still find $\lim_{r\to 0} f_q(k, r)$ divergent. If we consider the remaining part of the pertubation expansion we find (see Appendix) that for small r and large p

$$|R(p, r, k)| < \sum_{p+1}^{\infty} \left(\frac{\text{const}}{r^{n-1}} \exp\left(\frac{\eta}{2r^\gamma}\right) + \text{const} \right)^q \cdot \frac{q(\text{const})^q}{q!}$$

with all constants positive. Then we see that

$$\lim_{p\to\infty} R(p, r(p), k) \to 0 \quad \text{if} \quad r(p) \geq [\log p^{2(1-\epsilon)/\eta}]^{-1/\gamma} \quad (\epsilon \text{ small} > 0)$$

and [with the same limitation on $r(p)$] the Jost

function $f(k, 0)$ is the limit of sequences

$$f(k, 0) = 1 + \lim_{p\to\infty}\left[\sum_1^p f_q(k, r(p))\right].$$

VII. CONCLUSIONS

Thus we have shown, in this paper, that the method of convergence for the new Jost solution in coordinate space which consists mainly of connecting the radial coordinate and the order of the perturbation expansion, previously used[3] for potentials behaving like inverse powers near the origin, can be extended to potentials where the most singular term includes logarithms or exponentials and may be therefore of very large application.

Firstly we recall the results obtained for potentials which behave as $G^2(\log 1/r)^\beta r^{-2}$ as $r \to 0$.

In the case $-1 \leq \beta < 0$ we have found two main properties. On the one hand, with respect to r, the behavior of the solution near the origin is not the same as in the usual case (potentials which behave as $r^{-\lambda}$, $\lambda < 2$ as $r \to 0$). In the usual case the singularities are given only by the centrifugal term. On the contrary, for $-1 \leq \beta < 0$ although the potential is less singular than r^{-2}, the presence of the logarithmic term in the potential gives other singularities. On the other hand the factorization $Z(r)$ of the most singular part of the Jost solution is sufficient in order to obtain the Jost function as the sum of perturbative terms as in the usual case. Equivalently we have no limiting dependence $r_L(p)$. The reason being that $G = 0$ is not a singular point with respect to G. We remark that this situation is the same which occurs[1,3] for short range potentials behaving like Gr^{-2} near the origin.

On the contrary in the case $\beta > 0$, similarly to the power case more singular than r^{-2}, we have both singularities with respect to r for the Jost solutions and singularities[10] at $G = 0$ for the Jost functions which reflects in the fact that we have a limiting dependence $r_L(p) = \exp(-p^{-\epsilon+1/(1+\frac{1}{2}\beta)})$.

In the case when the most singular part of the potential behaves as $G^2(\log 1/r)^\beta r^{-2n}$ $(n > 1)$, as $r \to 0$ the limiting dependence $r_L(p)$ is practically the same as in the power case which behaves as G^2r^{-2n} as $r \to 0$. We find in both cases $r_L(p) \sim p^{\epsilon-1/(n-1)}$. This is easy to understand because the singular part of the perturbation expansion of the new Jost solution factorizes mainly the leading singularity of the new Jost solution. This leading term being

$$\exp\left[-2G\int_r^{\text{const}} r'^{-n}\left(\log\frac{1}{r'}\right)^{\frac{1}{2}\beta} dr'\right],$$

then for r real $\to 0$, the power term is the most important one.

Finally, we note that for the exponential case

$$V \underset{r\to 0}{\sim} G^2r^{-2n}\exp(\eta/r^\gamma) \qquad (\eta, \gamma > 0),$$

which is a stronger singularity than in all previous cases:

$$r_L(p) \sim [\log p^{2(1-\epsilon)/\eta}]^{-1/\gamma}$$

which is a higher limiting dependence than previously found.

Thus, if we consider potentials more and more singular, we find higher and higher limiting dependences and the range of the available $r(p)$ becomes narrower and narrower. In other words when we consider a perturbation expansion up to a certain order p (finite), if the potential becomes more singular, then the region of the interaction which has to be excluded at that order $p[r(p) \leq r_L(p)]$ becomes larger.

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APPENDIX

We want to investigate the remaining sequences $R(p, r, k)$ when p is large and $r \to 0$. We start from the integral equations (5), (45) and iterate. We consider only the singular part of $f(k, r)$ when r is small because for the regular part where we can invert the two limits ($p \to \infty$ and $r \to 0$) we can attribute an aribtrary $r(p)$ dependence such that $r(p) \to 0$ when $p \to \infty$.

The behavior near the origin of the singular part of the qth iteration of $f(k, r)$ is given from (5) and (45) by

$$f_q(r) \sim \int_r^a (r - r')\left(2\bar{\psi}(r')\frac{d}{dr'} + W(r')\right)f_{q-1}(r')\,dr', \tag{A1}$$

where a is a small finite positive constant.

We can rewrite (A1) keeping always only the singular part of $f_q(r)$

$$f_q(r) \sim \int_r^a [(r - r')(W - 2\bar{\psi}') + 2\bar{\psi}]f_{q-1}(r')\,dr'. \tag{A2}$$

We suppose now the two following conditions are

[10] We note that in the $\beta = 1$ case (S wave, zero energy) the singularity at $G = 0$ for the scattering length has been explicitly investigated by Calogero and Cassandro.[6]

verified

$$|\bar{\psi}(r')| \leq |\bar{\psi}^*(r')|\,(1 + O_1(r')), \tag{A3}$$

$$|(r - r')(W(r') - 2\bar{\psi}'(r'))| \leq |\bar{\psi}^*(r')| \quad (1 + O_2(r')) \tag{A4}$$

where $O_1(r')$ and $O_2(r')$ are bounded for $r' \in (0, a)$. We put

$$X(r) = \int_r^a |\bar{\psi}^*(r')|\,dr' \text{ and } |f_q(r)| = \frac{X^q}{q!}\,|g_q(r)|. \tag{A5}$$

First of all if (A3) and (A4) are satisfied we get

$$|f_q(r)| < \text{const} \int_r^a |\bar{\psi}^*(r')|\,|f_{q-1}(r')|\,dr'. \tag{A6}$$

Now we substitute (A5) in (A6) and we get

$$|g_q(r)| < \text{const} \max\,(|g_q(r')| + \text{const}, \qquad r' \in (r, a) \tag{A7}$$

where the constants in (A7) are finite: we iterate (A7) and get

$$|f_q(r)| < (X^q/q!)q(\text{const})^q \max\,|g_1(r')|, \qquad r' \in (r, a)$$

and for the remaining part $R(p, r, k)$

$$|R(p, r, k)| < \sum_{p+1}^{\infty} \frac{X^q}{q!}\,q(\text{const})^q \max\,|g_1(r')|, \qquad r' \in (r, a). \tag{A8}$$

(1) We consider the case of potentials (14′) such that

$$V(r) \underset{r\to 0}{\sim} \frac{G^2}{r^2}\left(\log\frac{1}{r}\right)^{\beta} + \frac{l(l+1)}{r^2}.$$

In this case [see Eqs. (15), (16)], $\bar{\psi}^* = 2G/r(\log 1/r)^{\frac{1}{2}\beta}$ and conditions (A3) and (A4) are satisfied. We have also $|g_1| < \text{const}$,

$$X \leq \frac{2G}{1 + \frac{1}{2}\beta}\left(\log\frac{1}{r}\right)^{1+\frac{1}{2}\beta} + \text{const}$$

and we get for small r and large p

$$|R(p, r, k)| < \sum_{p+1}^{\infty}\left[\frac{2G}{1 + \frac{1}{2}\beta}\left(\log\frac{1}{r}\right)^{1+\frac{1}{2}\beta} + \text{const}\right]^q \cdot\frac{q(\text{const})^q}{q!} \tag{A9}$$

with all constants positive.

(2) In the case of potentials (21) such that

$$V(r) \underset{r\to 0}{\sim} \frac{G^2}{r^{2n}}\left(\log\frac{1}{r}\right)^{\beta} + \frac{l(l+1)}{r^2}, \qquad (n > 1)$$

we have [see Eq. (22)] $\bar{\psi}^* = \text{const}/n\cdot(\log 1/r)^{\frac{1}{2}\beta}$ and conditions (A3) and (A4) are satisfied. We get $|g_1| < \text{const}$ and for large p and small r

$$|R(p, r, k)| < \sum_{p+1}^{\infty}\left[\frac{\text{const}}{r^{n-1}}\left(\log\frac{1}{r}\right)^{\frac{1}{2}\beta} + \text{const}\right]^q \cdot\frac{q(\text{const})^q}{q!} \tag{A10}$$

with all constants positive.

(3) for the case of potentials (23)

$$V(r) \underset{r\to 0}{\sim} \frac{G^2}{r^{2n}}\left[\left(\log\frac{1}{r}\right)^{\beta} + A^{\frac{1}{2}}h(r)\right] + \frac{l(l+1)}{r^2}$$

with conditions [see (23)] such that the behavior of the solution for $r \to \infty$ is given by the centrifugal term.

In first we consider $\delta > 0$ or $\delta = 0$ and $\beta > 0$. In this case [see Eq. (24)],

$$\bar{\psi}^* = \text{const}/r^n(\log 1/r)^{\frac{1}{2}\beta},$$

(A3) and (A4) are satisfied, $|g_1| < \text{const}$ and we have for $|R(p, r, k)|$ when p is large and r small, the same bound as (A10). Secondly we consider $\delta = 0$ and $\beta < 0$. In this case [see the conditions (25) on the potential and also (24)], $\bar{\psi}^* = \text{const}/r^n$, $|g_1| < \text{const}$, $A > 0$ and $X < \text{const}/r^{n-1} + \text{const}$. We get for large p and small r

$$|R(p, r, k)| < \sum_{p+1}^{\infty}\left[\frac{\text{const}}{r^{n-1}} + \text{const}\right]^q \frac{q(\text{const})^q}{q!} \tag{A11}$$

with all constants positive.

(4) Now we consider the case of exponentially singular potentials of finite range (25′) for the S wave

$$V = \left[\frac{G^2}{r^{2n}}\exp\left(\frac{\eta}{r^{\gamma}}\right) + \frac{A}{r^m}\right]\theta(r_0 - r) \qquad (\eta, \gamma > 0).$$

We have [see Eq. (26)]

$$\bar{\psi}^* = \frac{\text{const}}{r^{n+\gamma}}\exp\,(\eta r^{-\gamma}/2),$$

(A3) and (A4) are satisfied, $|g_1| < \text{const}$, $X <$ [const r^{1-n} exp $(\frac{1}{2}\eta r^{-\gamma})$ + const], and we get for large p and small r

$$|R(p, r, k)| < \sum_{p+1}^{\infty}\left[\frac{\text{const}}{r^{n-1}}\exp\,(\tfrac{1}{2}\eta r^{-\gamma}) + \text{const}\right]^q \cdot\frac{q(\text{const})^q}{q!} \tag{A12}$$

with all constants positive.

Perturbation Expansion for Lattice Thermal Conductivity

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A method is given for obtaining a perturbation expansion for the correlation function formula for thermal conductivity. The problem is reduced to the determination of the matrix elements of the products of resolvent operators $X_{ll'}$ and $Y_{ll'}$ to different orders in the perturbation $\lambda H'$. The coefficients in the general equations for $X_{ll'}$ and $Y_{ll'}$ derived by Van Hove, Janner, and Swenson are iterated, and the resulting approximate equations are used to deduce the formulas for the contributions to the lattice thermal conductivity proportional to λ^{-2} (lowest order) and to λ^{-1}.

1. INTRODUCTION

THIS is the second in a series of papers devoted to a rigorous quantum-mechanical formulation of the theory of lattice thermal conductivity. In the previous paper[1] the energy flux operator was derived for a lattice with imperfections and anharmonic forces. Here, the correlation function formula for the thermal conductivity K^{ij} is used to obtain formulas for the contributions to K^{ij} proportional to λ^{-2} and to λ^{-1}, where λ characterizes the strength of the interactions between the normal modes of a perfect, harmonic lattice. The equations obtained here for the lowest (or λ^{-2}) order contribution are used in the following paper[2] to derive the transport equations for K^{ij}. In a later paper, the λ^{-1} contributions will be expressed as corrections to this lowest-order result.[3]

Several alternate derivations of the correlation function formulas for transport coefficients have been given.[4] The formula of interest here is that for the thermal conductivity tensor[5]:

$$K^{ij} = \frac{V}{kT^2}\int_0^\infty dt\, e^{-\epsilon t}\ \mathrm{Re}\,\langle S^i S^j(\pm t)\rangle_0. \qquad (1.1)$$

Here, K^{ij} is the conductivity tensor. S^i is the ith component of the average energy flux operator, i.e., the local flux operator averaged over the entire volume of the system [see (2.13) in Ref. 1]. (The system is assumed to have zero local velocity so that S^i is also the heat flux.) $S^j(t)$ is the Heisenberg operator $\exp(iHt/\hbar)\ S^j \exp(-iHt/\hbar)$. The brackets $\langle\ \rangle_0$ indicate a canonical equilibrium average. Re designates that the real part is to be taken, V and T represent the volume and temperature of the system, and k is Boltzmann's constant. $e^{-\epsilon t}$ is a convergence factor. For a thermal conductivity to exist as an intrinsic property of the system, the value of (1.1) must be essentially independent of ϵ for a range of small values of ϵ; however, because of the recurrence properties of finite systems one cannot set $\epsilon = 0$.

Since the correlation function formulas are quite formal, they must be supplemented by appropriate many-body techniques in order to yield practical results. As examples of investigations in that direc-

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[5] Some authors [e.g., H. Mori, Phys. Rev. **112**, 1829 (1958)] give expression for K^{ij} similar to (1.1) but with $\mathrm{Re}\,\langle S^i S^j(\pm t)\rangle_0$ replaced by $\beta^{-1}\int_0^\beta d\xi\ \langle S^j S^i(t + i\hbar\xi)\rangle_0$, where $\beta = 1/kT$.

It can be shown [see Verboven, Ref. 8] that this latter expression equals $\frac{1}{2}[\langle S^i(t)S^j\rangle_0 + \langle S^i S^j(t)\rangle_0]$ in the case of steady-state transport coefficients. That $\frac{1}{2}[\langle S^i(t)S^j\rangle_0 + S^i\langle S^j(t)\rangle_0] = \mathrm{Re}\,\langle S^i S^j(\pm t)\rangle_0$ and that K^{ij} is independent of the sign in $S^j(\pm t)$ are consequences of the time-inversion symmetries of the operators involved [see, e. g., E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), pp. 325–348].

tion, we mention the following: The electrical conductivity of metals and the Wiedemann–Franz law have been discussed by Chester and Thellung[6], who used Van Hove's many-body techniques, and by Langer[7], who used a propagator method. The former work has been extended by Verboven[8], who obtained the second-order (or λ^0) corrections to the conductivity. Langer's results are valid to lowest order in the density of impurities and to all orders in the electron–electron interaction. Maradudin[9] has discussed the lattice thermal conductivity with Green's function techniques to lowest order in the density of impurities. Lattice thermal conductivity has also been treated by Schieve and Leaf[10] using the classical many-body methods of Prigogine, by Hardy[11] using Van Hove's generalized master equation and by Schieve and Peterson[12] who have shown that if the scattering of phonons can be characterized by a relaxation time, then (1.1) and the Boltzmann equation give the same results. The approach utilized here is most similar to that of McLennan and Swenson,[13] who obtained the thermal conductivity of a gas to lowest order in the density.

The special characteristic of the many-body treatment presented here is its simplicity. In Sec. 2 the correlation function formula is written out in the representation diagonalizing the unperturbed Hamiltonian, and the problem is reduced to that of finding expansions in powers of λ for $X_{ll'}$ and $Y_{ll'}$, products of matrix elements of resolvent operators. Van Hove[14] and Janner[15] first derived equations satisfied by $X_{ll'}$ and $Y_{ll'}$ by employing a perturbation expansion which is exact only for infinite systems. Later Swenson[16] and Peterson and Quay[17] deduced similar equations, valid for finite systems, which are simple algebraic consequences of the definitions of the quantities involved (see Appendix A). In Sec. 3 the coefficients of these equations, which hold to all orders in λ, are iterated to obtain sequences of approximate equations for determining $X_{ll'}$ and $Y_{ll'}$. The approximate equations are then used to deduce the formulas for the λ^{-2} and λ^{-1} contributions to K^{ij}; the results are compiled in Sec. 4.

Although the interest here is in the lattice thermal conductivity, the validity of the perturbation techniques used is not restricted to that problem. The resulting formulas apply to any correlation function of form (1.1) for which the fluxes (S^i and S^j) possess both diagonal and nondiagonal elements in the representation of the unperturbed energy and for system with perturbations $\lambda H'$ nondiagonal in the unperturbed representation. All results obtained are based on the iteration of exact equations to obtain perturbation series; no assumption about the convergence of any infinite series in powers of λ is necessary.

2. REDUCTION OF THE CORRELATION FUNCTION FORMULA

The first step in expanding K^{ij} in powers of λ is to express the operators in (1.1) as matrices in the representation diagonalizing H°, where

$$H = H^\circ + \lambda H' \tag{2.1}$$

and H° is the harmonic Hamiltonian. The eigenvalues and eigenfunctions of H° will be designated by $\mathcal{E}(\alpha)$ and $|\alpha\rangle$:

$$H^\circ\,|\alpha\rangle = \mathcal{E}(\alpha)\,|\alpha\rangle; \tag{2.2}$$

Greek letters indicate eigenstates. The perturbation $\lambda H'$ is assumed to be nondiagonal in the H°-representation:

$$\langle\alpha|\,\lambda H'\,|\alpha\rangle = 0. \tag{2.3}$$

The part of the Hamiltonian quadratic in the momentum and position operators can always be separated so that H° is a sum of plane-wave normal modes and the quadratic perturbation terms due modes and the quadratic perturbation terms due to lattice imperfections obeys (2.3) (see Ref. 1, p. 174). The cubic anharmonic-potential pertubation automatically satisfies (2.3).

In the H°-representation the correlation function expression (1.1) is

$$K^{ij} = (V/kT^2)\,\mathrm{Re}\,[\sum \langle\alpha|f_0|\mu\rangle\,\langle\mu|S^i|\gamma\rangle\,\langle\sigma|S^j|\beta\rangle \times \tilde{Z}_\bullet(\gamma\sigma\beta\alpha)], \tag{2.4}$$

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where the sum is to be carried over all states μ, β, α, γ, and σ, and where by definition

$$\tilde{Z}_\epsilon(\gamma\sigma\beta\alpha) \equiv \int_0^\infty dt\, e^{-\epsilon t} \times \langle\gamma|\exp(-iHt/\hbar)\,|\sigma\rangle\langle\beta|\exp(iHt/\hbar)\,|\alpha\rangle; \quad (2.5)$$

the minus sign in $S^i(\pm t)$ in (1.1) has been used here. Note that $\tilde{Z}_\epsilon(\alpha\beta\beta\alpha)$ is the Laplace transform of $|\langle\alpha|\exp(-iHt/\hbar)\,|\beta\rangle|^2$, the probability of a transition from state β to state α in time t.

The problem of expanding K^{ij} in powers of λ is now reduced to the separate problems of expanding f_0, $\mathbf{S}$, and $\tilde{Z}_\epsilon$. The expansions for f_0 and $\mathbf{S}$ are relatively easy to obtain and are given below. Expanding $\tilde{Z}_\epsilon$ is more difficult and is most easily done with the aid of resolvent operators.

The Expansions for f_0 and S

The canonical equilibrium density matrix is

$$f_0 = [\mathrm{Tr}\, e^{-H/kT}]^{-1} e^{-H/kT}; \quad (2.6)$$

Its perturbation expansion is[18]

$$\langle\alpha|f_0|\beta\rangle = \langle\alpha|f_0^\circ|\beta\rangle + \langle\alpha|\lambda f_0'|\beta\rangle + O(\lambda^2), \quad (2.7)$$

where

$$\langle\alpha|f_0^\circ|\beta\rangle = [Z^\circ]^{-1}\exp[-\mathcal{E}(\alpha)/kT]\,\delta_{\alpha\beta}, \quad (2.8)$$

$$\langle\alpha|\lambda f_0'|\beta\rangle = \frac{1}{Z^\circ}\frac{\exp[-\mathcal{E}(\alpha)/kT] - \exp[-\mathcal{E}(\beta)/kT]}{\mathcal{E}(\alpha) - \mathcal{E}(\beta)} \times \langle\alpha|\lambda H'|\beta\rangle, \quad (2.9)$$

and $Z^\circ \equiv \{\sum_\alpha \exp[-\mathcal{E}(\alpha)/kT]\}$; the remainder term $O(\lambda^2)$ is of order λ^2; $\delta_{\alpha\beta}$ is the Kronecker δ-function. Because of (2.3), $\langle\alpha|\lambda f_0'|\beta\rangle$ has no diagonal part.

The energy flux operator can always be written as [see Ref. 1: Eq. (3.2)]

$$\langle\alpha|\mathbf{S}|\beta\rangle = \langle\alpha|\mathbf{S}^\circ{}_d|\alpha\rangle\delta_{\alpha\beta} + \langle\alpha|\mathbf{S}^\circ{}_{nd}|\beta\rangle + \langle\alpha|\lambda\mathbf{S}'|\beta\rangle + \langle\alpha|\lambda^2\mathbf{S}''|\beta\rangle, \quad (2.10)$$

where $\mathbf{S}^\circ{}_d$ and $\mathbf{S}^\circ{}_{nd}$ are the diagonal and nondiagonal parts of the flux brought about by H°. In Ref. 1, formulas are given which express $\mathbf{S}^\circ{}_d$, $\mathbf{S}^\circ{}_{nd}$, and $\lambda\mathbf{S}'$ as explicit functions of the creation and annihilation operators for phonons (in Ref. 1, $\mathbf{S}^\circ{}_{nd} = \mathbf{S}^\circ{}_{2,nd} + \mathbf{S}^\circ{}_3$). In general, $\langle\alpha|\mathbf{S}^\circ{}_{nd}|\beta\rangle$ is not zero, and

$$\langle\alpha|\mathbf{S}^\circ{}_d|\alpha\rangle = V^{-1}\sum_{\mathbf{k}s}\langle\alpha|N_{\mathbf{k}s}|\alpha\rangle\hbar\omega_{\mathbf{k}s}\mathbf{v}_{\mathbf{k}s}, \quad (2.11)$$

where $N_{\mathbf{k}s}$, $\omega_{\mathbf{k}s}$, and $\mathbf{v}_{\mathbf{k}s}$ are the number operator, the frequency, and the group velocity of the normal mode with wave vector $\mathbf{k}$ and polarization index s.

Introduction of Resolvent Operators

The time-evolution operators are related to the resolvent operators $\langle\alpha|R_z|\beta\rangle$ by

$$\langle\alpha|\exp(\pm iHt/\hbar)\,|\beta\rangle = -(2\pi i)^{-1}\int_C dz\exp(\pm izt/\hbar)\langle\alpha|R_z|\beta\rangle, \quad (2.12)$$

where

$$\langle\alpha|R_z|\beta\rangle \equiv \langle\alpha|(H-z)^{-1}|\beta\rangle \quad (2.13)$$

and C is a contour enclosing the real axis in a counterclockwise direction. The poles of the resolvent operator are on the real axis. From (2.5) and (2.12) it follows that[19]

$$\begin{aligned}\tilde{Z}_\epsilon(\gamma\sigma\beta\alpha) &= -(2\pi)^{-2}\int_0^\infty dt\int_C dz\int_{C'} dz' \times \exp[-\epsilon t - i(z'-z)t/\hbar] \times \langle\gamma|R_{z'}|\sigma\rangle\langle\beta|R_z|\alpha\rangle \\ &= (\hbar/2\pi)\int_{-\infty}^\infty dE\,\langle\gamma|R_{E+\frac{1}{2}i\hbar\epsilon}|\sigma\rangle\langle\beta|R_{E-\frac{1}{2}i\hbar\epsilon}|\alpha\rangle.\end{aligned} \quad (2.14)$$

For the purpose of finding its λ dependence, the $\tilde{Z}_\epsilon(\gamma\sigma\beta\alpha)$ fall naturally into four categories which depend on the existance of identities among γ, σ, β, and α. First, introduce the following notation:

$$X_{ll'}(\alpha\beta) \equiv \langle\beta|R_l|\alpha\rangle\langle\alpha|R_{l'}|\beta\rangle; \quad (2.15)$$

$$Y_{ll'}(\alpha\beta\sigma) \equiv \langle\beta|R_l|\alpha\rangle\langle\alpha|R_{l'}|\sigma\rangle. \quad (2.16)$$

These four categories or types of $\tilde{Z}_\epsilon$ are

$$\tilde{Z}_\epsilon(\alpha\beta\beta\alpha) = (\hbar/2\pi)\int_{-\infty}^\infty dE\,X_{ll'}(\alpha\beta), \quad (2.17a)$$

$$\tilde{Z}_\epsilon(\alpha\sigma\beta\alpha) = (\hbar/2\pi)\int_{-\infty}^\infty dE\,Y_{ll'}(\alpha\beta\sigma)\ [\beta \neq \sigma], \quad (2.17b)$$

$$\tilde{Z}_\epsilon(\gamma\beta\beta\alpha) = (\hbar/2\pi)\int_{-\infty}^\infty dE\,Y_{l'l}(\beta\gamma\alpha)\ [\alpha \neq \gamma], \quad (2.17c)$$

$$\tilde{Z}_\epsilon(\gamma\sigma\beta\alpha) = (\hbar/2\pi)\int_{-\infty}^\infty dE\,\langle\gamma|R_{l'}|\sigma\rangle\langle\beta|R_l|\alpha\rangle. \quad (2.17d)$$

[18] This result is obtained by iterating the following identity to obtain a series in powers of λ and using the result to expand (2.6):

$$\exp[-\beta(A+\lambda B)] = \{1 - \textstyle\int_0^\beta d\xi \times \exp[-\xi(A+\lambda B)]\,\lambda B\exp[\xi A]\}\exp[-\beta A].$$

[19] To obtain the last member of (2.14), choose the countour C to be the lines $(-\infty - \frac{1}{2}i\hbar\epsilon, +\infty - \frac{1}{2}i\hbar\epsilon)$ and $(+\infty + \frac{1}{2}i\hbar\epsilon, -\infty + \frac{1}{2}i\hbar\epsilon)$, and C' to be $(-\infty - i\delta, +\infty - i\delta)$ and $(+\infty + i\delta, -\infty + i\delta)$, where $\delta < \frac{1}{2}\hbar\epsilon$. With these one has $\mathrm{Re}\,[i(z-z')/\hbar] < \epsilon$ so that the integration over t can be performed first; this introduces a pole at $i\hbar\epsilon + z - z' = 0$. Evaluate the z'-integration by taking the residues of the poles in the upper and lower halves of the complex z'-plane. Then, by taking the upper line of the contour C to infinity and making the substitution $E = z + \frac{1}{2}i\hbar\epsilon$, one obtains the last member of (2.14).

$[\beta \neq \sigma; \alpha \neq \gamma]$, where

$$l = E - \tfrac{1}{2}i\hbar\epsilon \quad \text{and} \quad l' = E + \tfrac{1}{2}i\hbar\epsilon. \tag{2.18}$$

The problem of expanding K^{ij} in powers of λ is now reduced to that of expanding $X_{ll'}$, $Y_{ll'}$, $Y_{l'l}$, and $\tilde{Z}_\epsilon$ of type (d).

3. THE PERTURBATION EXPANSION FOR $\tilde{Z}_\epsilon$

The exact equation for $X_{ll'}$ derived by Swenson[16] is

$$(l - l')X_{ll'}(\alpha\beta) - F_{ll'}(\alpha)\delta_{\alpha\beta} = \sum_\mu [F_{ll'}(\alpha)W_{ll'}(\alpha\mu)X_{ll'}(\mu\beta) - F_{ll'}(\mu)W_{ll'}(\mu\alpha)X_{ll'}(\alpha\beta)], \tag{3.1}$$

where $F_{ll'}$ and $W_{ll'}$ are defined by

$$F_{ll'}(\alpha) \equiv D_l(\alpha) - D_{l'}(\alpha), \tag{3.2}$$

$$W_{ll'}(\alpha\mu) \equiv U_l(\mu\alpha)U_{l'}(\alpha\mu) - \sum_\gamma W_{ll'}(\alpha\gamma)D_l(\gamma)D_{l'}(\gamma)U_l(\mu\gamma)U_{l'}(\gamma\mu), \tag{3.3}$$

where $D_l(\alpha)$ is the diagonal part of $\langle\alpha|R_l|\beta\rangle$ and

$$\langle\alpha|\, R_l \,|\beta\rangle \equiv \delta_{\alpha\beta}D_l(\beta) + D_l(\alpha)U_l(\alpha\beta)D_l(\beta). \tag{3.4}$$

The exact equation for $Y_{ll'}$ is found by introducing a quantity $V_{ll'}$ defined so that

$$Y_{ll'}(\alpha\gamma\sigma) \equiv \sum_\beta X_{ll'}(\alpha\beta)V_{ll'}(\beta\gamma\sigma). \tag{3.5}$$

Then, by multiplying (3.1) by $V_{ll'}(\beta\gamma\sigma)$ and summing over β, one obtains[16]

$$(l - l')Y_{ll'}(\alpha\gamma\sigma) - F_{ll'}(\alpha)V_{ll'}(\alpha\gamma\sigma) = \sum_\mu [F_{ll'}(\alpha)W_{ll'}(\alpha\mu)Y_{ll'}(\mu\gamma\sigma) - F_{ll'}(\mu)W_{ll'}(\mu\alpha)Y_{ll'}(\alpha\gamma\sigma)]. \tag{3.6}$$

By using (3.4) and definitions (2.15) and (2.16) for $X_{ll'}$ and $Y_{ll'}$, Eq. (3.5) can be rewritten as[16]

$$V_{ll'}(\alpha\gamma\sigma) = \delta_{\alpha\gamma}D_{l'}(\sigma)U_{l'}(\alpha\sigma) + \delta_{\alpha\sigma}D_l(\gamma)U_l(\gamma\alpha) + D_l(\gamma)U_l(\gamma\alpha)U_{l'}(\alpha\sigma)D_{l'}(\sigma) - \sum_\nu D_l(\nu)D_{l'}(\nu)U_l(\nu\alpha)U_{l'}(\alpha\nu)V_{ll'}(\nu\gamma\sigma). \tag{3.7}$$

It is apparent from the above comments and the very concise derivation of (3.1) given in Appendix A that the basic equations (3.1) and (3.6) are nothing more than simple algebraic consequences of the separation (3.4) and the definitions of $F_{ll'}$, $W_{ll'}$, and $V_{ll'}$. Thus, (3.1) and (3.6) contain neither more nor less information about $X_{ll'}$ and $Y_{ll'}$ than (2.15) and (2.16). Their usefulness lies in the fact that $F_{ll'}$ $W_{ll'}$, and $V_{ll'}$, can be expanded in powers of λ. This is done by iterating (3.3) and (3.7) to get series for $W_{ll'}$ and $V_{ll'}$ in terms of D_l and U_l and by expanded D_l and U_l in powers of λ (see Appendix B). The expansions which result are then used with (3.1) and (3.6) to form sequences of equations which determine $X_{ll'}$ and $Y_{ll'}$ to successive powers of λ. The approximate equations obtained in this way are well behaved for $l = E - \frac{1}{2}i\hbar\epsilon$ and $l' = E + \frac{1}{2}i\hbar\epsilon$ when ϵ is very small; by contrast, an attempt to expand $X_{ll'}$ and $Y_{ll'}$ directly in series of powers of λ yields series whose first terms are proportional to ϵ^{-1} (see comments at the end of this section).

The Approximate Equations for $X_{ll'}$ and $Y_{ll'}$

The interest here is in equations for $X_{ll'}$, $Y_{ll'}$, and $Y_{l'l}$ where l and l' are given by (2.18). To avoid concealing the essentials of the approach by a clutter of symbols, all indication of these subscripts will be dropped, and a new symbol $\bar{W}$ will be introduced:

$$\bar{W}(\alpha\mu) \equiv F_{ll'}(\alpha)W_{ll'}(\alpha\mu) - \delta_{\alpha\mu}[\sum_\nu F_{ll'}(\nu)W_{ll'}(\nu\alpha)]. \tag{3.8}$$

Remembering that $l - l' = -i\hbar\epsilon$, we can now express the exact equation (3.1) and (3.6) as

$$-i\hbar\epsilon X(\alpha\beta) - F(\alpha)\delta_{\alpha\beta} = \sum_\mu \bar{W}(\alpha\mu)X(\mu\beta) \tag{3.9}$$

and

$$\mp i\hbar\epsilon Y(\alpha\gamma\sigma) - F(\alpha)V(\alpha\gamma\sigma) = \sum_\mu \bar{W}(\alpha\mu)Y(\mu\gamma\sigma), \tag{3.10}$$

where by convention the upper sign in (3.10) corresponds to the case $Y_{ll'}$ and the lower sign to $Y_{l'l}$.

The exact forms of the expansions for $F_{ll'}$, $W_{ll'}$, and $V_{ll'}$ in powers at λ are given in Appendix B. The expansion for $\bar{W}$ follows immediately from that for $F_{ll'}$ and $W_{ll'}$. The results can be summarized as follows:

$$F(\alpha) = F^\circ(\alpha) + \lambda^2 F''(\alpha) + \cdots, \tag{3.11}$$

$$V(\alpha\gamma\sigma) = \lambda[V^\circ(\alpha\gamma\sigma) + \lambda V'(\alpha\gamma\sigma) + \cdots], \tag{3.12}$$

$$\bar{W}(\alpha\mu) = \lambda^2[\bar{W}^\circ(\alpha\mu) + \lambda\bar{W}'(\alpha\mu) + \cdots], \tag{3.13}$$

where there is no $\lambda F'(\alpha)$ term because of assumption (2.3).

The sequences of equations for $X(\alpha\beta)$ and $Y(\alpha\gamma\sigma)$ are formed by using the above to evaluate the coefficients in (3.9) and (3.10) to successively higher orders in λ; one obtains

$$-i\hbar\epsilon\, {}^\circ X(\alpha\beta) - F^\circ(\alpha)\delta_{\alpha\beta} = \sum_\mu \lambda^2\, \bar{W}^\circ(\alpha\mu)\, {}^\circ X(\mu\beta), \tag{3.14a}$$

$$-i\hbar\epsilon\,{}^1X(\alpha\beta) - F^\circ(\alpha)\delta_{\alpha\beta} = \sum_\mu \lambda^2\,[\bar{W}^\circ(\alpha\mu) + \lambda\bar{W}'(\alpha\mu)]\,{}^1X(\mu\beta), \tag{3.14b}$$

$$-i\hbar\epsilon\,{}^2X(\alpha\beta) - [F^\circ(\alpha) + \lambda^2 F''(\alpha)]\delta_{\alpha\beta} = \sum_\mu \lambda^2\,[\bar{W}^\circ(\alpha\mu) + \lambda\bar{W}'(\alpha\mu) + \lambda^2\bar{W}''(\alpha\mu)]^2\,X(\mu\beta), \tag{3.14c}$$

$$\text{etc.}; \tag{3.14n}$$

$$\mp i\hbar\,{}^0Y(\alpha\gamma\sigma) - F^\circ(\alpha)\,\lambda V^\circ(\alpha\gamma\sigma) = \sum_\mu \lambda^2\,\bar{W}^\circ(\alpha\mu)\,{}^0Y(\mu\gamma\sigma), \tag{3.15a}$$

$$\mp i\hbar\epsilon\,{}^1Y(\alpha\gamma\sigma) - F^\circ(\alpha)\,\lambda[V^\circ(\alpha\gamma\sigma) + \lambda V'(\alpha\gamma\sigma)] = \sum_\mu \lambda^2\,[\bar{W}^\circ(\alpha\mu) + \lambda\bar{W}(\alpha\mu)]\,{}^1Y(\mu\gamma\sigma), \tag{3.15b}$$

$$\text{etc.}$$

The left superscripts on ${}^2X(\alpha\beta)$, ${}^1Y(\alpha\gamma\sigma)$, etc. label the successive approximations to $X(\alpha\beta)$ and $Y(\alpha\beta\sigma)$. It is presumed, at least for the first few equations of the sequence, that ${}^nX(\alpha\beta)$ and ${}^nY(\alpha\beta\sigma)$ approach the exact $X(\alpha\beta)$ and $Y(\alpha\beta\sigma)$ determined by (3.9) and (3.10) as n increases.

A question now arises: How do the solutions of (3.14) and (3.15) depend on λ? To answer this, first consider (3.14a). If the term proportional to ϵ in it were omitted, it is apparent that the resulting ${}^0X(\alpha\beta)$ would be proportional to λ^{-2}. However, the term proportional to ϵ cannot be omitted: When it is omitted, $X(\alpha\beta) = (\text{constant})$ is a solution to the transposed homogeneous equation $\sum_\alpha \bar{W}^0(\alpha\mu)X(\alpha\beta)$ [see (3.8)] which is not orthogonal to the inhomogeneous term $-F^\circ(\alpha)\delta_{\alpha\beta}$; consequently, there is no solution to the thus altered (3.14a). Nevertheless, when (2.4), (2.17a), and ${}^0X(\alpha\beta)$ [as determined by (3.14a) with the term proportional to ϵ included] are used to evaluate K^{ij} along with the λ-independent parts of f_0 and $\mathbf{S}$, the resulting expression for K^{ij} is proportional to λ^{-2} in the limit $\epsilon \to 0$ and $V \to \infty$.[2] In other words, ${}^0X(\alpha\beta)$ gives the same contribution to the λ-dependence of the limiting value of K^{ij} as is suggested by neglecting the term proportional to ϵ. More satisfactorily, one can predict the λ-dependence for the resulting K^{ij} by treating the term proportional to ϵ as if it were proportional to λ^2. Of course, one must consider ϵ to be independent of λ (as it actually is) when the limit $\epsilon \to 0$ is finally taken.

To find the contribution of ${}^nX(\alpha\beta)$ for $n > 0$ to the λ-dependence of K^{ij}, consider the series

$${}^nX(\alpha\beta) = \lambda^{-2}[{}^nX^\circ(\alpha\beta) + \lambda\,{}^nX'(\alpha\beta) + \cdots + \lambda^i\,{}^nX^{(i)}(\alpha\beta) + \cdots]. \tag{3.16}$$

Substitute this into (3.14n) and equate coefficients of equal power of λ with the term proportional to ϵ treated as if ϵ were proportional to λ^2. In this way one obtains a collection of formulas for the ${}^nX^{(i)}(\alpha\beta)$. It is readily seen that the ${}^nX^{(i)}(\alpha\beta)$ with a given i but different values of n are all determined by the same equation provided that $i \leq n$. If $i > n$, all the ${}^nX^{(i)}(\alpha\beta)$'s with the same i but different n's are determined by different equations; thus, the ${}^nX^{(i)}(\alpha\beta)$ with $n > i$ have no consistent meaning. The ${}^iX^{(i)}(\alpha\beta) = {}^{i+1}X^{(i)}(\alpha\beta) = {}^{i+2}X^{(i)}(\alpha\beta) = \cdots$ are the parts of $X(\alpha\beta)$ which contribute to the limiting value of K^{ij} in the order λ^{i-2}.

Note that although the ${}^nX^{(i)}(\alpha\beta)$'s are in general all nonzero, the ${}^0X^{(i)}(\alpha\beta)$ determined by (3.14a) vanish for $i > 0$ and $\lambda^{-2}\,{}^0X^\circ(\alpha\beta)$ is equivalent to ${}^0X(\alpha\beta)$. Equation (3.14a) determines the λ^{-2}-contribution to K^{ij} from $X(\alpha\beta)$.[2] Now, the formulas for $\lambda^{-1}\,{}^nX'(\alpha\beta)$ depend on $\lambda^{-2}\,{}^nX^\circ(\alpha\beta)$, but the solution for $\lambda^{-2}\,{}^nX^\circ(\alpha\beta) = {}^0X(\alpha\beta)$ is not available; thus, to find a useful expression for the λ^{-1} contribution to K^{ij} it is necessary to use the complete ${}^1X(\alpha\beta)$ determined by (3.14b). To proceed, one uses Eq. (3.14b) in conjunction with (2.4) and (2.17a) to find an expression for K^{ij}, takes the limits $V \to \infty$ and $\epsilon \to 0$, expands the resulting expression in powers of λ, and neglects all terms proportional to λ^i with $i > -1$. This, of course, gives both the λ^{-2} (lowest order) and λ^{-1} contributions from $X(\alpha\beta)$.

Statements similar to the above also apply to (3.15) with ${}^nY(\alpha\beta\sigma) = \lambda^{-1}[{}^nY^\circ(\alpha\beta\sigma) + \cdots]$. The λ^{-1} (lowest-order) contribution to the limiting value of K^{ij} from $Y(\alpha\beta\sigma)$ is determined with (3.15a). [Note: (3.14a), (3.14b), and (3.15a) are given in unabbreviated notation by (4.2), (4.9), and (4.11).]

The Expansion of $\tilde{Z}_\epsilon$

The expansion of $\tilde{Z}_\epsilon$ for $\beta \neq \sigma$ and $\alpha \neq \gamma$ has still to be found; it is easily obtained by a straightforward expansion of the resolvent operators. From (2.13) and (2.18) it follows that

$$\langle\gamma|\,R_{i'}\,|\sigma\rangle\langle\beta|\,R_i\,|\alpha\rangle = \frac{\delta_{\gamma\sigma}}{\mathcal{E}(\gamma) - E - \frac{1}{2}i\hbar\epsilon}\,\frac{\delta_{\beta\alpha}}{\mathcal{E}(\alpha) - E + \frac{1}{2}i\hbar\epsilon} + O(\lambda). \tag{3.17}$$

Performing the integration over E specified in (2.17d) by finding the residue of the pole at $E = \mathcal{E}(\alpha) + \frac{1}{2}i\hbar\epsilon$, one obtains

$$\tilde{Z}_\epsilon(\gamma\sigma\beta\alpha) = \frac{i\hbar\delta_{\gamma\sigma}\delta_{\beta\alpha}}{\mathcal{E}(\alpha) - \mathcal{E}(\gamma) + i\hbar\epsilon} + O(\lambda). \tag{3.18}$$

This result can also be obtained by iterating the

identity in footnote 18 to obtain a series in powers of λ, using the result to expand the integrand of (2.5), and then performing the integration over t.

Note that all four types of $\tilde{Z}_\epsilon$ given in (2.17) cannot be expanded directly as type (d) was above. If one treats type (a) where $\beta = \sigma$ and $\alpha = \gamma$ as above, one obtains $\mathcal{E}(\alpha) - \mathcal{E}(\alpha) + i\hbar\epsilon = i\hbar\epsilon$ in (3.18), so that the first term is proportional to ϵ^{-1} With types (b) and (c) the first term in (3.18) vanishes, but the second ($\propto\lambda$) term becomes proportional to ϵ^{-1}. Since ϵ^{-1} increases without bound as ϵ decreases, such series are not usuable. In contrast, (3.18) for type (d) becomes a (δ_+ or) ζ-function[20] in the limits $\epsilon \to 0$ and $V \to \infty$.

The integrations over E specified in Eqs. (2.17) do not affect the λ-dependence, so that the λ-dependence of $\tilde{Z}_\epsilon$ of types (a)–(c), is the same as that of $X(\alpha\beta)$ and $Y(\alpha\gamma\sigma)$. Consequently, the contributions of $\tilde{Z}_\epsilon$ to the λ-dependence of K^{ij} (in the limit $\epsilon \to 0$) are as follows:

$$\text{(a) } \tilde{Z}_\epsilon(\alpha\beta\beta\alpha) = \lambda^{-2}[\tilde{Z}_\epsilon^\circ + \lambda\tilde{Z}_\epsilon' + \cdots]; \tag{3.19a}$$

$$\text{(b) } \tilde{Z}_\epsilon(\alpha\sigma\beta\alpha) = \lambda^{-1}[\tilde{Z}_\epsilon^\circ + \cdots] \quad [\beta \neq \sigma]; \tag{3.19b}$$

$$\text{(c) } \tilde{Z}_\epsilon(\gamma\beta\beta\alpha) = \lambda^{-1}[\tilde{Z}_\epsilon^\circ + \cdots] \quad [\alpha \neq \gamma]; \tag{3.19c}$$

$$\text{(d) } \tilde{Z}_\epsilon(\gamma\sigma\beta\alpha) = \tilde{Z}_\epsilon^\circ + \lambda\tilde{Z}_\epsilon' + \cdots \quad [\beta \neq \sigma;\ \alpha \neq \gamma]. \tag{3.19d}$$

4. CONCLUSIONS

The necessary information is now available for writing down all of the λ^{-2} and λ^{-1} contributions to the lattice thermal conductivity.

The λ^{-2} Contribution to K^{ij}

From (3.19) for $\tilde{Z}_\epsilon$ and from (2.8) for f_0, it follows that $\gamma = \alpha$, $\sigma = \beta$, and $\mu = \alpha$ in the λ^{-2} part of (2.4). Substituting the first terms of the expansions of f_0, $\mathbf{S}$, and $\tilde{Z}_\epsilon$ into (2.4) and using (2.17a), one obtains

$$K^{ij} = \frac{V}{kT^2}\sum_{\alpha\beta}\langle\alpha|\, f_0^\circ\,|\alpha\rangle\langle\alpha|\, S^{\circ i}\,|\alpha\rangle\langle\beta|\, S^{\circ j}\,|\beta\rangle \times \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dE\, {}^0X_{E,\epsilon}(\alpha\beta), \tag{4.1}$$

where ${}^0X_{E,\epsilon}(\alpha\beta)$ represents the lowest order approximation to $X(\alpha\beta)$, which is determined by (3.14a). In unabbreviated notation (3.14a) is [combine (3.14a), (3.8), (B3), and (B4)]

$$(\hbar\epsilon/2\pi)\,{}^0X_{E,\epsilon}(\alpha\beta) - \delta_\epsilon(\mathcal{E}(\alpha) - E)\delta_{\alpha\beta} = \sum_\mu |\langle\alpha|\,\lambda H'\,|\mu\rangle|^2\,[\delta_\epsilon(\mathcal{E}(\alpha) - E)\,{}^0X_{E,\epsilon}(\mu\beta) - \delta_\epsilon(\mathcal{E}(\mu) - E)\,{}^0X_{E,\epsilon}(\alpha\beta)], \tag{4.2}$$

where $|\langle\alpha|\,\lambda H'\,|\mu\rangle|^2 = |\langle\mu|\,\lambda H'\,|\alpha\rangle|^2$ has been used, and where $\delta_\epsilon(x)$ is defined by

$$\pi\delta_\epsilon(x) \equiv \tfrac{1}{2}\hbar\epsilon[x^2 + (\tfrac{1}{2}\hbar\epsilon)^2]^{-1}. \tag{4.3}$$

$\delta_\epsilon(x)$ becomes a Dirac δ-function in the limit $\epsilon \to 0$. f_0° and $\langle\alpha|\,\mathbf{S}^\circ\,|\alpha\rangle$ (the subscript d is omitted here) are given by (2.8) and (2.11). The above are the formulas for determining the lowest order contribution to the lattice thermal conductivity.[21]

The λ^{-1} Contributions to K^{ij}

This contribution is obtained by combining terms from the expansions of f_0, S^i, S^j, and $\tilde{Z}_\epsilon$ [see (2.7), (2.10), and Sec. 3] so that the resulting contribution to K^{ij} is proportional to λ^{-1}. There are six such contributions.

First, consider those contributions with $\tilde{Z}_\epsilon \propto \lambda^{-2}$. For these, one has $\gamma = \alpha$ and $\sigma = \beta$ in (2.4). There are three contributions of this type:

$$K_1^{ij} = \frac{V}{kT^2}\sum_{\alpha\beta}\langle\alpha|f_0^\circ|\alpha\rangle\langle\alpha|S^{\circ i}|\alpha\rangle\langle\beta|\lambda S'^j|\beta\rangle \times \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dE\, {}^0X_{E,\epsilon}(\alpha\beta), \tag{4.4}$$

$$K_2^{ij} = \frac{V}{kT^2}\sum_{\alpha\beta}\langle\alpha|f_0^\circ|\alpha\rangle\langle\alpha|\lambda S'^i|\alpha\rangle\langle\beta|S^{\circ j}|\beta\rangle \times \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dE\, {}^0X_{E,\epsilon}(\alpha\beta), \tag{4.5}$$

and the contribution containing the diagonal part of $\lambda f_0' S^{0i}$:

$$K_3^{ij} = \frac{V}{kT^2}\,\mathrm{Re}\sum_{\alpha\beta\mu}\langle\alpha|\,\lambda f_0'\,|\mu\rangle\langle\mu|S^\circ{}_{nd}{}^i|\alpha\rangle\langle\beta|S^{\circ j}|\beta\rangle \times \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dE\, {}^0X_{E,\epsilon}(\alpha\beta). \tag{4.6}$$

$\lambda f_0'$ is defined in (2.9); the nondiagonal $\mathbf{S}^\circ{}_{nd}$ occurs here since $\langle\alpha|\,\lambda f_0'\,|\alpha\rangle = 0$. The quantity ${}^0X_{E,\epsilon}$ is the solution of (4.2); the detailed forms of $\lambda\mathbf{S}'$ and $\mathbf{S}^\circ{}_{nd}$ are given in Ref. 1.

[20] W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, London, 1954), pp. 69–71.

[21] If one uses the plus sign in the $S^i(\pm t)$ from (1.1) in writing (2.4) and (2.5), the roles of z and z' in the exponential in (2.14) and of the l and l' in (2.17) are interchanged. This, in turn, implies the replacement of ${}^nX_{E,\epsilon}(\alpha\beta)$ by ${}^nX_{E,\epsilon}(\beta\alpha)$ and of ${}^0Y_{E,\pm\epsilon}(\alpha\beta\sigma)$ by ${}^0Y_{E,\mp\epsilon}(\alpha\beta\sigma)$ [these are defined below (4.1), (4.8), and (4.10)]. Thus, by using the $+t$ instead of the $-t$ from (1.1), the ${}^nX_{E,\epsilon}(\alpha\beta)$ in (4.1), (4.4), (4.5), (4.6), and (4.10) can be replaced by ${}^nX_{E,\epsilon}(\beta\alpha)$ with the ${}^0Y_{E,\pm\epsilon}(\alpha\beta\sigma)$ in (4.7) and (4.8) being replaced by ${}^0Y_{E,\mp\epsilon}(\alpha\beta\sigma)$ without changing the value of K^{ij}.

Next, consider the contributions with $\tilde{Z}_\epsilon \propto \lambda^{-1}$ and depending on $Y_{E,\pm\epsilon}(\alpha\beta\sigma)$ through (2.17b) and (2.17c). There are two contributions of this type:

$$K_4^{ij} = \frac{V}{kT^2}\,\mathrm{Re}\sum_{\alpha\beta\sigma}\langle\alpha|f_0^\circ|\alpha\rangle\,\langle\alpha|S^{\circ i}|\alpha\rangle\,\langle\sigma|S^\circ{}_{nd}{}^j|\beta\rangle \times\frac{\hbar}{2\pi}\int_{-\infty}^{\infty}dE\,{}^0Y_{E,+\epsilon}(\alpha\beta\sigma); \quad (4.7)$$

$$K_5^{ij} = \frac{V}{kT^2}\,\mathrm{Re}\sum_{\alpha\beta\gamma}\langle\alpha|f_0^\circ|\alpha\rangle\,\langle\alpha|S^\circ{}_{nd}{}^i|\gamma\rangle\langle\beta|S^{\circ j}|\beta\rangle \times\frac{\hbar}{2\pi}\int_{-\infty}^{\infty}dE\,{}^0Y_{E,-\epsilon}(\beta\gamma\alpha). \quad (4.8)$$

Here, ${}^0Y_{E,+\epsilon}$ and ${}^0Y_{E,-\epsilon}$ represent the lowest order approximations to $Y_{ll'}$ and $Y_{l'l}$, respectively, where $l = E - \frac{1}{2}i\hbar\epsilon$ and $l' = E + \frac{1}{2}i\hbar\epsilon$. This lowest-order approximation is determined by (3.15a) which in unabbreviated notation is [combine (3.15a), (3.8), (B3), (B4), and (B5)]

$$\begin{aligned}&(\hbar\epsilon/2\pi)\,{}^0Y_{E,\pm\epsilon}(\alpha\gamma\sigma) - \delta_\epsilon(\mathcal{E}(\alpha) - E)\,\lambda V^\circ_{E,\pm\epsilon}(\alpha\gamma\sigma)\\ &= \sum_\mu |\langle\alpha|\,\lambda H'\,|\mu\rangle|^2\,[\delta_\epsilon(\mathcal{E}(\alpha) - E)\,{}^0Y_{E,\pm\epsilon}(\mu\gamma\sigma)\\ &\quad - \delta_\epsilon(\mathcal{E}(\mu) - E)\,{}^0Y_{E,\pm\epsilon}(\alpha\gamma\sigma)],\end{aligned} \quad (4.9)$$

where $\lambda V^\circ_{E,\pm\epsilon}$ is given by (B7).

The remaining λ^{-1} contribution to K^{ij} comes from ${}^1X(\alpha\beta)$ and is

$$K_6^{ij} = \frac{V}{kT^2}\sum_{\alpha\beta}\langle\alpha|f_0^\circ|\alpha\rangle\,\langle\alpha|S^{\circ i}|\alpha\rangle\,\langle\beta|S^{\circ j}|\beta\rangle \times\frac{\hbar}{2\pi}\int_{-\infty}^{\infty}dE\,{}^1X_{E,\epsilon}(\alpha\beta), \quad (4.10)$$

where ${}^1X_{E,\epsilon}(\alpha\beta)$ is the solution of (3.14b). In unabbreviated notiation (3.14b) is [combine (3.14b), (3.8), (B3), and (B4)]

$$\begin{aligned}&(\hbar\epsilon/2\pi)\,{}^1X_{E,\epsilon}(\alpha\beta) - \delta_\epsilon(\mathcal{E}(\alpha) - E)\,\delta_{\alpha\beta}\\ &= \sum_\mu [|\langle\alpha|\,\lambda H'\,|\mu\rangle|^2 - \lambda^3 F_{E,\epsilon}(\alpha\mu)]\\ &\quad\times\delta_\epsilon(\mathcal{E}(\alpha) - E)\,{}^1X_{E,\epsilon}(\mu\beta)\\ &\quad - \sum_\mu [|\langle\mu|\,\lambda H'\,|\alpha\rangle|^2 - \lambda^3 F_{E,\epsilon}(\mu\alpha)]\\ &\quad\times\delta_\epsilon(\mathcal{E}(\mu) - E)\,{}^1X_{E,\epsilon}(\alpha\beta),\end{aligned} \quad (4.11)$$

where $\lambda^3 F_{E,\epsilon}(\alpha\mu)$ is defined by (B6). As discussed in Sec. 3, the contribution to the thermal conductivity involving ${}^1X(\alpha\beta)$ (in this case K_6^{ij}) is to be expanded in powers of λ after the limits $V \to \infty$ and $\epsilon \to 0$ have been taken. (The limit $V \to \infty$ must be taken first so that the arguments of the δ_ϵ-functions depend on a continuous variable, the wave vector, which is integrated over. Then, in the limit $\epsilon \to 0$ the δ_ϵ-functions become Dirac δ-functions.) The lowest-order term in this expansion of K_6^{ij} will be the λ^{-2} approximation determined by (4.1) and (4.2); the next term will be the sixth λ^{-1} contribution to K^{ij}; the remaining terms will have no significance.

Discussion

The formulas for the λ^{-2} contribution to K^{ij} lead to equations for the thermal conductivity that are equivalent to those of kinetic therory[2], i.e., the Boltzmann equation and

$$\mathbf{s}(\mathbf{x}) = V^{-1}\sum_{\mathbf{k}s} n_{\mathbf{k}s}\hbar\omega_{\mathbf{k}s}\mathbf{v}_{\mathbf{k}s}.$$

The equations for the λ^{-1} contributions give corrections that can be expressed as modifications to the Boltzmann equation.[3] Also, with the formulation presented above one can determine the relative importance of various corrections to the lowest order results without carrying out detailed calculations. For example: the correction to energy flux labeled $\lambda\mathbf{S}_3'$ in Ref. 1 is nondiagonal in the H°-representation so that the evaluation of its contribution requires the use of $\tilde{Z}_\epsilon(\alpha\sigma\beta\alpha)$ and $\tilde{Z}_\epsilon(\gamma\beta\beta\alpha)$ [see Sec. 2.], which according to (3.19b) and (3.19c) are of order λ^{-1} and higher; then, since $\lambda\mathbf{S}_3'$ is proportional to λ, the lowest-order correction to K^{ij} due to $\lambda\mathbf{S}_3'$ is of order λ^0. The effect of a correction to the flux analogous to $\lambda\mathbf{S}_3'$ has been considered by Henin and Blum,[22] who, it appears, missed the several corrections of order λ^{-1} given above.

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APPENDIX A: DERIVATION OF (3.1)

The essentials of the derivation of (3.1) are more clearly seen if one temporarily omits all indication of the subscripts l and l' and introduces the following abbreviations:

$$\bar{D}(\alpha) = D_l(\alpha)D_{l'}(\alpha);\ \bar{U}(\alpha\beta) = U_l(\beta\alpha)U_{l'}(\alpha\beta). \quad (A1)$$

[22] F. Henin and L. Blum, Bull. Classe Sci. Acad. Roy. Belg. 46, 862 (1960).

Then, the substitution of (3.4) into (2.15), the definition of $X(\alpha\beta)$, gives

$$X(\alpha\beta) = \bar{D}(\alpha)\delta_{\alpha\beta} + \bar{D}(\alpha)\bar{U}(\alpha\beta)\bar{D}(\beta). \quad \text{(A2)}$$

Equation (3.3) becomes

$$W(\alpha\mu) = \bar{U}(\alpha\mu) - \sum_{\gamma} W(\alpha\gamma)\bar{D}(\gamma)\bar{U}(\gamma\mu). \quad \text{(A3)}$$

And, it follows from (2.13), (2.15), and (3.2) that

$$\begin{aligned} F(\alpha) &= \langle\alpha|\ (H - l)^{-1} - (H - l')^{-1}\ |\alpha\rangle \\ &= (l - l')\langle\alpha|\ (H - l')^{-1}(H - l)^{-1}\ |\alpha\rangle \\ &= (l - l')\sum_{\beta} X(\alpha\beta). \end{aligned} \quad \text{(A4)}$$

Multiplying (A2) by $W(\gamma\alpha)$, summing over α, and using (A3), one obtains

$$\sum_{\alpha} W(\gamma\alpha)X(\alpha\beta) = \bar{U}(\gamma\beta)\bar{D}(\beta). \quad \text{(A5)}$$

The substitution of this into (A2) gives

$$X(\alpha\beta) = \bar{D}(\alpha)[\delta_{\alpha\beta} + \sum_{\mu} W(\alpha\mu)X(\mu\beta)]. \quad \text{(A6)}$$

Summing this over β and utilizing (A4), one finds

$$F(\alpha) = \bar{D}(\alpha)[(l - l') + \sum_{\mu} W(\alpha\mu)F(\mu)]. \quad \text{(A7)}$$

Then, the multiplication of (A6) by $[(l - l') + \sum_{\mu} W(\alpha\mu)F(\mu)]$ with the aid of (A7) gives

$$\begin{aligned} (l - l')X(\alpha\beta) - F(\alpha)\delta_{\alpha\beta} &= \sum_{\mu} F(\alpha)W(\alpha\mu)X(\mu\beta) \\ &\quad - \sum_{\mu} W(\alpha\mu)F(\mu)X(\alpha\beta). \end{aligned} \quad \text{(A8)}$$

By using (A1) and indicating subscripts, (A7) becomes

$$F_{ll'}(\alpha) = D_l(\alpha)D_{l'}(\alpha)[(l - l') + \sum_{\mu} W_{ll'}(\alpha\mu)F_{ll'}(\mu)]. \quad \text{(A9)}$$

Exchanging l and l' in this and using $F_{ll'}(\alpha) = -F_{l'l}(\alpha)$ [which follows from (3.2)] and $W_{ll'}(\alpha\beta) = W_{l'l}(\beta\alpha)$ [which can be shown by iterating (3.3)],[16] one obtains

$$-F_{ll'}(\alpha) = D_{l'}(\alpha)D_l(\alpha)\cdot[(l' - l) - \sum_{\mu} W_{ll'}(\mu\alpha)F_{ll'}(\mu)]. \quad \text{(A10)}$$

The addition of (A9) and (A10) yields

$$\sum_{\mu} W_{ll'}(\alpha\mu)F_{ll'}(\mu) = \sum_{\gamma} W_{ll'}(\mu\alpha)F_{ll'}(\mu). \quad \text{(A11)}$$

Then, by writing out (A8) with subscripts indicated and using (A11) to alter the last term on its right, one obtains the desired result: (3.1).

APPENDIX B: $F_{ll'}$, $W_{ll'}$, AND $V_{ll'}$

It is a simple consequence of definitions (2.13) and (3.4) [see Swenson,[16] Eqs. (14), (15), and (16)] that

$$D_l(\alpha) = (\mathcal{E}(\alpha) - l)^{-1} + O(\lambda^2); \quad \text{(B1)}$$

$$\begin{aligned} U_l(\beta\alpha) &= -\langle\beta|\ \lambda H'\ |\alpha\rangle \\ &\quad + \sum_{\nu} \langle\beta|\ \lambda H'\ |\nu\rangle\ [\mathcal{E}(\nu) - l]^{-1}\ \langle\nu|\ \lambda H'\ |\alpha\rangle \\ &\quad + O(\lambda^3) \qquad [\alpha \neq \beta]. \end{aligned} \quad \text{(B2)}$$

From these, (3.2), and the iteration of (3.3) and (3.7), it follows that:

$$F_{E\mp\frac{1}{2}i\hbar\epsilon, E\pm\frac{1}{2}i\hbar\epsilon}(\alpha) = \mp 2\pi i\delta_{\epsilon}(\mathcal{E}(\alpha) - E) + O(\lambda^2); \quad \text{(B3)}$$

$$W_{E\mp\frac{1}{2}i\hbar\epsilon, E\pm\frac{1}{2}i\hbar\epsilon}(\alpha\mu) = |\langle\alpha|\ \lambda H'\ |\mu\rangle|^2 - \lambda^3 F_{E,\pm\epsilon}(\alpha\mu) + O(\lambda^4); \quad \text{(B4)}$$

$$V_{E\mp\frac{1}{2}i\hbar\epsilon, E\pm\frac{1}{2}i\hbar\epsilon}(\alpha\gamma\sigma) = \lambda V^{\circ}_{E,\pm\epsilon}(\alpha\gamma\sigma) + O(\lambda^3). \quad \text{(B5)}$$

$\delta_{\epsilon}(x)$ is defined by (4.3) and $\lambda^3 F_{E,\pm\epsilon}(\alpha\mu)$ and $\lambda V_{E,\pm\epsilon}$ are defined by

$$\lambda^3 F_{E,\pm\epsilon}(\alpha\mu) = \sum_{\nu} \frac{\langle\mu|\ \lambda H'\ |\alpha\rangle\langle\alpha|\ \lambda H'\ |\nu\rangle\langle\nu|\ \lambda H'\ |\mu\rangle}{\mathcal{E}(\nu) - E \mp \frac{1}{2}i\hbar\epsilon} + \text{c.c.}, \quad \text{(B6)}$$

where +c.c. indicates that the complex conjugate is to be added, and

$$\lambda V^{\circ}_{E,\pm\epsilon}(\alpha\gamma\sigma) = -\langle\gamma|\ \lambda H'\ |\sigma\rangle \times \left[\frac{\delta_{\alpha\gamma}}{\mathcal{E}(\sigma) - E \mp i\hbar\epsilon} + \frac{\delta_{\alpha\sigma}}{\mathcal{E}(\gamma) - E \pm i\hbar\epsilon}\right]. \quad \text{(B7)}$$

Lowest-Order Contribution to the Lattice Thermal Conductivity*

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In a previous paper the correlation function formula for the thermal conductivity was used to derive equations for the lowest-order contribution to the lattice thermal conductivity K^{ij}. An explicit but formal solution of these equations is obtained here, and it is shown how this solution simplifies in the limit of infinite volume. Transport equations equivalent to the familiar Boltzmann equation are derived for perturbations describing both anharmonic forces and lattice imperfections. No approximations are made beyond the restriction to lowest order in the perturbation. It is demonstrated that K^{ij} is symmetric.

1. INTRODUCTION

In previous papers the energy flux operator for a lattice with imperfections and anharmonic forces was derived[1], and the formulas for determining the λ^{-2} and λ^{-1} contributions to the lattice thermal conductivity K^{ij} were obtained[2]: λ characterizes the strength of the interaction between the normal modes of a perfect, harmonic lattice. Here, the formulas for the lowest order, or λ^{-2}, contribution to K^{ij} are used to derive the transport equations for lattice thermal conductivity. The methods used are similar to those employed by McLennan and Swenson[3] in their analysis of the thermal conductivity of a low-density gas.

The transport[4], or Boltzmann, equations for lattice thermal conductivity were first derived by Peierls[5] by using arguments of the kinetic-theory type. Since its presentation, this approach has been extensively applied and discussed, but its theoretical basis has changed little[6]; review articles on the subject have been written by, to mention a few, Carruthers,[7] Klemens,[8] and Leibfried.[9] In kinetic theory it is assumed that "the number of phonons per mode changes for two reasons: (1) collisions of phonons with each other and impurities; (2) transport of phonons due to the presence of a temperature gradient."[10] Although these assumptions arise from a plausible physical picture, they are nevertheless *ad hoc* and are difficult to incorporate consistently into a mathematical formulation, particularly due to the necessity of having "localized phonons" in order to describe the spatial variations of the temperature. Furthermore, the usual treatment of change (1) depends on arguments that are equivalent to assuming the Pauli equation (7.3) which in turn depends on several assumptions not required here, e.g., "random phases at initial time," "course grained distribution functions," etc.[11] In treating charge (1), one must also assume "factorization," i.e., that the nonequilibrium average of a product of occupation numbers can be written as a product of their averages. In most discussions "factorization" is assumed without comment; however, its justification is a problem of fundamental importance and has given rise to extensive discussion in the Boltzmann equation treatment of gases.

None of the above-mentioned assumptions, including "factorization," are required in the treatment of lattice thermal conductivity given here. The transport equations follow as a direct mathe-

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[4] Here, "Boltzmann equation" refers only to the kinetic theory equations for determining what is interpreted as the deviation of the number of phonons per mode from the equilibrium value, while "transport equation" is used to refer to any equation having a similar form; e.g., compare the "transport equation" (2.21) with the "Boltzmann equation" (2.22a).

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[7] P. Carruthers, Rev. Mod. Phys. **33**, 92 (1961).

[8] P. G. Klemens in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. XIV, pp. 198–281; and in *Solid State Physics*, edited by S. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 7, pp. 1–98.

[9] G. Leibfried in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1955), Vol. VII 1, pp. 293–316.

[10] P. Carruthers, Ref. 9. pp. 101–102.

[11] See, e. g., L. Van Hove in *The Theory of Neutral and Ionized Gases* edited by C. De Witt and J. Detoeuf (John Wiley & Sons, Inc., New York, 1960), pp. 151–183.

metical consequence of the correlation function formula for the thermal conductivity, the assumption of a Hamiltonian, and the decision to consider only the contribution to K^{ij} which is lowest order in λ in the limits $V \to \infty$ and $\epsilon \to 0$ (V is the volume of the system; ϵ comes in through a convergence factor $e^{-\epsilon t}$, where t is time). The correlation function formula itself is a general result derived from basic assumptions about the meaning of thermal conductivity; its use avoids any problems with localization.

The essentials of the present derivation are contained in Sec. 2 and the first parts of Sec. 3; most of the remainder of the article deals with calculations for specific perturbations.

In Sec. 2 an explicit solution for the lowest-order contribution to K^{ij} is obtained from the formulas in Ref. 2. The limits $V \to \infty$ and $\epsilon \to 0$ are then taken, and the solution is written as

$$\lim_{\epsilon \to 0} \lim_{V \to \infty} K^{ij} = V^{-1} \sum_k \eta_k^i \hbar \omega_k v_k^i, \tag{1.1}$$

where ω_k and v_k^i are the frequency and group velocity of mode k ($V^{-1} \sum_k$ is an integral in this limit). It is shown that the quantity η_k^i is determined by a transport equation. The relation of η_k^i to the kinetic-theory quantity $\hat{n}_k$ is discussed, where $\hat{n}_k$ is the deviation of the number of phonons in mode k from the equilibrium value. It is shown that the thermal conductivities predicted by kinetic theory and by the present approach are the same.

In Sec. 3 the detailed form of the transport equation for anharmonic forces is deduced, and the critical role of the limits $V \to \infty$ and $\epsilon \to 0$ in obtaining it is made clear. The form of the transport equation which results most naturally is more symmetric than the usual Boltzmann equation [see (3.37)]; however, it is shown that a transport equation with the form of the usual result is also possible [see (3.38)]. The additional information needed to treat imperfection scattering is given in Sec. 4. In Sec. 5 the generalization to systems with both imperfections and anharmonic forces is discussed. The symmetry of the tensor K^{ij} is proved in Sec. 6.

Notation

Before proceeding, the notation to be employed and some necessary standard results will be summarized:

The Hamiltonian for the system is

$$H = H^\circ + \lambda H', \tag{1.2}$$

where H° is the harmonic Hamiltonian for a perfect lattice. The eigenvalues and eigenvectors of H° are represented by $\mathcal{E}(\gamma)$ and $|\gamma\rangle$, where the Greek letters designate eigenstates: $H^\circ|\gamma\rangle = \mathcal{E}(\gamma)|\gamma\rangle$, where $\mathcal{E}(\gamma) \equiv \sum_k [N_k(\gamma) + \frac{1}{2}]\hbar\omega_k$ and $N_k(\gamma)$ and ω_k are, respectively, the occupation number and frequency of mode k. Subscripts j, k, l, etc., designate the plane-wave normal modes of H°; in particular, k stands for $\mathbf{k}$ and s where $\mathbf{k}$ is the wave vector and s is the polarization index ($s = 1, 2, 3$). The specification of the occupation numbers for every mode completely determines the eigenstate, and conversely:

$$|\gamma\rangle = |N_{k_1}(\gamma), N_{k_2}(\gamma), \cdots\rangle. \tag{1.3}$$

Let $\mathfrak{N}$ be the number of particles in the system. $V/\mathfrak{N}$ is the volume of a unit cell of the lattice, which is constant; thus, the limit $V \to \infty$ implies the limit $\mathfrak{N} \to \infty$.

The perturbation to be considered is $\lambda H' = \lambda T' + \lambda V_2 + \lambda V_3$. The perturbation to the kinetic energy due to the presence of more than one isotope, etc. is $\lambda T'$; the perturbation to the potential energy due to lattice imperfections is λV_2. Their sum has the form[12]

$$\lambda T' + \lambda V_2 = \sum_{jk} c_{j-k} a_j a_k^\dagger + \tfrac{1}{2} \sum_{jk} c_{jk}{}^* (a_j a_k + a_{-j}^\dagger a_{-k}^\dagger), \tag{1.4}$$

where $a_k^\dagger$ and a_k are, respectively, the creation and annihilation operators for phonons.[13] The coefficients c_{jk} are such that

$$|c_{j-k}|^2 = |c_{-jk}|^2 = |c_{k-j}|^2 \propto V^{-1}. \tag{1.5}$$

In Ref. 1 (p. 124) it was shown that the separation (1.2) can always be made so that $c_{k-k} = 0$. The perturbation due to anharmonic forces is[12]

$$\lambda V_3 = \frac{1}{3!} \sum_{jkl} b_{jkl} [3(a_j a_{-k}^\dagger a_{-l}^\dagger - a_{-j}^\dagger a_k a_l) + (a_j a_k a_l - a_{-j}^\dagger a_{-k}^\dagger a_{-l}^\dagger)], \tag{1.6}$$

where $k = (\mathbf{k}, s)$ and $-k = (-\mathbf{k}, s)$. To obtain (1.6) the condition $b_{jk-k} = b_{jk-j} = b_{j-jk} = 0$ was imposed for all values of j and k: Since this condition affects only one out of every $\mathfrak{N}$ of the coefficients b_{jkl}, any error introduced by it vanishes when the limit $V \to \infty$ is taken. Because of the symmetry of the lattice, b_{jkl} is proportional to $\Delta_{\mathbf{j}+\mathbf{k}+\mathbf{l}}$, which equals one when $\mathbf{j} + \mathbf{k} + \mathbf{l}$ equals zero or a member of the reciprocal lattice and which is zero otherwise. The dependence

[12] In Ref. 1 (p. 173) $\lambda T'$, λV_2 and λV_3 are given as functions of the particle momentum and position operators. For more details about the coefficients in $\lambda T'$, λV_2 and λV_3 see: Carruthers, Ref. 10; M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, London, 1954), pp. 217–223.

[13] The commutation relation is $[a_j, a_k^\dagger] = \delta_{jk}$.

of b_{jkl} on V is such that

$$|b_{j_s,k_{s'},l_{s''}}|^2 \propto V^{-1}\Delta_{j+k+l}. \tag{1.7}$$

λV_3 is Hermitian and b_{jkl} is independent of the order of j, k, and l; as a result

$$|b_{-j-k-l}|^2 = |b_{jkl}|^2 = |b_{kjl}|^2 = |b_{klj}|^2. \tag{1.8}$$

$\mathbf{S}(\alpha)$ represents the diagonal part of the lowest-order contribution to the energy flux:

$$\mathbf{S}(\alpha) = V^{-1}\sum_k N_k(\alpha)\hbar\omega_k\mathbf{v}_k. \tag{1.9}$$

where $\mathbf{v}_k$ is the group velocity of mode k. Note that

$$\mathbf{v}_k = -\mathbf{v}_{-k} \quad \text{and} \quad \omega_k = \omega_{-k} \geq 0. \tag{1.10}$$

Because of this, the frequencies will be written without a sign before their subscripts. The symbol $f(\alpha)$ designates the lowest-order contribution to the density matrix, which is diagonal:

$$f(\alpha) = [Z^\circ]^{-1}\exp[-\mathcal{E}(\alpha)/kT], \tag{1.11}$$

where $Z^\circ = \sum_\alpha \exp[-\mathcal{E}(\alpha)/kT]$. Averages formed with $f(\alpha)$ will be indicated by $\langle\ \rangle_0$, e.g.,

$$\sum_\alpha f(\alpha)N_k(\alpha) \equiv \langle N_k\rangle_0 = [\exp(\hbar\omega_k/kT) - 1]^{-1}. \tag{1.12}$$

Since $\omega_k = \omega_{-k}$, the averages $\langle\cdots N_jN_k\cdots\rangle_0$ of a number of occupation numbers are independent of the signs before the subscripts; consequently, such signs will often be omitted. If all of the occupation numbers except perhaps two (k and k') belong to different modes, one has

$$\begin{aligned}&\langle\cdots N_jN_kN_{k'}N_l\cdots\rangle_0\\ &= [\cdots\langle N_j\rangle_0\langle N_k\rangle_0\langle N_{k'}\rangle_0\langle N_l\rangle_0\cdots]\\ &+ \delta_{kk'}[\cdots\langle N_j\rangle_0\langle N_{k'}\rangle_0(\langle N_{k'}\rangle_0 + 1)\langle N_l\rangle_0\cdots].\end{aligned} \tag{1.13}$$

Also, it can be shown that

$$\sum_j \langle N_kN_j\rangle_0\hbar\omega_j\mathbf{v}_j = \tfrac{1}{4}\mathfrak{s}_k^{-2}\hbar\omega_k\mathbf{v}_k = kT^2[d\langle N_k\rangle_0/dT]\mathbf{v}_k = \mathfrak{v}_k, \tag{1.14}$$

where this defines $\mathfrak{v}_k$ and where

$$\mathfrak{s}_k = \sinh(\hbar\omega_k/2kT). \tag{1.15}$$

2. LATTICE THERMAL CONDUCTIVITY

In this section an explicit, formal solution of the lowest order equations for the thermal conductivity is obtained and is expressed in the form of a transport equation. The lowest order equations from Ref. 2 [(4.1) and (4.2)] are

$$K^{ij} = \frac{V}{kT^2}\sum_{\alpha\beta} f(\alpha)S^i(\alpha)S^j(\beta)\frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dE\,{}^0X_{E,\epsilon}(\alpha\beta), \tag{2.1}$$

where (1.9) and (1.11) have been used (the superscripts $i, j = 1, 2, 3$ specify vector components), and

$$\begin{aligned}&(\hbar\epsilon/2\pi)\,{}^0X_{E,\epsilon}(\alpha\beta) - \delta_\epsilon(\mathcal{E}(\alpha) - E)\delta_{\alpha\beta}\\ &= \sum_\gamma |\langle\alpha|\ \lambda H'\ |\gamma\rangle|^2[\delta_\epsilon(\mathcal{E}(\alpha) - E)\,{}^0X_{E,\epsilon}(\gamma\beta)\\ &\quad - \delta_\epsilon(\mathcal{E}(\gamma) - E)\,{}^0X_{E,\epsilon}(\alpha\beta)],\end{aligned} \tag{2.2}$$

where ϵ is a small positive number and

$$\pi\delta_\epsilon(x) \equiv \tfrac{1}{2}\hbar\epsilon[x^2 + (\tfrac{1}{2}\hbar\epsilon)^2]^{-1}. \tag{2.3}$$

The Formal Solution for K^{ij}

It is convenient to introduce quantities $Q_{E,\epsilon}(\alpha\beta)$ and $\mathfrak{S}_{E,\epsilon}(\alpha)$ defined as follows:

$$(\hbar/2\pi)\,{}^0X_{E,\epsilon}(\alpha\beta) \equiv \delta_\epsilon(\mathcal{E}(\alpha) - E)\,Q_{E,\epsilon}(\alpha\beta); \tag{2.4}$$

$$\mathfrak{S}_{E,\epsilon}(\alpha) \equiv \sum_\beta Q_{E,\epsilon}(\alpha\beta)\mathbf{S}(\beta). \tag{2.5}$$

Then, by multiplying (2.2) by $\mathbf{S}(\beta)$, and summing over β one obtains

$$\begin{aligned}&-\mathbf{S}(\alpha) + \epsilon\mathfrak{S}_{E,\epsilon}(\alpha)\\ &= \frac{2\pi}{\hbar}\sum_\gamma |\langle\alpha|\ \lambda H'\ |\gamma\rangle|^2\delta_\epsilon(\mathcal{E}(\gamma) - E)\\ &\quad\times[\mathfrak{S}_{E,\epsilon}(\gamma) - \mathfrak{S}_{E,\epsilon}(\alpha)].\end{aligned} \tag{2.6}$$

This can also be expressed as

$$\mathbf{S}(\alpha) = \epsilon\mathfrak{S}_{E,\epsilon}(\alpha) - \sum_\gamma \langle\alpha|\ \bar{W}\ |\gamma\rangle\mathfrak{S}_{E,\epsilon}(\gamma), \tag{2.7}$$

where

$$\begin{aligned}\langle\alpha|\ \bar{W}\ |\gamma\rangle &\equiv (2\pi/\hbar)\{|\langle\alpha|\ \lambda H'\ |\gamma\rangle|^2\delta_\epsilon(\mathcal{E}(\gamma) - E)\\ &\quad - \delta_{\alpha\gamma}\sum_\mu |\langle\alpha|\ \lambda H'\ |\mu\rangle|^2\delta_\epsilon(\mathcal{E}(\mu) - E)\}.\end{aligned} \tag{2.8}$$

Now, multiply (2.7) by $e^{-\epsilon s}$ and by

$$\langle\beta|\exp[\bar{W}s]\ |\alpha\rangle \equiv \sum_{m=0}^{\infty}\frac{s^m}{m!}\langle\beta|\ \bar{W}^m\ |\alpha\rangle, \tag{2.9}$$

where $\langle\beta|\bar{W}^0|\alpha\rangle \equiv \delta_{\beta\alpha}$ and $\langle\beta|\bar{W}^m|\alpha\rangle$ is the product of m matrices $\langle\beta|\bar{W}|\alpha\rangle$. Then, by summing over α and integrating over s, one obtains

$$\begin{aligned}&\int_0^\infty ds\,e^{-\epsilon s}\sum_\alpha\langle\beta|\exp[\bar{W}s]\ |\alpha\rangle\mathbf{S}(\alpha)\\ &= -\int_0^\infty ds\sum_\gamma\{e^{-\epsilon s}\sum_\alpha\langle\beta|\exp[\bar{W}s]\ |\alpha\rangle\\ &\quad\times(-\epsilon\delta_{\alpha\gamma} + \langle\alpha|\ \bar{W}\ |\gamma\rangle)\}\mathfrak{S}_{E,\epsilon}(\gamma).\end{aligned} \tag{2.10}$$

Since the quantity inside the braces $\{\ \}$ is the derivative with respect to s of $e^{-\epsilon s}\langle\alpha|\ \exp\ [\bar{W}s]\ |\gamma\rangle$, Eq. (2.10) integrates to

$$\mathfrak{S}_{E,\epsilon}(\beta) = \int_0^\infty ds\, e^{-\epsilon s} \times \sum_\alpha \langle\beta|\ \exp\ [\bar{W}s]\ |\alpha\rangle \mathrm{S}(\alpha). \quad (2.11)$$

It is apparent from (2.1), (2.4), and (2.5) that

$$K^{ij} = \frac{V}{kT^2} \sum_\alpha f(\alpha) S^i(\alpha) \times \int_{-\infty}^\infty dE\ \delta_\epsilon(\mathcal{E}(\alpha) - E)\, \mathfrak{S}^j_{E,\epsilon}(\alpha). \quad (2.12)$$

This in conjunction with (2.11) gives K^{ij} as an explicit function of the interaction mechanism described by $\langle\alpha|\ \bar{W}\ |\gamma\rangle$.

The Effect of the Limits $V \to \infty$ and $\epsilon \to 0$

Before proceeding, introduce a quantity $\mathfrak{n}_{k'}$ (or $\eta^1_{k'}$ where $j = 1, 2, 3$) defined by

$$\mathfrak{n}_{k'} \equiv \lim_{\epsilon\to 0}\lim_{V\to\infty} \frac{V}{kT^2} \sum_{\alpha\gamma} f(\alpha) N_{k'}(\alpha) \int_{-\infty}^\infty dE \times \delta_\epsilon(\mathcal{E}(\alpha) - E) \int_0^\infty ds\, e^{-\epsilon s}\langle\alpha|\ \exp\ [\bar{W}s]\ |\gamma\rangle \mathrm{S}(\gamma). \quad (2.13)$$

From this, (1.9), (2.11), and (2.12), it follows that

$$\lim_{\epsilon\to 0}\lim_{V\to\infty} K^{ij} = V^{-1} \sum_{k'} \eta^i_{k'} \hbar\omega_{k'} v^j_{k'}. \quad (2.14)$$

One now needs the important result, which will be proved in Secs. 3–5, that the second member of the following can be written in the limits $V \to \infty$ and $\epsilon \to 0$ in the form of the third member (the first equality defines $\mathbf{W}^{(m)}{}_{k'}$):

$$\mathbf{W}^{(m)}{}_{k'} \equiv \lim_{\epsilon\to 0}\lim_{V\to\infty} e^{-\epsilon s} V \sum_{\alpha\gamma} f(\alpha) N_{k'}(\alpha) \times \int_{-\infty}^\infty dE\ \delta_\epsilon(\mathcal{E}(\alpha) - E)\, \langle\alpha|\ \bar{W}^m\ |\gamma\rangle\ \mathrm{S}(\gamma) = (-1)^m V^{-1} \sum_l \Omega^m{}_{k'l} \mathfrak{v}_l, \quad (2.15)$$

where $\Omega^0{}_{jk} \equiv V\delta_{jk}$ and where for $m > 0$

$$\Omega^m{}_{jk} = V^{1-m} \sum_{j_{m-1}} \cdots \sum_{j_1} \Omega_{jj_{m-1}} \cdots \Omega_{j_2 j_1} \Omega_{j_1 k}. \quad (2.16)$$

$\mathfrak{v}_l$ is defined by (1.14). Since the limit $V \to \infty$ has been taken, Ω_{jk} with $j = (\mathbf{j}, s)$ and $k = (\mathbf{k}, s')$ is a function of two discrete indices ($s, s' = 1, 2, 3$) and two continuously varying vectors $\mathbf{j}$ and $\mathbf{k}$. The density of wave vectors in k-space is $V(2\pi)^{-3}$; thus, as $V \to \infty$

$$V^{-1} \sum_k \to (2\pi)^{-3} \sum_s \int d\mathbf{k}, \quad (2.17a)$$

$$V\delta_{jk} \to (2\pi)^3 \delta_{ss'} \delta(\mathbf{j} - \mathbf{k}), \quad (2.17b)$$

and

$$V\Delta_{\mathbf{j}+\mathbf{k}+1} \to (2\pi)^3 \delta(\mathbf{j} + \mathbf{k} + 1 - \mathbf{K}), \quad (2.17c)$$

where $\delta(\mathbf{k})$ is a Dirac δ-function and $\mathbf{K}$ equals zero or a member of the reciprocal lattice. To obtain a convergent result in the limit $V \to \infty$, all factors of V, all summations over $\mathbf{k}$ space, and all Kronecker δ-functions and Δ-functions must occur in the combinations prescribed on the left of (2.17); if one or more factors of V is missing, the quantity involved will either trivially converge to zero or diverge. The notation on the left of (2.17) will be used in what follows; the integrals over k-space and the Dirac δ-functions will be left implicit.

The use of (2.15) in (2.13) yields

$$\mathfrak{n}_{k'} = (kT^2V)^{-1} \int_0^\infty ds \sum_l \{e^{-\Omega s}\}_{k'l} \mathfrak{v}_l \quad (2.18a)$$

where

$$\{e^{-\Omega s}\}_{kl} \equiv \sum_{m=0}^\infty \frac{(-s)^m}{m!} \Omega^m{}_{kl}. \quad (2.18b)$$

The Transport Equation

To obtain the transport equation, multiply (2.18a) by $\Omega_{jk'}$, sum over k', and perform the s-integration over the infinite series in powers of s; one finds

$$V^{-1} \sum_{k'} \Omega_{jk'} \mathfrak{n}_{k'} = \frac{1}{kT^2V} \sum_l [-\{e^{-\Omega s}\}_{jl} + V\delta_{jl}] \mathfrak{v}_l \Big|_0^\infty, \quad (2.19)$$

where $\Omega^0{}_{jl} \equiv V\ \delta_{jl}$ has been used. Now, provided that

$$\lim_{s\to\infty} V^{-1} \sum_l \{e^{-\Omega s}\}_{jl} \mathfrak{v}_l = 0, \quad (2.20)$$

Eq. (2.19) can be written with the aid of (1.14) as

$$[d\langle N_j\rangle_0/dT]\mathbf{v}_j = V^{-1} \sum_{k'} \Omega_{jk'} \mathfrak{n}_{k'}, \quad (2.21)$$

where $[d\ \langle N_j\rangle_0\ /dT]\mathbf{v}_j$ enters as simply a more meaningful way of writing $\mathfrak{v}_j/kT^2$. Equation (2.21) is the *transport equation* for $\mathfrak{n}_{k'}$; its solution in conjunction with (2.14) determines the lattice thermal conductivity. Condition (2.20) is discussed in Sec. 6.

Comparison with Kinetic Theory

In kinetic theory the lattice thermal conductivity is determined by the Boltzmann equation and the equation relating $\langle\mathbf{s}\rangle$ (the heat flux) to $\hat{n}_k$ (the devia-

tion of the average number of phonons in mode k from $\langle N_k\rangle_0$); these equations are, respectively,

$$[d\langle N_j\rangle_0/dT]\mathbf{v}_j\cdot\nabla T = -V^{-1}\sum_{k'}\tilde{\Omega}_{jk'}\hat{n}_{k'} \tag{2.22a}$$

and

$$\langle\mathbf{s}\rangle = V^{-1}\sum_k \hat{n}_k\hbar\omega_k\mathbf{v}_k. \tag{2.22b}$$

Equations (2.22) can be transformed into equations of the form of (2.21) and (2.14) by assuming that

$$\hat{n}_k = -\tilde{\mathbf{n}}_k\cdot\nabla T \tag{2.23a}$$

and

$$\langle s^i\rangle = -\sum_j K^{ij}\frac{\partial T}{\partial x^j}, \tag{2.23b}$$

where $\tilde{\mathbf{n}}_k$ and K^{ij} are independent of ∇T. Thus, provided $\tilde{\Omega}_{jk} = \Omega_{jk}$, the thermal conductivity determined by kinetic theory is simply the lowest-order contribution to K^{ij}. The equality $\tilde{\Omega}_{jk} = \Omega_{jk}$ is verified in Secs. 3–5.

3. PROOF OF (2.15): ANHARMONIC FORCES

The perturbation with anharmonic forces alone is $\lambda H' = \lambda V_3$.

The elements $\langle\alpha|\,\lambda V_3\,|\gamma\rangle$ vanish unless $N_k(\alpha) = N_k(\gamma)$ for all modes except three, say j', k', and l', for which

$$N_{j'}(\alpha) = N_{j'}(\gamma)\mp 1;\quad N_{k'}(\alpha) = N_{k'}(\gamma)\pm 1;$$
$$N_{l'}(\alpha) = N_{l'}(\gamma)\pm 1. \tag{3.1}$$

Then, from (1.6) it is apparent that the value of the element $\langle\alpha|\,\lambda V_3\,|\gamma\rangle$ with α and γ connected by the upper set of signs in (3.1) is

$$\tfrac{1}{2}(b_{j'-k'-l'} + b_{j'-l'-k'})$$
$$\times\{N_{j'}(\gamma)[N_{-k'}(\gamma)+1][N_{-l'}(\gamma)+1]\}^{\frac{1}{2}},$$

and since b_{jkl} is independent of the order of its subscripts, one has

$$\tfrac{1}{2}(b_{j'-k'-l'} + b_{j'-l'-k'}) = b_{j'-k'-l'}. \tag{3.2}$$

Similar results hold for the element with α and γ connected by the lower set of signs. Thus, with the aid of (1.8), the square of the magnitude of $\langle\alpha|\,\lambda V_3\,|\gamma\rangle$ for all α and γ can be written as

$$|\langle\alpha|\,\lambda V_3\,|\gamma\rangle|^2 = \tfrac{1}{2}\sum_{jkl}|b_{jkl}|^2$$
$$\times\{N_j(\gamma)[N_{-k}(\gamma)+1][N_{-l}(\gamma)+1]\langle\alpha|\,A_jA_{-k}^\dagger A_{-l}^\dagger\,|\gamma\rangle$$
$$+ [N_j(\gamma)+1]N_{-k}(\gamma)N_{-l}(\gamma)\langle\alpha|\,A_j^\dagger A_{-k}A_{-l}\,|\gamma\rangle\}$$
$$+ \text{parts with } A_jA_kA_l \text{ or } A_{-j}^\dagger A_{-k}^\dagger A_{-l}^\dagger, \tag{3.3}$$

where

$$\langle\cdots, N_k(\alpha), \cdots|A_k^\dagger|\cdots, N_k(\gamma), \cdots\rangle$$
$$\equiv \delta_{N_k(\alpha),N_k(\gamma)+1}\prod_{j(\neq k)}\delta_{N_j(\alpha),N_j(\gamma)} \tag{3.4a}$$

and

$$\langle\cdots, N_k(\alpha), \cdots|A_k|\cdots, N_k(\gamma), \cdots\rangle$$
$$\equiv \delta_{N_k(\alpha),N_k(\gamma)-1}\prod_{j(\neq k)}\delta_{N_j(\alpha),N_j(\gamma)}. \tag{3.4b}$$

Note that $A_k^\dagger = a_k^\dagger(N_k+1)^{-\frac{1}{2}}$ and $A_k = a_k(N_k)^{-\frac{1}{2}}$. The factor of $\frac{1}{2}$ in (3.3) compensates for the existence of two combinations of j, k, and l [i.e., j', $-k'$, $-l'$ and j', $-l'$, $-k'$] which contribute to $|\langle\alpha|\,\lambda V_3\,|\gamma\rangle|^2$ for each α and γ satisfying (3.1).

When $\lambda H' = \lambda V_3$, the quantity $\langle\alpha|\,\tilde{W}\,|\gamma\rangle$ defined by (2.8) will be represented by $\langle\alpha|\,\tilde{G}\,|\gamma\rangle$. Using the relations between $N_k(\alpha)$ and $N_k(\gamma)$ given in (3.4), one obtains

$$\langle\alpha|\,\tilde{G}\,|\gamma\rangle = \frac{\pi}{\hbar}\sum_{jkl}|b_{jkl}|^2$$
$$\times\{\delta_\epsilon(\hbar\omega_j - \hbar\omega_k - \hbar\omega_l + \mathcal{E}(\alpha) - E)$$
$$\times[N_j(\alpha)+1]N_{-k}(\alpha)N_{-l}(\alpha)$$
$$\times[\langle\alpha|\,A_jA_{-k}^\dagger A_{-l}^\dagger\,|\gamma\rangle - \delta_{\alpha\gamma}]$$
$$+ \delta_\epsilon(\hbar\omega_j - \hbar\omega_k - \hbar\omega_l - \mathcal{E}(\alpha) + E)$$
$$\times N_j(\alpha)[N_{-k}(\alpha)+1][N_{-l}(\alpha)+1]$$
$$\times[\langle\alpha|\,A_j^\dagger A_{-k}A_{-l}\,|\gamma\rangle - \delta_{\alpha\gamma}]\}$$

$+$ parts proportional to

$$\delta_\epsilon(\hbar\omega_j + \hbar\omega_k + \hbar\omega_l \pm \mathcal{E}(\alpha)\mp E). \tag{3.5}$$

The Effect of the Limits $V\to\infty$ and $\epsilon\to 0$

For anharmonic forces, the first two members of (2.15) will be written as

$$\mathbf{G}^{(m)}{}_{k'} \equiv \lim_{\epsilon\to 0}\lim_{V\to\infty} V\sum_{\alpha\gamma} f(\alpha)N_{k'}(\alpha)\int_{-\infty}^{\infty}dE'\,\delta_\epsilon(E')$$
$$\times\langle\alpha|\,\tilde{G}^m\,|\gamma\rangle\mathbf{S}(\gamma)|_{E=E'+\mathcal{E}(\alpha)}, \tag{3.6}$$

where the limits have been commuted with the $e^{-\epsilon s}$ specified in (2.15) and the substitution $E = E' + \mathcal{E}(\alpha)$ has been made. $\langle\alpha|\,\tilde{G}^0\,|\gamma\rangle$ equals $\delta_{\alpha\gamma}$ by definition; it then follows immediately from (1.9) and (1.14) that

$$\mathbf{G}^{(0)}{}_{k'} = \sum_k\langle N_{k'}N_k\rangle_0\hbar\omega_k\mathbf{v}_k = \mathfrak{v}_{k'}. \tag{3.7}$$

The general properties of $\mathbf{G}^{(m)}{}_{k'}$ which make possible its simplification can be seen be considering just $\mathbf{G}^{(2)}{}_{k'}$ and the contribution to it from the part of $\langle\alpha|\ \bar{G}\ |\gamma\rangle$ containing $[\langle\alpha|\ A_jA^\dagger_{-k}A^\dagger_{-l}\ |\gamma\rangle - \delta_{\alpha\gamma}]$. First consider the effect of $[\langle\alpha|\ A_jA^\dagger_{-k}A^\dagger_{-l}\ |\gamma\rangle - \delta_{\alpha\gamma}]$ on $\mathbf{S}(\gamma)$:

$$\sum_\gamma [\langle\alpha|\ A_jA^\dagger_{-k}A^\dagger_{-l}\ |\gamma\rangle - \delta_{\alpha\gamma}]V^{-1}\sum_{j'} N_{j'}(\gamma)\hbar\omega_{j'}\mathbf{v}_{j'}$$

$$= V^{-1}\sum_{j'}[(N_{j'}(\alpha) + \delta_{jj'} - \delta_{-kj'} - \delta_{-lj'}) - N_{j'}(\alpha)]\hbar\omega_{j'}\mathbf{v}_{j'} = \left(\frac{\partial}{\partial N_j(\alpha)} - \frac{\partial}{\partial N_{-k}(\alpha)} - \frac{\partial}{\partial N_{-l}(\alpha)}\right)\mathbf{S}(\alpha), \quad (3.8)$$

where the partial derivatives are included as simply an alternate notation. Now, by using (3.8) and the above mentioned part of $\langle\alpha|\ \bar{G}\ |\gamma\rangle$ [see (3.5)], one obtains the following contribution to $\mathbf{G}^{(2)}{}_{k'}$:

$$\lim_{\epsilon\to 0}\lim_{V\to\infty} V\int_{-\infty}^{\infty} dE'\ \delta_\epsilon(E')\sum_\alpha f(\alpha)N_{k'}(\alpha)\frac{\pi}{\hbar}\sum_{j_sk_sl_s}|b_{j_sk_sl_s}|^2\ \delta_\epsilon(\hbar\omega_{j_s} - \hbar\omega_{k_s} - \hbar\omega_{l_s} - E')$$
$$\times [N_{j_s}(\alpha) + 1]N_{-k_s}(\alpha)N_{-l_s}(\alpha)\sum_\beta [\langle\alpha|\ A_{j_s}A^\dagger_{-k_s}A^\dagger_{-l_s}\ |\beta\rangle - \delta_{\alpha\beta}]$$
$$\times\frac{\pi}{\hbar}\sum_{j_1k_1l_1}|b_{j_1k_1l_1}|^2\ \delta_\epsilon(\hbar\omega_{j_1} - \hbar\omega_{k_1} - \hbar\omega_{l_1} + \mathcal{E}(\beta) - \mathcal{E}(\alpha) - E')$$
$$\times [N_{j_1}(\beta) + 1]N_{-k_1}(\beta)N_{-l_1}(\beta)V^{-1}\hbar(\omega_{j_1}\mathbf{v}_{j_1} - \omega_{k_1}\mathbf{v}_{-k_1} + \omega_{l_1}\mathbf{v}_{-l_1}). \quad (3.9)$$

It is readily demonstrated that the sum over β here has the following effect:

$$\sum_\beta [\langle\alpha|\ A_{j_s}A^\dagger_{-k_s}A^\dagger_{-l_s}\ |\beta\rangle - \delta_{\alpha\beta}]\delta_\epsilon(\hbar\omega_{j_1} - \hbar\omega_{k_1} - \hbar\omega_{l_1} + \mathcal{E}(\beta) - \mathcal{E}(\alpha) - E')[N_{j_1}(\beta) + 1]N_{-k_1}(\beta)N_{-l_1}(\beta)$$
$$= \{\hbar^{-1}\ \delta_\epsilon(\omega_{j_s} - \omega_{k_s} - \omega_{l_s} + \omega_{j_1} - \omega_{k_1} - \omega_{l_1} - E'/\hbar)$$
$$\times [N_{j_1}(\alpha) + 1 + \delta_{j_sj_1} - \delta_{-k_sj_1} - \delta_{-l_sj_1}][N_{-k_1}(\alpha) + \delta_{j_s-k_1} - \delta_{k_sk_1} - \delta_{l_sk_1}]$$
$$\times [N_{-l_1}(\alpha) + \delta_{j_s-l_1} - \delta_{k_sl_1} - \delta_{l_sl_1}]\} - \{\hbar^{-1}\ \delta_\epsilon(\omega_{j_1} - \omega_{k_1} - \omega_{l_1} - E'/\hbar)[N_{j_1}(\alpha) + 1]N_{-k_s}(\alpha)N_{-l_s}(\alpha)\}. \quad (3.10)$$

Now, since the arguments of the δ_ϵ-functions in the second member of (3.10) do not depend on α, the only dependence on α of the result obtained by substituting (3.10) into (3.9) is in the occupation numbers and in $f(\alpha)$. Thus, the summation over α simply causes an averaging of the occupation numbers, so that the limit $V\to\infty$ can be taken without difficulty. The summations over the wave vectors $\mathbf{j}_1$, $\mathbf{k}_1$, $\mathbf{l}_1$, $\mathbf{j}_2$, $\mathbf{k}_2$, and $\mathbf{l}_2$ become integrations, and the arguments of the δ_ϵ-functions become continuous functions of $\mathbf{j}_1$, $\mathbf{k}_1$, etc. In this situation, the limit $\epsilon\to 0$ can be taken and the δ_ϵ-functions become Dirac δ-functions. The arguments of Dirac-δ's can be altered as follows:

$$\delta(x - x_1)\delta(x - x_2) = \delta(x - x_1)\delta(x_1 - x_2). \quad (3.11)$$

Then, using this and neglecting the parts of (3.10) which contain more than one Kronecker δ-function factor (this is justified below), one can rewrite (3.9) as

$$\frac{\pi}{\hbar^2}\sum_{j_sk_sl_s}|b_{j_sk_sl_s}|^2\delta(\omega_{j_s} - \omega_{k_s} - \omega_{l_s})\frac{\pi}{\hbar^2}\sum_{j_1k_1l_1}|b_{j_1k_1l_1}|^2\delta(\omega_{j_1} - \omega_{k_1} - \omega_{l_1})$$
$$\times\langle N_{k'}(N_{j_s} + 1)N_{-k_s}N_{-l_s}[(\delta_{j_sj_1} - \delta_{-k_sj_1} - \delta_{-l_sj_1})N_{-k_1}N_{-l_1}$$
$$+ (\delta_{j_s-k_1} - \delta_{k_sk_1} - \delta_{l_sk_1})(N_{j_1} + 1)N_{-l_1} + (\delta_{j_s-l_1} - \delta_{k_sl_1} - \delta_{l_sl_1})(N_{j_1} + 1)N_{-k_1}]\rangle_0$$
$$\times\hbar(\omega_{j_1}\mathbf{v}_{j_1} - \omega_{k_1}\mathbf{v}_{-k_1} - \omega_{l_1}\mathbf{v}_{-l_1}); \quad (3.12)$$

because of the $\delta_\epsilon(E')$ and $\delta_\epsilon(\hbar\omega_{j_s} - \hbar\omega_{k_s} - \hbar\omega_{l_s} + E')$ in (3.9), the $\delta_\epsilon(\omega_{j_s} - \omega_{k_s} - \omega_{l_s} + \omega_{j_1} - \omega_{k_1} - \omega_{l_1} - E'/\hbar)$ has become $\delta(\omega_{j_1} - \omega_{k_1} - \omega_{l_1})$ in (3.12).

From the definition of the average $\langle\ \rangle_0$, it follows that

$$\langle N_{k'}(\cdots N_j N_k \cdots)\rangle_0 = \langle N_{k'}(\cdots N_{-j} N_{-k} \cdots)\rangle_0, \quad (3.13)$$

provided that k' and $-k'$ are different from $\cdots j, k, \cdots$, etc., otherwise the two members of (3.13) are unequal. Because of this and since $\mathbf{v_k}$ is the only odd function of k in (3.12) [see (1.8) and (1.10)], each term in the sums in (3.12) with k' and $-k'$ different from any of the subscripts j_1, k_1, l_2, j_2, k_2, and l_2 is equal to the negative of the term with the subscripts $-j_1, -k_2, -l_2, -j_2, -k_2$, and $-l_2$; such terms cancel. Thus, only those terms for which k' or $-k'$ equals j_1, k_1, l_1, j_2, k_2, or l_2 contributes to $\mathbf{G}^{(2)}{}_{k'}$. This property in essence introduces another Kronecker δ-function factor into (3.12). Now, because of the factors V^{-1} and Δ_{j+k+l} in $|b_{jkl}|^2$ and of the various Kronecker δ-functions, (3.12) contains the correct number of factors of V for nontrivial convergence in the limit $V \to \infty$ [see (2.17) and below]. The contributions to (3.12) from those parts of (3.10) with more than one Kronecker-δ factor lack one or more factors of V for nontrivial convergence, and thus do not contribute to $\mathbf{G}^{(2)}{}_{k'}$. Note that the quantity in square brackets in (3.12) could also have been expressed as

$$\left(\frac{\partial}{\partial N_{j_1}} - \frac{\partial}{\partial N_{-k_2}} - \frac{\partial}{\partial N_{-l_1}}\right)(N_{j_1}+1)N_{-k_2}N_{-l_1}. \quad (3.14)$$

Three additional contributions similar to (3.12) exist in the complete expression for $\mathbf{G}^{(2)}{}_{k'}$. However, there are no contributions from the "parts proportional to $\delta_\epsilon(\hbar\omega_j + \hbar\omega_k + \hbar\omega_l \pm \mathcal{E}(\alpha) \mp E)$" in $\langle\alpha|\ \tilde{G}\ |\gamma\rangle$ [see (3.5)]. Their contributions vanish because in the limits $V \to \infty$ and $\epsilon \to 0$ the above δ_ϵ-functions become $\hbar^{-1}\delta(\omega_j+\omega_k+\omega_l)$. Since $\omega_k \geq 0$, this Dirac-δ vanishes unless $\omega_j = \omega_k = \omega_l = 0$ which implies (at least for the acoustic modes) that $\mathbf{j} = \mathbf{k} = \mathbf{l} = 0$; but when this is true $|b_{jkl}|^2$ vanishes.

Now, consider the generalization to $\mathbf{G}^{(m)}{}_{k'}$ with arbitrary m:

First, note that each additional $\langle\alpha|\ \tilde{G}\ |\gamma\rangle$ introduces: three additional summations over $\mathbf{k}$-space; one factor of V^{-1}; one Δ-function; and one Kronecker-δ factor which originates from the $[\langle\alpha|\ A_j A^\dagger_{-k} A^\dagger_{-l}\ |\gamma\rangle - \delta_{\alpha\gamma}]$, etc. As a result, $\mathbf{G}^{(m)}{}_{k'}$ will always have the correct number of factors of V for nontrivial convergence in the limit $V \to \infty$.

Second, each term in the expansion of $\mathbf{G}^{(m)}{}_{k'}$ contains a product of m δ_ϵ-functions. After performing the $m-1$ intermediate sums over eigenstates in $\langle\alpha|\ \tilde{G}^m\ |\gamma\rangle$, taking the limits $V \to \infty$ and $\epsilon \to 0$, and repeatedly using (3.11), these δ_ϵ-functions all become Dirac δ's of the form $\delta(\omega_j - \omega_k - \omega_l)$, just as in (3.12). Thus, *for the purpose evaluating* $\mathbf{G}^{(m)}{}_{k'}$ *one can replace the* δ_ϵ*-functions from the parts of* $\langle\alpha|\ \tilde{G}\ |\gamma\rangle$ *written out in* (3.5) *by* $\hbar^{-1}\delta(\omega_j - \omega_k - \omega_l)$. Since the δ_ϵ-function from the "parts proportional to $\delta_\epsilon(\hbar\omega_j + \hbar\omega_k + \hbar\omega_l \pm (\cdots))$" becomes $\hbar^{-1}\delta(\omega_j + \omega_k + \omega_l)$, and since $|b_{jkl}|^2$ vanishes when $\delta(\omega_j + \omega_k + \omega_l)$ is nonzero: only the parts of $\langle\alpha|\ \tilde{G}\ |\gamma\rangle$ written out in (3.5) contribute to $\mathbf{G}^{(m)}{}_{k'}$.

Third, the maximum number of factors of occupation numbers in any term in the expansion of $\mathbf{G}^{(m)}{}_{k'}$ is a function of m, say $f(m)$. The number of different normal modes of H° is $3\mathfrak{N}$. Neither the Δ-functions in $|b_{jkl}|^2$, which connect three wave vectors, nor the Kronecker δ's which arise in the evaluation of $\mathbf{G}^{(m)}{}_{k'}$ and which occur in place of occupation numbers as in, e.g., (3.10), favor combinations of occupation numbers in which more than one is from the same mode. Thus, there are $(3\mathfrak{N})^{f(m)}$ different possible combinations of modes to which $f(m)$ occupation numbers can belong. Of these combinations, the fraction which does *not* have every occupation number from a different mode is

$$\frac{(3\mathfrak{N})^{f(m)} - (3\mathfrak{N})(3\mathfrak{N}-1)\cdots(3\mathfrak{N}-f(m)+1)}{(3\mathfrak{N})^{f(m)}}. \quad (3.15)$$

In the limit $V \to \infty$ this is proportional to $\frac{1}{2}[f(m)-1]\, f(m)/3\mathfrak{N}$; this fraction will be smaller for those terms in the expansion of $\mathbf{G}^{(m)}{}_{k'}$ having fewer occupation numbers than $f(m)$. Because of the limit $V \to \infty$ which implies $\mathfrak{N} \to \infty$ any error made in the calculation of terms not having every occupation number from a different made does not affect the value of $\mathbf{G}^{(m)}{}_{k'}$. Thus, *the average of any product of occupation numbers in* $\mathbf{G}^{(m)}{}_{k'}$ *can be replaced by the product of the averages* [see (1.13)] *unless more than one of the occupation numbers is from mode* k'. This latter proviso is necessary because without it every term will cancel with some other term for the reasons discussed below (3.13) (More than one occupation number from any mode other than k' or $-k'$ will not prevent this cancellation).

Fourth, since the number of operators of the type A_k and $A^\dagger_k$ is fixed at $3m$, while the number of modes goes to infinity in the limit, the A_k and $A^\dagger_k$ may all be considered to be from different modes for the purpose of evaluating $\mathbf{G}^{(m)}{}_{k'}$. Now, if all modes $j, -k, -l$ are different, and if all modes $\cdots j', l', \cdots$ are also different, it can be shown that

$$\sum_\gamma [\langle\alpha|\ A_j A^\dagger_{-k} A^\dagger_{-l}\ |\gamma\rangle - \delta_{\alpha\gamma}][\cdots N_{j'}(\gamma) N_{l'}(\gamma) \cdots]$$
$$= \left[\frac{\partial}{\partial N_j} - \frac{\partial}{\partial N_{-k}} - \frac{\partial}{\partial N_{-l}}\right]$$

$$\times [\cdots N_{j'}, N_{l'}, \cdots]\Big|_{N_k=N_k(\alpha)}, \qquad (3.16)$$

where $[\cdots N_{j'}(\gamma)N_{l'}(\gamma)\cdots]$ represents any product of occupation numbers. If $A_j^\dagger A_{-k}A_{-l}$ is used in (3.16) instead of $A_jA_{-k}^\dagger A_{-l}^\dagger$, then the last member will differ by a factor of -1. Because of this, *the factors*

$$[\langle\alpha|\ A_jA_{-k}^\dagger A_{-l}^\dagger\ |\gamma\rangle - \delta_{\alpha\gamma}]$$

and $[\langle\alpha|\ A_j^\dagger A_{-k}A_{-l}\ |\gamma\rangle - \delta_{\alpha\gamma}]$ *in* $\langle\alpha|\ \bar{G}\ |\gamma\rangle$ *can be replaced in the calculation of* $\mathbf{G}^{(m)}{}_{k'}$ *by*

$$\frac{\partial}{\partial N_j} - \frac{\partial}{\partial N_{-k}} - \frac{\partial}{\partial N_{-l}}$$

and the negative of this, respectively. The writing out of the arguments α, γ, etc. of the occupation numbers no longer serves any useful purpose and henceforth will not be done.

Applying the several conclusions obtained above, one finds that (3.6) can be simplified to

$$G^{(m)}{}_{k'} = \lim_{\epsilon\to 0}\lim_{V\to\infty} V\sum_\alpha f(\alpha)N_{k'}(\alpha)$$
$$\times B_mP_mD_m\cdots B_2P_2D_2B_1P_1D_1\mathbf{S}|_{N_k=N_k(\alpha)}, \qquad (3.17)$$

where

$$B_i \equiv \frac{\pi}{\hbar^2}\sum_{j_ik_il_i}|b_{j_ik_il_i}|^2, \qquad (3.18)$$

$$P_i \equiv \delta_\epsilon(\omega_{j_i} - \omega_{k_i} - \omega_{l_i})\,[(N_{j_i}+1)N_{-k_i}N_{-l_i}$$
$$- N_{j_i}(N_{-k_i}+1)(N_{-l_i}+1)], \qquad (3.19)$$

and

$$D_i \equiv \frac{\partial}{\partial N_{j_i}} - \frac{\partial}{\partial N_{-k_i}} - \frac{\partial}{\partial N_{-l_i}}\,; \qquad (3.20)$$

it is understood that the summations over j_i, k_i, *and* l_i *in* B_i *are simultaneous summations over the* j_i, k_i, *and* l_i *in* P_i, *in* D_i, *and in* B_i. Every differential operator D_i in (3.17) operates on all of the P_i's to its right.

Proof of (2.15)

The application of the product rule for differentiation gives

$$B_nP_nD_nB_{n-1}P_{n-1}D_{n-1}\cdots\mathbf{S}$$
$$= B_nP_nB_{n-1}(D_nP_{n-1})D_{n-1}\cdots\mathbf{S}$$
$$+ B_nP_nB_{n-1}P_{n-1}(D_nD_{n-1}\cdots\mathbf{S}), \qquad (3.21)$$

where the D's inside the parenthesis operate only on those P's within the same parenthesis. The successive use of (3.21) in (3.17) yields

$$\mathbf{G}^{(m)}{}_{k'} = \lim_{\epsilon\to 0}\lim_{V\to\infty} V$$
$$\times [\langle N_{k'}B_mP_mB_{m-1}(D_mP_{m-1})$$
$$\times B_{m-2}(D_{m-1}P_{m-2})\cdots B_1(D_2P_1)(D_1\mathbf{S})\rangle_0$$
$$+ \langle N_{k'}B_mP_mB_{m-1}P_{m-1}(D_mD_{m-1}\cdots B_1P_1D_1\mathbf{S})\rangle_0$$
$$+ \langle N_{k'}B_mP_mB_{m-1}(D_mP_{m-1})$$
$$\times B_{m-2}P_{m-2}(D_{m-1}D_{m-2}\cdots\mathbf{S})\rangle_0$$
$$+\cdots$$
$$+ \langle N_{k'}B_mP_mB_{m-1}(D_mP_{m-1})\cdots B_1P_1(D_2D_1\mathbf{S})\rangle_0]. \qquad (3.22)$$

Note that all of the m averages within the square brackets, except the first and last, contain two factors of P not operated on by a D.

Using the properties of Dirac δ-functions, one can prove that

$$\delta(\omega_j - \omega_k - \omega_l)\,[\langle N_k\rangle_0\langle N_l\rangle_0$$
$$- \langle N_j\rangle_0(\langle N_k\rangle_0 + \langle N_l\rangle_0 + 1)] = 0, \qquad (3.23a)$$

$$\delta(\omega_j - \omega_k - \omega_l)(\langle N_k\rangle_0 + \langle N_l\rangle_0 + 1)$$
$$= \delta(\omega_j - \omega_k - \omega_l)\,\mathfrak{s}_j^2/2\mathfrak{s}_j\mathfrak{s}_k\mathfrak{s}_l, \qquad (3.23b)$$

and

$$\delta(\omega_j - \omega_k - \omega_l)(\langle N_l\rangle_0 - \langle N_j\rangle_0)$$
$$= \delta(\omega_j - \omega_k - \omega_l)\,\mathfrak{s}_k^2/2\mathfrak{s}_j\mathfrak{s}_k\mathfrak{s}_l; \qquad (3.23c)$$

$\mathfrak{s}_k$ is defined by (1.15). From these and (1.13), it follows that

$$\lim_{\epsilon\to 0}\lim_{V\to\infty}\langle N_{k'}P\rangle_0 = -\langle N_{k'}\rangle_0(\langle N_{k'}\rangle_0 + 1)$$
$$\times(\delta_{k'j} - \delta_{k'-k} - \delta_{k'-l})\,(\mathfrak{s}_{k'}^2/2\mathfrak{s}_j\mathfrak{s}_k\mathfrak{s}_l)$$
$$\times\delta(\omega_j - \omega_k - \omega_l) \qquad (3.24)$$

and

$$\lim_{\epsilon\to 0}\lim_{V\to\infty}\langle P\rangle_0 = 0, \qquad (3.25)$$

Since the average of a product of occupation numbers, unless two are from mode k', may be replaced in $\mathbf{G}^{(m)}{}_{k'}$ by the product of their averages, i.e., (1.13) may be used, the evaluation of (3.22) yields at least one factor of $\langle P\rangle_0$ in each of the averages having two P's not operated on by a D. Then, because of (3.25), all but the first and last of the averages in the square brackets in (3.22) vanish; the last average vanishes because it contains the second derivative of a linear function, i.e., $\mathbf{S}$. Thus, (3.22) can be simplified to

$$\mathbf{G}^{(m)}{}_{k'} = \lim_{\epsilon\to 0}\lim_{V\to\infty} VB_m\langle N_{k'}P_m\rangle_0B_{m-1}\langle D_mP_{m-1}\rangle_0$$
$$\times B_{m-2}\cdots B_1\langle D_2P_1\rangle_0(D_1\mathbf{S}), \qquad (3.26)$$

where it is understood that the D's only operate on the P within the same bracket.

The various quantities in (3.26) are readily evaluated. First, it follows from (1.9) and (3.20) that

$$(D_1\mathbf{S}) = V^{-1}\sum_j(\delta_{j_1j} + \delta_{k_1j} + \delta_{l_1j})4\mathfrak{s}_j^2\mathfrak{v}_j, \qquad (3.27)$$

where (1.14) has been used. Note that $(D_1\mathbf{S})$ has the following properties under transformations of its free subscripts j_1, k_1, and l_1 (this defines J_{jkl}):

$$-J_{-j-k-l} = J_{jkl} = J_{kjl} = J_{jlk}. \tag{3.28}$$

It follows from (3.18), (3.19), and (3.20) that

$$\begin{aligned} B\langle D'P\rangle_0 = &-\frac{\pi}{\hbar^2}\sum_{jkl}|b_{jkl}|^2\delta_\epsilon(\omega_j-\omega_k-\omega_l)\\ &\times[(\delta_{j'j}-\delta_{-k'j}-\delta_{-l'j})(\langle N_k\rangle_0+\langle N_l\rangle_0+1)\\ &+(\delta_{j'-k}-\delta_{k'k}-\delta_{l'k})(\langle N_j\rangle_0-\langle N_l\rangle_0)\\ &+(\delta_{j'-l}-\delta_{k'l}-\delta_{l'l})(\langle N_j\rangle_0-\langle N_k\rangle_0)]. \end{aligned} \tag{3.29}$$

Let J denote J_{jkl}; then, using (1.8), (3.23), and (3.28), one obtains

$$\begin{aligned} &\lim_{\epsilon\to 0}\lim_{V\to\infty} B\langle D'P\rangle_0 J\\ &\quad=(-1)V^{-1}\sum_j(\delta_{j'j}+\delta_{k'j}+\delta_{l'j})\mathfrak{s}_j^2\sum_{kl}\mathfrak{B}_{jkl}J_{jkl}, \end{aligned} \tag{3.30}$$

where

$$\begin{aligned} \mathfrak{B}_{jkl} = &(\pi/2\hbar^2)V\,|b_{jkl}|^2(\mathfrak{s}_j\mathfrak{s}_k\mathfrak{s}_l)^{-1}\\ &\times[\delta(\omega_j-\omega_k-\omega_l)+\delta(\omega_k-\omega_l-\omega_j)\\ &\qquad+\delta(\omega_l-\omega_j-\omega_k)]. \end{aligned} \tag{3.31}$$

$\mathfrak{B}_{jkl}$ is independent of the order of its subscripts and is such that $\mathfrak{B}_{jkl}\geq 0$. Note that $B\,\langle D'P\rangle_0\,J$ changes under transformations of its free subscripts j', k', and l' according to (3.28). Consequently, (3.30) not only determines the $B_1\langle D_2P_1\rangle_0$ in (3.26) correctly, but can also be used to evaluate the quantities $B_i\,\langle D_{i+1}P_i\rangle_0$ for all value of i.

It can be shown that

$$\langle N_{k'}\rangle_0\,(\langle N_{k'}\rangle_0+1)=\tfrac{1}{4}\mathfrak{s}_{k'}^{-2}. \tag{3.32}$$

From this, (3.24) and (3.28) it follows that

$$\begin{aligned} &\lim_{\epsilon\to 0}\lim_{V\to\infty} VB_m\langle N_{k'}P_m\rangle_0 J_m\\ &\qquad=-\tfrac{1}{4}\sum_{k_ml_m}\mathfrak{B}_{k'k_ml_m}J_{jmk_ml_m}. \end{aligned} \tag{3.33}$$

The substitutions of (3.27), (3.30), and (3.33) into (3.26) yield

$$\begin{aligned} \mathbf{G}^{(m)}{}_{k'} = &-\tfrac{1}{4}\sum_{k_ml_m}\mathfrak{B}_{k'k_ml_m}\\ &\times(-1)V^{-1}\sum_{j_{m-1}}(\delta_{j_mj_{m-1}}+\delta_{k_mj_{m-1}}\delta_{l_mj_{m-1}})\mathfrak{s}_{j_{m-1}}^2\\ &\qquad\times\sum_{k_{m-1}l_{m-1}}\mathfrak{B}_{j_{m-1}k_{m-1}l_{m-1}}\\ &\times\cdots\\ &\times(-1)V^{-1}\sum_{j_1}(\delta_{j_2j_1}+\delta_{k_2j_1}+\delta_{l_2j_1})\mathfrak{s}_{j_1}^2\sum_{k_1l_1}\mathfrak{B}_{j_1k_1l_1}\\ &\times V^{-1}\sum_j(\delta_{j_1j}+\delta_{k_1j}+\delta_{l_1j})4\mathfrak{s}_j^2\mathfrak{v}_j. \end{aligned} \tag{3.34}$$

Regrouping the various parts of this, one obtains

$$\mathbf{G}^{(m)}{}_{k'}=(-1)^mV^{-1}\sum_l\Gamma^m{}_{k'l}\mathfrak{v}_l, \tag{3.35}$$

where

$$\Gamma_{jk'}\equiv\sum_{kl}\mathfrak{B}_{jkl}(\delta_{jk'}+\delta_{kk'}+\delta_{lk'})\mathfrak{s}_{k'}^2; \tag{3.36}$$

from (3.7) it is apparent that $\Gamma^0{}_{k'l}=V\delta_{k'l}$. Compare (3.35) with (2.15). One sees when the perturbation is due to anharmonic forces alone that (2.15) is indeed valid and that $\Omega_{jk}=\Gamma_{jk}$.

The Transport Equation; Comparison with Kinetic Theory

The use of (3.31) and (3.36) in (2.21) gives

$$\begin{aligned} [d\langle N_j\rangle_0/dT]\nabla_j = &\frac{\pi}{2\hbar^2}\sum_{kl}|b_{jkl}|^2\,(\mathfrak{s}_j\mathfrak{s}_k\mathfrak{s}_l)^{-1}\\ &\times[\delta(\omega_j-\omega_k-\omega_l)+\delta(\omega_k-\omega_l-\omega_j)\\ &\qquad+\delta(\omega_l-\omega_j-\omega_k)]\\ &\times(\mathbf{n}_j\mathfrak{s}_j^2+\mathbf{n}_j\mathfrak{s}_j^2+\mathbf{n}_l\mathfrak{s}_l^2). \end{aligned} \tag{3.37}$$

This is the *transport equation* for anharmonic forces.

Equation (3.37) does not have the form of the Boltzmann equation from kinetic theory. However, (3.34) does not uniquely determine the form of Γ_{jk}. For example, instead of Γ_{jk} one could have used the quantity defined by

$$\begin{aligned} \tilde{\Gamma}_{jk'} = &\frac{\pi}{2\hbar^2}\sum_{kl}V\,|b_{jkl}|^2(\mathfrak{s}_j\mathfrak{s}_k\mathfrak{s}_l)^{-1}\\ &\times[\delta(\omega_j-\omega_k-\omega_l)(\delta_{jk'}-\delta_{-kk'}-\delta_{-lk'})\\ &+\delta(\omega_k-\omega_l-\omega_j)(\delta_{jk'}-\delta_{-kk'}+\delta_{lk'})\\ &+\delta(\omega_l-\omega_j-\omega_k)(\delta_{jk'}+\delta_{kk'}-\delta_{-lk'})]\mathfrak{s}_{k'}^2. \end{aligned} \tag{3.38}$$

One can verify that $\tilde{\Gamma}_{jk'}$ is consistent with (3.34) and (3.35) by using $\mathfrak{v}_j=-\mathfrak{v}_{-j}$ and the following readily demonstrated relation:

$$V^{-1}\sum_k\Gamma_{jk}f_k=V^{-1}\sum_k\tilde{\Gamma}_{jk}f_k, \tag{3.39}$$

where f_k is any odd function of k, i.e., $f_k=-f_{-k}$; note that both sides of (3.39) are odd functions of their free subscript j. When $\tilde{\Gamma}_{jk}$ is used in (2.21) instead of Γ_{jk}, the resulting transport equation does have the usual form of the Boltzmann equation from kinetic theory.[14]

The value of K^{ij}, as determined by (2.14), is only sensitive to the odd part of $\mathbf{n}_k$, i.e., to $\frac{1}{2}(\mathbf{n}_k-\mathbf{n}_{-k})$. By using the transport equation (2.21), the

[14] See Leibfried (Ref. 9), Eqs. (90.1), (90.5), and (93.6).

easily verified relations $\Gamma_{jk} = \Gamma_{-j-k}$ and $\tilde{\Gamma}_{jk} = \tilde{\Gamma}_{-j-k}$, and $\mathbf{v}_j = -\mathbf{v}_{-j}$, one can show that

$$[d\langle N_j\rangle_0/dT]\mathbf{v}_j = V^{-1}\sum_k \Gamma_{jk}\tfrac{1}{2}(\mathbf{n}_k - \mathbf{n}_{-k}) \tag{3.40}$$

and similarly for $\tilde{\Gamma}_{jk}$. Thus, the odd part of any solution to the transport equation is also a solution. Furthermore: because of (3.39), the odd part of any solution of the transport equation with Γ_{jk} is a solution of the transport equation with $\tilde{\Gamma}_{jk}$, and vice versa. Hence, to the extent that the odd part of the solution is unique, both Γ_{jk} and $\tilde{\Gamma}_{jk}$ predict the same lattice thermal conductivity. This uniqueness has not been proved. However, for it not to be unique, a solution to the homogeneous part of (2.21) when $\Omega_{jk} = \Gamma_{jk}$ with an odd part must exist. No such solution is known (the subject of solutions to the homogeneous part of the transport equation is discussed briefly in Sec. 6).

4. PROOF OF (2.15): IMPERFECTIONS

The perturbation describing the effect of imperfections is $\lambda H' = \lambda T' + \lambda V_2$; the proof of (2.15) with this perturbation proceeds through the same steps as the proof for $\lambda H' = \lambda V_3$. It follows from (1.4) that

$$\begin{aligned}&|\langle\alpha|\,\lambda T' + \lambda V_2\,|\gamma\rangle|^2\\ &= \sum_{jk}|c_{j-k}|^2\,N_j(\gamma)[N_k(\gamma)+1]\langle\alpha|\,A_jA_k^\dagger\,|\gamma\rangle\\ &\qquad + \text{parts with } A_jA_k \text{ or } A_{-j}^\dagger A_{-k}^\dagger.\end{aligned} \tag{4.1}$$

With imperfections alone, $\langle\alpha|\,\bar{W}\,|\gamma\rangle$ *will be represented by* $\langle\alpha|\,\bar{L}\,|\gamma\rangle$. Using (1.5), (2.8), and (3.4), one obtains

$$\begin{aligned}&\langle\alpha|\,\bar{L}\,|\gamma\rangle = \frac{\pi}{\hbar}\sum_{jk}|c_{j-k}|^2\\ &\times\{\delta_\epsilon(\hbar\omega_j - \hbar\omega_k + \mathcal{E}(\alpha) - E)[N_j(\alpha)+1]N_k(\alpha)\\ &\qquad\times[\langle\alpha|\,A_jA_k^\dagger\,|\gamma\rangle - \delta_{\alpha\gamma}]\\ &+\delta_\epsilon(\hbar\omega_j - \hbar\omega_k - \mathcal{E}(\alpha) + E)N_j(\alpha)[N_k(\alpha)+1]\\ &\qquad\times[\langle\alpha|\,A_j^\dagger A_k\,|\gamma\rangle - \delta_{\alpha\gamma}]\}\\ &+\text{parts proportional to } \delta_\epsilon(\hbar\omega_j + \hbar\omega_{k\epsilon} \pm\mathcal{E}(\alpha) \mp E).\end{aligned} \tag{4.2}$$

The quantity of interest here is

$$\begin{aligned}\mathbf{L}^{(m)}{}_{k'} \equiv \lim_{\epsilon\to0}\lim_{V\to\infty} V\sum_{\alpha\gamma} f(\alpha)N_{k'}(\alpha)\int_{-\infty}^{\infty}dE'\,\delta_\epsilon(E')\\ \times\langle\alpha|\,\bar{L}^m\,|\gamma\rangle\mathbf{S}(\gamma)\big|_{E=E'+\mathcal{E}(\alpha)}.\end{aligned} \tag{4.3}$$

Then, using arguments exactly analogous to those given to obtain (3.17)–(3.20), one can show that the effect of the limits $V\to\infty$ and $\epsilon\to0$ makes it possible to express $\mathbf{L}^{(m)}{}_{k'}$ as

$$\begin{aligned}\mathbf{L}^{(m)}{}_{k'} = \lim_{\epsilon\to0}\lim_{V\to\infty} V\sum_\alpha f(\alpha)N_{k'}(\alpha)\\ \times C_mQ_mE_m\cdots C_2Q_2E_2C_1Q_1E_1\mathbf{S}|_{N_k=N_k(\alpha)},\end{aligned} \tag{4.4}$$

where

$$C_i \equiv \frac{\pi}{\hbar^2}\sum_{j_ik_i}|c_{j_i-k_i}|^2, \tag{4.5}$$

$$Q_i \equiv \delta_\epsilon(\omega_{j_i} - \omega_{k_i})[(N_{j_i}+1)N_{k_i} - N_{j_i}(N_{k_i}+1)], \tag{4.6}$$

and

$$E_i \equiv \partial/\partial N_{j_i} - \partial/\partial N_{k_i}; \tag{4.7}$$

the summation symbol in C_i *implies the simultaneous summation over the* j_i *and* k_i *in* Q_i, E_i, *and* C_i.

With the aid of (1.13) it can be shown that

$$\begin{aligned}\lim_{\epsilon\to0}\lim_{V\to\infty}\langle N_{k'}Q\rangle_0 = \langle N_{k'}\rangle_0(\langle N_{k'}\rangle_0+1)\\ \times(\delta_{k'k} - \delta_{k'j})\delta(\omega_j - \omega_k)\end{aligned} \tag{4.8}$$

and

$$\lim_{\epsilon\to0}\lim_{V\to\infty}\langle Q\rangle_0 = 0\,. \tag{4.9}$$

Using these results—the product rule for differentiation, and the fact that the average of a product of occupation numbers, unless two are from mode k', may be replaced in $\mathbf{L}^{(m)}{}_{k'}$ by the product of their averages—one can rewrite (4.4) as

$$\begin{aligned}\mathbf{L}^{(m)}{}_{k'} = \lim_{\epsilon\to0}\lim_{V\to\infty} VC_m\langle N_{k'}Q_m\rangle_0C_{m-1}\langle E_mQ_{m-1}\rangle_0\\ \times C_{m-2}\cdots C_1\langle E_2Q_1\rangle_0(E_1S).\end{aligned} \tag{4.10}$$

It is readily demonstrated that

$$(E_1\mathbf{S}) = V^{-1}\sum_j(\delta_{j_1j} - \delta_{k_1j})4\mathfrak{s}_j^2\mathfrak{v}_j. \tag{4.11}$$

From $\mathfrak{v}_j = -\mathfrak{v}_j$ it is apparent that $(E_1\mathbf{S})$ changes under transformations of its free subscripts j_1 and k_1 according to (this defines K_{jk})

$$-K_{-j_1-k_1} = K_{j_1k_1} = -K_{k_1j_1}. \tag{4.12}$$

Let K denote K_{jk}; then, it follows from (1.5), (4.5)–(4.7), and (4.12) that

$$\begin{aligned}C\langle E'Q\rangle_0K = (-1)V^{-1}\sum_j(\delta_{j'j} - \delta_{k'j})\mathfrak{s}_j^2\mathfrak{s}_j^{-2}\\ \times\frac{2\pi}{\hbar^2}\sum_k V|c_{j-k}|^2\,\delta_\epsilon(\omega_j - \omega_k)K_{jk},\end{aligned} \tag{4.13}$$

where factors of V and $\mathfrak{s}_j^2$ have been multiplied in

and divided out. Since (4.13) changes under transformations of j' and k' according to (4.12), Eq. (4.13) not only determines the $C_1\langle E_2Q_1\rangle_0$ in (4.10) correctly, but can also be used to evaluate the quantities $C_i\langle E_{i+1}Q_i\rangle_0$ for all values of i. Finally, by combining (4.5), (4.8), and (4.12), one can show that

$$\lim_{\epsilon\to 0}\lim_{V\to\infty} VC_m\langle N_{k'}Q_m\rangle_0 K_m = -\tfrac{1}{4}\mathfrak{s}_{k'}^{-2}\frac{2\pi V}{\hbar^2}\sum_{km}|c_{k'-km}|^2\,\delta(\omega_{k'}-\omega_{km})K_{k'km}. \quad (4.14)$$

The substitutions of (4.11), (4.13), and (4.14) into (4.10) yields

$$\begin{aligned}\mathbf{L}^{(m)}{}_{k'} &= -\tfrac{1}{4}\mathfrak{s}_{k'}^{-2}\frac{2\pi}{\hbar^2}\sum_{km} V\,|c_{k'-km}|^2\delta(\omega_{k'}-\omega_{km})\\ &\times(-1)V^{-1}\sum_{j_{m-1}}(\delta_{k'j_{m-1}}-\delta_{kmj_{m-1}})\mathfrak{s}_{j_{m-1}}^2\mathfrak{s}_{j_{m-1}}^{-2}\frac{2\pi}{\hbar^2}\sum_{km-1} V\,|c_{j_{m-1}-km-1}|^2\delta(\omega_{j_{m-1}}-\omega_{km-1})\\ &\times\cdots\\ &\times(-1)V^{-1}\sum_{j_1}(\delta_{j_2j_1}-\delta_{k_2j_1})\mathfrak{s}_{j_1}^2\mathfrak{s}_{j_1}^{-2}\frac{2\pi}{\hbar^2}\sum_{k_1} V\,|c_{j_1-k_1}|^2\,\delta(\omega_{j_1}-\omega_{k_1})\\ &\times V^{-1}\sum_j(\delta_{j_1j}-\delta_{k_1j})4\mathfrak{s}_j^2\mathfrak{v}_j. \end{aligned} \quad (4.15)$$

The various parts of this can be regrouped to give

$$\mathbf{L}^{(m)}{}_{k'} = (-1)^m V^{-1}\sum_i \Lambda^m{}_{k'i}\mathfrak{v}_i, \quad (4.16)$$

where

$$\Lambda_{jk'} \equiv \mathfrak{s}_j^{-2}\frac{2\pi}{\hbar^2}\sum_k V\,|c_{j-k}|^2\,\delta(\omega_j-\omega_k)(\delta_{jk'}-\delta_{kk'})\mathfrak{s}_{k'}^2. \quad (4.17)$$

Comparing (4.16) with (2.15), one sees that (2.15) is indeed valid when the perturbation is $\lambda H' = \lambda T' + \lambda V_2$. In this case $\Omega_{jk} = \Gamma_{jk}$, and the *transport equation* (2.21) becomes

$$[d\langle N_j\rangle_0/dT]\mathfrak{v}_j = \frac{2\pi}{\hbar^2}\sum_k |c_{j-k}|^2\,\delta(\omega_j-\omega_k)(\mathfrak{n}_j-\mathfrak{n}_k), \quad (4.18)$$

where the factors of $\mathfrak{s}_j^{-2}$ and $\mathfrak{s}_k^2$ cancel because of the Dirac δ. Equation (4.18) has the same form as the corresponding Boltzmann equation from kinetic theory.[15]

5. PROOF OF (2.15): $\lambda H' = \lambda T' + \lambda V_2 + \lambda V_3$

In general, the perturbation to the harmonic Hamiltonian includes contributions both from anharmonic forces and from imperfections. Here, the additional information necessary to prove (2.15) when $\lambda H' = \lambda T' + \lambda V_2 + \lambda V_3$ is given.

Since $\lambda T' + \lambda V_2$ is a quadratic function of the creation and annihilation operators for phonons while λV_3 is a cubic function, there are no states α and γ for which both $\langle\alpha|\,\lambda T' + \lambda V_2\,|\gamma\rangle$ and $\langle\alpha|\,\lambda V_3\,|\gamma\rangle$ are nonzero; hence,

$$|\langle\alpha|\,\lambda T' + \lambda V_2 + \lambda V_3\,|\gamma\rangle|^2 = |\langle\alpha|\,\lambda V_3\,|\gamma\rangle|^2 + \langle\alpha|\,\lambda T' + \lambda V_2\,|\gamma\rangle|^2. \quad (5.1)$$

The use of this in definition (2.8) for $\langle\alpha|\,\bar{W}\,|\gamma\rangle$ yields

$$\langle\alpha|\,\bar{W}\,|\gamma\rangle = \langle\alpha|\,\bar{G}\,|\gamma\rangle + \langle\alpha|\,\bar{L}\,|\gamma\rangle, \quad (5.2)$$

where $\langle\alpha|\,\bar{G}\,|\gamma\rangle$ and $\langle\alpha|\,\bar{L}\,|\gamma\rangle$ are given by (3.5) and (4.2). After taking into account the effect of the limits $V\to\infty$ and $\epsilon\to 0$, one obtains

$$\begin{aligned}\mathbf{W}^{(m)}{}_{k'} &= \lim_{\epsilon\to 0}\lim_{V\to\infty} V\sum_\alpha f(\alpha)N_{k'}(\alpha)\\ &\times(B_mP_mD_m + C_mQ_mE_m)\cdots(B_2P_2D_2 + C_2Q_2E_2)\\ &\times(B_1P_1D_1 + C_1Q_1E_1)\mathbf{S}|_{N_k=N_k(\alpha)}\end{aligned} \quad (5.3)$$

where $B_mP_mD_m$ and $C_mQ_mE_m$ are given by (3.18)–(3.20) and (4.5)–(4.7).

Using (3.25) and (4.9), the product rule for differentiation, and the fact that average of a product of occupation numbers in $\mathbf{W}^{(m)}{}_{k'}$ can be evaluated with (1.13), one can rewrite (5.3) formally as

$$\begin{aligned}\mathbf{W}^{(m)}{}_{k'} &= \lim_{\epsilon\to 0}\lim_{V\to\infty} V[B_m\langle N_{k'}P_m\rangle_0\langle D_m + C_m\langle N_{k'}Q_m\rangle_0\langle E_m]\\ &\times[B_{m-1}P_{m-1}\rangle_0\langle D_{m-1} + C_{m-1}Q_{m-1}\rangle_0\langle E_{m-1}]\\ &\times\cdots[B_1P_1\rangle_0D_1 + C_1Q_1\rangle_0E_1]\mathbf{S}.\end{aligned} \quad (5.4)$$

Two typical terms in the expansion of this are

$$VB_m\langle N_{k'}P_m\rangle_0C_{m-1}\langle D_mQ_{m-1}\rangle_0 \times B_{m-2}\langle E_{m-1}P_{m-2}\rangle_0\cdots B_1\langle D_2P_1\rangle_0(D_1\mathbf{S}) \quad (5.5a)$$

and

$$VC_m\langle N_{k'}Q_m\rangle_0C_{m-1}\langle E_mQ_{m-1}\rangle_0 \times B_{m-2}\langle E_{m-1}P_{m-2}\rangle_0\cdots C_1\langle D_2Q_1\rangle(E_1\mathbf{S}). \quad (5.5b)$$

[15] Compare (4.18) with Klemens (Ref. 8): Eqs. (4.3) and (5.6).

To evaluate (5.4), $B\langle E'P\rangle_0$ and $C\langle D'Q\rangle_0$ must be calculated: It follows from (3.18), (3.19), (4.7), (3.23), (1.8), (3.28), and (3.31) that

$$\lim_{\epsilon\to 0}\lim_{V\to\infty} B\langle E'P\rangle_0 J = (-1)V^{-1}\sum_j(\delta_{j'j}-\delta_{k'j})\mathfrak{s}_j^2\sum_{kl}\mathfrak{B}_{jkl}J_{jkl}; \quad (5.6)$$

this changes under transformations of j' and k' in the same way as $K_{j'k'}$ [see (4.12)]. It follows from (3.20), (4.5), (4.6), (4.12), and (1.5) that

$$C\langle D'Q\rangle_0 K = (-1)V^{-1}\sum_j(\delta_{j'j}+\delta_{k'j}+\delta_{l'j})\mathfrak{s}_j^2\mathfrak{s}_j^{-2} \times\frac{2\pi}{\hbar}\sum_k V|c_{j-k}|^2\,\delta_\epsilon(\omega_j-\omega_k)K_{jk}; \quad (5.7)$$

this transforms under changes of j', k', and l' in the same way as $J_{j'k'l'}$ [see (3.28)]. Since (5.6) and (5.7) behave correctly under transformations of their free subscripts, Eqs. (5.6) and (5.7) can be used along with (3.30) and (4.13) to evaluate the quantities

$$B_i\,\langle E_{i+1}P_i\rangle_0, \quad C_i\,\langle D_{i+1}Q_i\rangle_0, \quad B_i\,\langle D_{i+1}P_i\rangle_0,$$

and $C_i\,\langle E_{i+1}Q_i\rangle_0$ in the expansion of (5.4) for all values of i. Of course, (3.27), (3.33), (4.11), and (4.14) are necessary for the evaluation of the first and last parts of (5.4). By using these equations and regrouping parts as in the derivation of (3.35) and (4.16), it can be shown that the typical terms (5.5) can be written as

$$(-1)^m V^{-1}\sum_j\{\Gamma\Lambda\Gamma\cdots\Gamma\Gamma\}_{k'j}\,\mathfrak{v}_j \quad (5.8)$$

and

$$(-1)^m V^{-1}\sum_j\{\Lambda\Lambda\Gamma\cdots\Gamma\Lambda\}_{k'j}\,\mathfrak{v}_j, \quad (5.9)$$

where Γ and Λ are given by (3.36) and (4.17). By evaluating all of the terms in the expansion of (5.4) and combining them, one obtains

$$\mathbf{W}^{(m)}{}_{k'} = (-1)^m V^{-1}\sum_j\{\Gamma+\Lambda\}^m{}_{k'j}\,\mathfrak{v}_j, \quad (5.10)$$

which has the form of (2.15). The *transport equation* (2.21) becomes

$$[d\langle N_i\rangle_0/dT]\mathbf{v}_i = V^{-1}\sum_k\{\Gamma_{ik}+\Lambda_{ik}\}\mathfrak{n}_k, \quad (5.11)$$

where the second member of this is sum of the second members from (3.37) and (4.18). Of course, $\tilde{\Gamma}_{ik}$ could be used here instead of Γ_{ik}, so that (5.11) would have the same form as the analogous Boltzmann equation from kinetic theory.

6. PROPERTIES OF THE SOLUTION FOR K^{ij}

Since the kinetic theory equations for K^{ij} are the same as the lowest-order equations determined from the correlation function formula, those properties of the thermal conductivity deduced in the kinetic theory analysis also apply here. However, the explicit solution (2.18) for $\mathfrak{n}_{k'}$ makes the discussion of these properties particularly simple. To see this, transform Ω_{kl} according to

$$\Omega'_{kl} = \mathfrak{s}_k\Omega_{kl}\mathfrak{s}_l^{-1}, \quad (6.1)$$

where Ω_{kl} may represent either Γ_{kl}, $\tilde{\Gamma}_{kl}$, Λ_{kl}, $\Gamma_{kl}+\Lambda_{kl}$, or $\tilde{\Gamma}_{kl}+\Lambda_{kl}$. With this, Eqs. (2.14) and (2.18) can be combined to give

$$\lim_{\epsilon\to 0}\lim_{V\to\infty} K^{ij} = \frac{\hbar^2}{4kT^2V^2}\sum_{kl}(\omega_k v_k^i/\mathfrak{s}_k)\{e^{-\Omega' s}\}_{kl}(\omega_l v_l^i/\mathfrak{s}_l). \quad (6.2)$$

Onsager's Relations

As mentioned in Ref. 2, the correlation function formula for K^{ij} is consistent with Onsager's relations, i.e., K^{ij} is a symmetric tensor. If the approximation procedure used there to obtain the lowest order equations for K^{ij} is valid for arbitrary interaction strengths λ, the lowest order result (6.2) will also be such that $K^{ij} = K^{ji}$. That this is indeed true follows from the symmetric form of (6.2) and the fact that Γ'_{jk}, $\tilde{\Gamma}'_{jk}$, and Λ'_{jk} are symmetric, i.e.,

$$\Omega'_{jk} = \Omega'_{kj}. \quad (6.3)$$

This latter symmetry is readily verified by using definitions (3.36), (3.38), and (4.17) and (6.1).

Proof of (2.20)

By using Ω'_{kl} and introducing the eigenfunctions $\Theta_k(a)$ and eigenvalues $\Omega(a)$ of Ω'_{jk}, condition (2.20) can be expressed as

$$\lim_{s\to\infty} V^{-1}\sum_l\{e^{-\Omega' s}\}_{kl}(\omega_l\mathbf{v}_l/\mathfrak{s}_l) = \lim_{s\to\infty}\sum_a e^{-\Omega(a)s}\mathbf{A}(a)\Theta_k(a) = 0, \quad (6.4)$$

where a labels the different eigenstates and the $\mathbf{A}_k(a)$ are the coefficients of the expansion of $(\omega_k\mathbf{v}_k/\mathfrak{s}_k)$ in a series of the eigenfunctions $\Theta_k(a)$. Obviously, for condition (6.4) to be satisfied one must have either $\Omega(a) > 0$ or $A_k(a) = 0$ for all a. The eigenvalues $\Omega(a)$ will be greater than or equal to zero if

$$V^{-2}\sum_{kl}\Omega'_{kl}h_k h_l \geq 0 \quad (6.5)$$

for every vector h_k. The proof of (6.5) for $\Omega'_{kl} = \tilde{\Gamma}'_{kl}$ is given by Leibfried,[16] and it is easily proved

[16] Leibfried, Ref. 9, pp. 307–309. Note that Leibfried's symmetric $P_{\mathfrak{s}\mathfrak{s}',\mathfrak{r}\mathfrak{r}'}$ is equivalent to $4\,kV^{-1}\mathfrak{s}_k\Omega'_{kk'}\mathfrak{s}_{k'}$ where $k = (\mathfrak{r}, s)$ and $k' = (\mathfrak{r}', s')$.

for other choices for Ω'_{kl} by similar arguments. The requirement that $A_k(a) = 0$ if $\Omega(a)$ is equal to zero is equivalent to the condition that any solution $(\vartheta_l\eta_l)$ to the homogeneous part of the transport equation (2.21) as modified by (6.1) be orthogonal to the modified inhomogeneous part $(\hbar/4kT^2)(\omega_k\nabla_k/\vartheta_k)$.

This latter condition has also been studied in kinetic theory.[16] Note that the solution to the homogeneous equation which is interpreted in kinetic theory as a small uniform temperature increase has an analog here when $\Omega'_{kl} = \Gamma'_{kl}$ but not when $\Omega'_{kl} = \Gamma'_{kl}$.

7. DISCUSSION

The equality of the thermal conductivities predicted here and by kinetic theory is not particularly surprising when one considers the basic equations used in the two approaches for treating the many-body aspect of the problem. The equation used here is (2.2). If the ${}^0X_{E,\epsilon}(\alpha\beta)$'s in it had δ-function singularities at $E = \mathcal{E}(\alpha)$ and no other singularities, and if δ_ϵ-functions could be treated as Dirac δ's, Eq. (2.2) could be integrated from $E = -\infty$ to $E = +\infty$ to yield

$$\epsilon\tilde{P}_\epsilon(\alpha\beta) - \delta_{\alpha\beta} = \frac{2\pi}{\hbar}\sum_\gamma |\langle\alpha|\,\lambda H'\,|\gamma\rangle|^2 \times \delta(\mathcal{E}(\alpha) - \mathcal{E}(\gamma))[\tilde{P}_\epsilon(\gamma\beta) - \tilde{P}_\epsilon(\alpha\beta)], \quad (7.1)$$

where $\tilde{P}_\epsilon(\alpha\beta) = (\hbar/2\pi)\int dE\ {}^0X_{E,\epsilon}(\alpha\beta)$. It follows from the discussion in Ref. 2 that to lowest order in λ the quantity $\tilde{P}_\epsilon(\alpha\beta)$ defined above is the Laplace transform of the probability of a transition from state β to state α in time t,[17] that is,

$$\tilde{P}_\epsilon(\alpha\beta) = \int_0^\infty dt\, e^{-\epsilon t}P_t(\alpha\beta), \quad (7.2)$$

where $P_t(\alpha\beta) = |\langle\alpha|\exp(-iHt/\hbar)\,|\beta\rangle|^2$. It is now obvious that (7.1) has the form of the Laplace transform of the Pauli equation[18]

$$\frac{\partial P_t(\alpha\beta)}{\partial t} = \frac{2\pi}{\hbar}\sum_\gamma |\langle\alpha|\,\lambda H'\,|\gamma\rangle|^2 \times \delta(\mathcal{E}(\alpha) - \mathcal{E}(\gamma))[P_t(\gamma\beta) - P_t(\alpha\beta)]. \quad (7.3)$$

The arguments used in kinetic theory to calculate the rate of change of the number of phonons per mode due to collisions are equivalent to assuming the Pauli equation, which may be considered as the basic many-body equation of the kinetic-theory derivation. Thus, although the presumptions made to obtain (7.1) from (2.2) would be very difficult to justify, the above considerations do illustrate the essential similarity in the structures of the many-body equations of the two approaches.

It is apparent from their derivation in Ref. 2 and Secs. 2–5 that the transport equations (3.37), (4.18), and (5.11) are direct consequences of the correlation function formula, the choice of the Hamiltonian, and the decision to consider the limiting value of the thermal conductivity to lowest order in λ. The many additional assumptions used in previous derivations are now seen to be unnecessary. The present work thus establishes the theory of lattice thermal conductivity on a firmer theoretical foundation as well as facilitating the unambiguous generalization to higher orders in λ.[19]

ACKNOWLEDGMENTS

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[17] This follows from the definition of ${}^0X_{E,\epsilon}(\alpha\beta)$ given in Ref. 2 below (4.1) and from Ref. 2: (2.5), (2.17a), and (2.18). Note that $\tilde{P}_\epsilon(\alpha\beta)$ is the lowest order part of the quantity $\tilde{Z}_\epsilon(\alpha\beta\beta\alpha)$.

[18] L. Van Hove (Ref. 11): Eqs. (10.15) and (11.1).

[19] For a preliminary report on the extension to order λ^{-1} see W. C. Schieve and R. J. Hardy: Technical Report 675 (1963), U. S. Naval Radiological Defense Laboratory, San Francisco, California; Bull. Am. Phys. Soc. 8, 15 (1963).

One-Particle Singularities of the S-Matrix in Quantum Field Theory*

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In the framework of the Haag–Ruelle collision theory one-particle singularities are proved to exist in the physical region of any connected scattering amplitude. They occur with the causal propagator $(p^2 - m^2 + i\epsilon)^{-1}$ in the dominant term and have a residue, which factors into the product of two connected amplitudes for subprocesses. The remainder of the amplitude is infinitely often differentiable in the critical variable. These results rely essentially on short-range forces and the one-particle spectrum, but neither depend on analyticity nor on unitarity.

I. INTRODUCTION

IN any reasonable framework of relativistic quantum mechanics[1] one expects all stable elementary and bound massive particles to appear as poles in the physical region of the connected scattering amplitudes $\langle \mathbf{p}_1 \cdots \mathbf{p}_m^{\text{out}} \mid \mathbf{q}_1 \cdots \mathbf{q}_n^{\text{in}} \rangle^{\text{T}}$ for $m, n \geq 3$.

The existence of one-particle singularities in many-body amplitudes is implied by the experimental feasibility of successive reactions with a large time-like separation. For instance in a three-body reaction $p_4 + p_5 + p_6 \to p_1 + p_2 + p_3$, some singularity should occur for $\omega(\mathbf{p}_1) + \omega(\mathbf{p}_2) - \omega(\mathbf{p}_4) = \omega(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_4)$, where two successive two-body reactions $p_5 + p_6 \to p_3 + p$ and $p_4 + p \to p_1 + p_2$ are kinematically possible. In a macroscopic space–time description the dominant rescattering term should appear most clearly in processes where no causal relation exists between the noninteracting particles, as illustrated in Fig. 1. Here particles 5 and 6 interact first, with 4 remaining in large spacelike separation. Then one outgoing particle interacts with 4 to give 1 and 2, while 3 passes in a large distance from their interaction region. Particles 3 and 4 are causally independent in the sense that, while 4 is still in large spacelike separation to 5 and 6 "before they interact" (asymptotically, as specified in Sec. 2) and while 3 is far spacelike from the "region of emergence" of 1 and 2, the separation between 3 and 4 is large and spacelike.

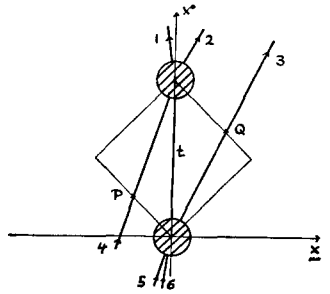
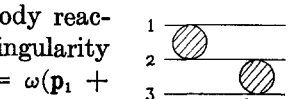


FIG. 1. Causal Independence.

By translating the intersection of the wave packets f_1, f_2, f_4 of particles 1, 2, 4 in x space along the classical orbit of the possible real intermediate particle, the dominant contribution



$$= \int \frac{d\mathbf{p}}{2\omega} \langle \hat{f}_1 \hat{f}_2^{\text{out}} \mid \hat{f}_4 \mathbf{p}^{\text{in}} \rangle^{\text{T}} \langle \hat{f}_3 \mathbf{p}^{\text{out}} \mid \hat{f}_5 \hat{f}_6^{\text{in}} \rangle^{\text{T}} \tag{1.1}$$

should be obtained in the limit $t \to +\infty$ faster than any power of t in a theory of short-range forces. The amplitude should converge rapidly to zero for $t \to -\infty$, since no real intermediate particle of negative energy can be exchanged. In momentum space the rapid convergence of $\langle \hat{f}_1^t \hat{f}_2^t \hat{f}_3^{\text{out}} \mid \hat{f}_4^t \hat{f}_5^t \hat{f}_6^{\text{in}} \rangle^{\text{T}}$ for $t \to \pm\infty$ implies that the connected three-body amplitude has the following one-particle structure with respect to $(p_1 + p_2 - p_4)^2 \approx m^2$:

$$\langle \mathbf{p}_1\mathbf{p}_2\mathbf{p}_3^{\text{out}} \mid \mathbf{p}_4\mathbf{p}_5\mathbf{p}_6^{\text{in}} \rangle^{\text{T}} = \langle \mathbf{p}_1\mathbf{p}_2\mathbf{p}_3^{\text{out}} \mid \mathbf{p}_4\mathbf{p}_5\mathbf{p}_6^{\text{in}} \rangle^{\text{T}}_{\text{irr}} + \lim_{\epsilon \downarrow 0} [(p_1 + p_2 - p_4)^2 - m^2 + i\epsilon]^{-1} \times \int \frac{d\mathbf{p}}{2\omega} \langle \mathbf{p}_1\mathbf{p}_2^{\text{out}} \mid \mathbf{p}_4\mathbf{p}^{\text{in}} \rangle^{T} \langle \mathbf{p}_3\mathbf{p}^{\text{out}} \mid \mathbf{p}_5\mathbf{p}_6^{\text{in}} \rangle^{\text{T}}, \tag{1.2}$$

where the first term on the right-hand side is smooth in the variable $\omega(\mathbf{p}_1) + \omega(\mathbf{p}_2) - \omega(\mathbf{p}_4) - \omega(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_4)$.

This one-particle structure is well known from perturbation theory, and the causal nature of the propagator $(p^2 - m^2 + i\epsilon)^{-1}$ has been elucidated by the discussions of Stueckelberg,[2] Feynman,[3] and

* Research supported by the National Science Foundation.
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especially by Fierz.[4] The structure analysis of the truncated time-ordered distributions $\langle \bar{T}(p_1, \cdots, p_n)\rangle_0^T$ in quantum field theory[5] has revealed one-particle singularities in any cross energy $q^2 = (\sum p_i - \sum p_j)^2$, with the residue factorizing into the product of time-ordered distributions with the causal propagator and the regularity of the remainder in $q^0 - \omega(\mathbf{q})$. Although $\prod (p_i^2 - m^2)\langle \bar{T}(p_1, \cdots -p_n)\rangle_0^T$ can be shown[6] to be regular around the origin in $p_i^0 - \omega(\mathbf{p}_i)$, $1 \leq i \leq n$, and gives restricted to the mass shell the connected scattering amplitudes, the singularity structure of these Green's functions uniformly in all $p_i^0 - \omega(\mathbf{p}_i)$ and in any cross energy q^2 has not been determined from general principles.

In analytic S-matrix theory the one-particle structure is of great importance. Arguments of various generality[7,8] have been given to derive (1.2) from unitarity and from a Landau-type singularity structure of the connected scattering amplitudes at the critical points. It can be understood entirely in terms of mass shell quantitites that only the propagator $(q^2 - m^2 + i\epsilon)^{-1}$ is consistent with macroscopic causality.[9-11]

We shall derive in the framework of the Haag–Ruelle collision theory[12,13] that the connected many-body amplitudes have physical region singularities of the type (1.2) in any cross energy q^2, with the remainder being C^∞ in the critical variable $q^0 - \omega(\mathbf{q})$. The proof holds for causally independent scattering configurations and uses neither analyticity nor unitarity (in the sense of asymptotic completeness). Essential is the existence of massive one-particle states created from the vacuum by almost local fields, whose truncated vacuum expectation values (VEV) decrease strongly in spacelike directions, as it is characteristic for a theory with short-range interactions.

In Sec. 2 the one-particle singularities of the three-body scattering amplitude will be investigated as well as the generalization to many-body amplitudes. In the concluding Sec. 3, we shall discuss the connection of these results with other timelike cluster properties of the S matrix[14] and with the work of Goldberger, Watson, and Froissart[15] on a coarse-grained space–time structure in S-matrix theories.

II. ONE-PARTICLE SINGULARITIES

Sacrificing generality for clarity we shall study in this section the one-particle structure of the three-body amplitude in a theory of only one kind of scalar particle of mass $m > 0$. The necessary modifications for more general particle spectra and for many-body amplitudes will become clear in the discussion.

We assume that the mass spectrum consists of the nondegenerated eigenvalue 0 corresponding to the vacuum Ω, then $m > 0$ corresponding to the one-particle space $\mathfrak{H}_1$ and a continuum starting at $2m$. A neutral scalar field[16] $A(x)$ is assumed to satisfy $(\Phi, A(x)\Omega) \neq 0$ for all $\Phi \in \mathfrak{H}_1$. $A(x)$ need not be local, but only almost local in the sense that the VEV $\langle A(x_1) \cdots [A(x_m), A(x_{m+1})] \cdots A(x_n)\rangle_0$ should decrease rapidly for $(x_m - x_{m+1})^2 \to -\infty$, belonging (as tempered distributions[17] in the variables $\xi_i = x_i - x_{i+1}$, $1 \leq i \leq n-1$) to $\mathcal{O}_C$ in ξ_m for $|\xi_m^0| < \delta|\xi_m|$, with $0 < \delta < 1$ and $1 \leq m \leq n-1$. Almost locality and the mass spectrum conditions allow the construction of scattering states and an S matrix by the Haag–Ruelle theorem.[12,13] It is not necessary to assume asymptotic completeness (unitarity).

Let us discuss a three-body process $p_4 + p_5 + p_6 \to p_1 + p_2 + p_3$ around $\omega(\mathbf{p}_1) + \omega(\mathbf{p}_2) - \omega(\mathbf{p}_4) = \omega(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_4)$, for convenience in the rest frame $\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_4 = \mathbf{0}$. In order to approximate the scattering amplitude uniformly in terms of VEV of products of almost-local fields and to guarantee the causal independence of particles 3 and 4, we impose the following kinematical restrictions on $\mathbf{p}_1, \cdots, \mathbf{p}_6$.

(a) Uniformly nonoverlapping velocities $\mathbf{v}_i = \mathbf{p}_i\omega(\mathbf{p}_i)^{-1}$: $\mathbf{v}_1 \neq \mathbf{v}_2$, $\mathbf{v}_1 \neq \lambda\mathbf{v}_3 \neq \mathbf{v}_2$ for all $\lambda \geq 0$, $\mathbf{v}_5 \neq \mathbf{v}_6$, $\mathbf{v}_5 \neq \mu\mathbf{v}_4 \neq \mathbf{v}_6$ for all $-\infty < \mu < +\infty$;

(b) causal independence:

The intersection P (see Fig. 1) of the foreward light cone from 0 with the line $\{(t, \mathbf{0}) + \rho p_4, \rho \in R^1\}$

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[11] Recently G. Wanders [Helv. Phys. Acta **38**, 142 (1965)] has given a particularly lucid discussion of this fact, based on asymptotic causality and assuming the dominance of the rescattering term.
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[15] M. L. Goldberger, K. M. Watson, Phys. Rev. **127**, 2284 (1962); M. Froissart, M. L. Goldberger, K. M. Watson, Phys. Rev. **131**, 2820 (1963).
[16] A. S. Wightman, Phys. Rev. **101**, 860 (1956).
[17] L. Schwartz, *Théorie des distributions* (Paris, 1957/59), Vols. I, II.

and the intersection Q of the backward light cone from $(t, \mathbf{0})$ with $\{\rho p_3, \rho \in R^1\}$ should determine a spacelike segment $[PQ]$ for $t > 0$ (we shall denote segments by enclosing the endpoints in brackets). Then the three-body amplitude satisfies the following timelike cluster decomposition property.

Theorem. Let $\mathbf{p}_1, \cdots, \mathbf{p}_6$ be some three-body scattering configuration satisfying (a) and (b). Let

$$T(t) = \int \prod_{i=1}^{3} \frac{d\mathbf{q}_i}{2\omega_i} \hat{f}_i^*(\mathbf{q}_i) \prod_{i=4}^{6} \frac{d\mathbf{q}_i}{2\omega_i} \hat{f}_i(\mathbf{q}_i) \times \exp[-i(\omega_1 + \omega_2 - \omega_4 - \omega)t] \langle \mathbf{q}_1\mathbf{q}_2\mathbf{q}_3^{\text{out}} \mid \mathbf{q}_4\mathbf{q}_5\mathbf{q}_6^{\text{in}} \rangle^{\mathrm{T}}. \tag{2.1}$$

Then there exists an $\epsilon = \epsilon(\mathbf{p}_1, \cdots, \mathbf{p}_6) > 0$ such that for all $\hat{f}_i \in \mathfrak{D}(U_\epsilon(\mathbf{p}_i))$,

$$T(t) - \int \frac{d\mathbf{q}}{2\omega} \langle \hat{f}_1 \hat{f}_2^{\text{out}} \mid \hat{f}_4 \mathbf{q}^{\text{in}} \rangle^{\mathrm{T}} \times \langle \mathbf{q} \hat{f}_3^{\text{out}} \mid \hat{f}_5 \hat{f}_6^{\text{in}} \rangle^{\mathrm{T}} = o(|t|^{-\infty}) \tag{2.2}$$

for $t \to +\infty$ and $T(t) = o(|t|^{-\infty})$ for $t \to -\infty$. The one-particle irreducible amplitude with respect to $(q_1 + q_2 - q_4)^2 = q^2$

$$\langle \mathbf{q}_1\mathbf{q}_2\mathbf{q}_3^{\text{out}} \mid \mathbf{q}_4\mathbf{q}_5\mathbf{q}_6^{\text{in}} \rangle^{\mathrm{T}} - \lim_{\epsilon \downarrow 0} (q^2 - m^2 + i\epsilon)^{-1} \times \int \frac{d\mathbf{q}}{2\omega} \langle \mathbf{q}_1\mathbf{q}_2^{\text{out}} \mid \mathbf{q}_4\mathbf{q}^{\text{in}} \rangle^{T} \langle \mathbf{q}_3\mathbf{q}^{\text{out}} \mid \mathbf{q}_5\mathbf{q}_6^{\text{in}} \rangle^{\mathrm{T}} \tag{2.3}$$

is C^∞ in $\omega_1 + \omega_2 - \omega_4 - \omega$ in a neighborhood of the origin, when integrated over the remaining variables with test functions of sufficiently small support around $\mathbf{p}_1, \cdots, \mathbf{p}_6$.

Notation. $\mathfrak{D}(U_\epsilon(\mathbf{p}_i))$ is the space[17] of C^∞ wavefunctions $\hat{f}_i$ with support in $\{\mathbf{q}: |\mathbf{q} - \mathbf{p}_i| < \epsilon\}$ and $o(|t|^{-\infty})$ denotes $o(|t|^{-N})$, $N > 0$ arbitrary, and $\omega_i = \omega(\mathbf{q}_i)$, $\omega = \omega(\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_4)$.

Proof. We use similar majorizations as in the derivation of the Haag–Ruelle theorem[12,13] and of the reduction formulas of Lehmann, Symanzik and Zimmermann. By assumption one has $\langle \mathbf{q} | A(x)\Omega \rangle = \alpha^{-1}(2\pi)^{-2} \exp[i(\omega x^0 - \mathbf{q}\mathbf{x})] \neq 0$. Let $G = \{q: q^0 > 0, 0 < q^2 < 4m^2\}$ and for $\tilde{f} \in \mathcal{S}(G)$ define $A(f, t)^* = \alpha \int dq \tilde{A}(-q)\tilde{f}(q) \exp[i(q^0 - \omega)t]$. Then the connected scattering amplitudes are given by

$$\langle \hat{f}_1 \cdots \hat{f}_m^{\text{out}} \mid \hat{f}_{m+1} \cdots \hat{f}_n^{\text{in}} \rangle^{\mathrm{T}} = \lim_{s \to \infty} \left\langle \prod_{i=1}^{m} A(f_i, s) \prod_{i=m+1}^{n} A(f_i, -s)^* \right\rangle_0^{\mathrm{T}}, \tag{2.4}$$

with $\hat{f}_i(\mathbf{q}) = \tilde{f}_i(\omega, \mathbf{q})$.

Consider $t \geq 0$. We choose $\epsilon > 0$ so small that all $U_\epsilon(p_i) \subset G$ and that $(q_1 + q_2 - q_4)$, $(q_5 + q_6 - q_3) \in G$ for all $q_i \in U_\epsilon(p_i)$. Then $T(t)$ is the limit $s = u = v \to +\infty$ of some

$$F(s, u, v, t) = \alpha^6 \int dq \prod_{i=1}^{2} f_i^*(q_i) \exp[-i(q_i^0 - \omega_i) \times (s + t)] \tilde{f}_3^*(q_3) \exp[-i(q_3^0 - \omega_3)(u + t)] \times \tilde{f}_4(q_4) \exp[-i(q_4^0 - \omega_4)v] \prod_{i=5}^{6} \tilde{f}_i(q_i) \times \exp[-i(q_i^0 - \omega_i)s] \exp[-i(\omega_1 + \omega_2 - \omega_4 - \omega)t] \times \langle \tilde{A}(q_1)\tilde{A}(q_2)\tilde{A}(q_3)\tilde{A}(-q_4)\tilde{A}(-q_5)\tilde{A}(-q_6) \rangle_0^{\mathrm{T}}. \tag{2.5}$$

One sees from Fig. 1 that for $\mathbf{p}_1, \cdots, \mathbf{p}_6$ satisfying (a) and (b) there exist $\eta_1 > 0$, $\eta_2, \eta_3 < \eta_1$ such that the points

$$\begin{aligned} P_1 &= (1 + \eta_1, \eta_1 \mathbf{p}_1 \omega(\mathbf{p}_1)^{-1}), \\ P_2 &= (1 + \eta_1, \eta_1 \mathbf{p}_2 \omega(\mathbf{p}_2)^{-1}), \\ P_3 &= (1 + \eta_2, (1 + \eta_2)\mathbf{p}_3 \omega(\mathbf{p}_3)^{-1}), \\ P_4 &= (-\eta_3, -(1 + \eta_3)\mathbf{p}_4 \omega(\mathbf{p}_4)^{-1}), \\ P_5 &= (-\eta_1, -\eta_1 \mathbf{p}_5 \omega(\mathbf{p}_5)^{-1}), \\ P_6 &= (-\eta_1, -\eta_1 \mathbf{p}_6 \omega(\mathbf{p}_6)^{-1}). \end{aligned} \tag{2.6}$$

determine spacelike intervals $[P_1P_2]$, $[P_1P_3]$, $[P_2P_3]$, $[P_4P_5]$, $[P_4P_6]$, $[P_5P_6]$, $[P_3P_4]$. We shall prove (2.1) by showing that for sufficiently small $\epsilon > 0$ and for all $\hat{f}_i \in \mathfrak{D}(U_\epsilon(p_i))$ one has in the limit $t \to \infty$

$$T(t) - F(\eta_1 t, \eta_2 t, \eta_3 t, t) = o(|t|^{-\infty}) \tag{2.7}$$

and

$$F(\eta_1 t, \eta_2 t, \eta_3 t, t) - \int \frac{d\mathbf{q}}{2\omega} \langle \hat{f}_1 \hat{f}_2^{\text{out}} \mid \hat{f}_4 \mathbf{q}^{\text{in}} \rangle^{\mathrm{T}} \times \langle \hat{f}_3 \mathbf{q}^{\text{out}} \mid \hat{f}_5 \hat{f}_6^{\text{in}} \rangle^{\mathrm{T}} = o(|t|^{-\infty}). \tag{2.8}$$

By the asymptotic condition one obtains the estimate

$$|T(t) - F(\eta_1 t, \eta_1 t, \eta_1 t, t)| \leq \int_{\eta_1 t}^{\infty} ds \left| \frac{d}{ds} F(s, s, s, t) \right|, \tag{2.9}$$

and the right-hand side is $o(|t|^{-\infty})$, if one can show that there exists an $M < \infty$, such that for all $N > 0$

$$|(d/ds)F(s, s, s, t)| < c(1 + s)^{-N}(1 + t)^M \tag{2.10}$$

uniformly for all $t \geq 0$, $s \geq \eta_1 t$ with $c = c(\eta_1, N) < \infty$. Since $\tilde{f}_i \in \mathfrak{D}(G)$, the terms in $(d/ds)F(s, s, s, t)$ vanish, where d/ds operates on $\exp[-i(q_i^0 - \omega_i)s]$, $i = 1, 6$. Let us consider the contribution from $(d/ds) \exp[-i(q_3^0 - \omega_3)s]$, where for the same reason

one can replace the VEV $\langle \tilde{A}(q_1) \cdots \tilde{A}(-q_6)\rangle_0^T$ in (2.5) by

$$\langle \tilde{A}(q_1)[\tilde{A}(q_2), \tilde{A}(q_3)] \cdots \tilde{A}(-q_6)\rangle_0^T + \langle [\tilde{A}(q_1), \tilde{A}(q_3)]\tilde{A}(q_2) \cdots \tilde{A}(-q_6)\rangle_0^T.$$

The first tempered distribution has in x-space the global representation[15] (using translation invariance)

$$\sum_{r=1}^{R} D_r \prod_{i=1}^{5} (1 + \|\xi_i\|^2)^K T_r(\xi_1, \cdots, \xi_5) \quad (2.11)$$

and (using almost locality) in $\{|\xi_2^0| < \delta|\xi_2|, 0 < \delta < 1 \text{ fixed}\}$ for any integer $L > 0$ as

$$\sum_{s=1}^{S(L)} D_{s,L} \prod_{i\neq 2} (1 + \|\xi_i\|^2)^K \times (1 + \|\xi_2\|^2)^{-L} T_{s,L}(\xi_1, \cdots, \xi_5). \quad (2.12)$$

Here $\|\xi_i\|^2 = \sum_{j=0}^{3} (\xi_i^j)^2$. The integers R, K depend only on the order of $\langle \cdots \rangle_0^T$, while $S(L)$ increases with L. D_r and $D_{s,L}$ are differential monomials in the $\partial/\partial\xi_i^j$ and T_r, $T_{s,L}$ are bounded continuous functions. The distribution $\langle A(x_1)[A(x_2), A(x_3)] \cdots A(x_6)\rangle_0^T$ is integrated over the test function

$$f(x, s, t) = -\frac{i\alpha^6}{(2\pi)^{12}} \int dq(q_3^0 - \omega_3) \prod_{i=1}^{3} \tilde{f}_i^*(q_i) \times \exp\{-i[(q_i^0 - \omega_i)(s + t) - q_i x_i]\} \times \exp\{-i(\omega_1 + \omega_2 - \omega_4 - \omega)t\} \prod_{i=4}^{6} \tilde{f}_i(q_i) \times \exp\{-i[(q_i^0 - \omega_i)s + q_i x_i]\}, \quad (2.13)$$

whose essential support in x-space varies with s and t. Obviously $D_r f$ and $D_{s,L} f$ are of the type (2.13), while for any polynomial P in the x_i^j Pf can be represented by a finite sum $\sum f_{m,n} s^m t^n$ with $f_{m,n}(x, s, t)$ as in (2.13). Using (2.11) and (2.12) one sees after partial integration that it is sufficient to show that every $f(x, s, t)$ of the type (2.13) satisfies

$$\sup_{\{|\xi_2^0| \geq \delta|\xi_2|\}} |f(x, s, t)| < c_N(1 + |s|)^{-N}, \quad (2.14)$$

$$\sup_{\{|\xi_2^0| \leq \delta|\xi_2|\}} |(1 + \|\xi_2\|^2)^{-\frac{1}{2}N} f(x, s, t)| < c_N(1 + |s|)^{-N}, \quad (2.15)$$

where for all $N > 0$ $c_N < \infty$ uniformly for all $s \geq \eta_1 t \geq 0$.

With $t = \tau s$, $0 \leq \tau \leq \eta_1^{-1}$, it follows from (2.13) by partial integration that $f(x, s, \tau s)$ decreases uniformly faster than any power of $[x_i^0 - (1 + \tau)s]^{-1}$, $i = 2, 3$, and is bounded in the other variables. In the set of $\mathbf{x}_2$, $\mathbf{x}_3$, for which

$$\mathbf{x}_2 \neq [\mathbf{q}_2\omega_2^{-1} + (\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_4)\tau\omega^{-1}]s$$

for all

$$\mathbf{q}_i \in U_{2\epsilon}(\mathbf{p}_i), \quad i = 1, 2, 4, \quad (2.16)$$

$$\mathbf{x}_3 \neq \mathbf{q}_3(1 + \tau)s\omega_3^{-1} \quad \text{for all} \quad \mathbf{q}_3 \in U_{2\epsilon}(\mathbf{p}_3); \quad (2.17)$$

$f(x, s, \tau s)$ decreases uniformly stronger than any power of $(s^2 + \mathbf{x}_2^2)$ or $(s^2 + \mathbf{x}_3^2)$, respectively, with bounds depending continuously on τ. For $\eta_1 > 0$ fixed satisfying (2.6), there exists and $\epsilon = \epsilon(\mathbf{p}_1, \cdots, \mathbf{p}_6) > 0$ such that the distance between

$$\{\mathbf{q}_2\omega_2^{-1} + (\mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_4)\tau\omega^{-1} : \mathbf{q}_i \in U_{2\epsilon}(\mathbf{p}_i)\}$$

and

$$\{(1 + \tau)\mathbf{q}_3\omega_3^{-1} : \mathbf{q}_3 \in U_{2\epsilon}(\mathbf{p}_3)\}$$

exceeds some $\eta > 0$ for all $0 \leq \tau \leq \eta_1^{-1}$, since $\mathbf{p}_1, \cdots, \mathbf{p}_6$ were chosen to satisfy (a) and (b). Then the essential supports of $f(x, s, \tau s)$ in x_2, x_3, where neither (2.16) nor (2.17) holds, separate linearly in s in spacelike direction, uniformly for $0 \leq \tau \leq \eta_1^{-1}$. This proves (2.14) and (2.15) for a sufficiently large $\delta < 1$, and one obtains (2.10), since the other terms in $(d/ds)F(s, s, s, t)$ behave similarly.

It follows by the same majorizations that

$$|F(\eta_1 t, \eta_1 t, \eta_1 t, t) - F(\eta_1 t, \eta_2 t, \eta_3 t, t)| \leq \int_{\eta_3 t}^{\eta_1 t} du \left|\frac{d}{du} F(\eta_1 t, u, \eta_1 t, t)\right| + \int_{\eta_3 t}^{\eta_1 t} dv \left|\frac{d}{dv} F(\eta_1 t, \eta_2 t, v, t)\right| = o(|t|^{-\infty}) \quad (2.18)$$

for sufficiently small $\epsilon > 0$. There exists an $\epsilon > 0$, for which the essential supports of the wave packets of particles 3 and 4 in $F(\eta_1 t, \eta_2 t, \eta_3 t, t)$ separate linearly in t in spacelike direction. Therefore by almost-locality, $F(\eta_1 t, \eta_2 t, \eta_3 t, t)$ equals up to $o(|t|^{-\infty})$

$$\left\langle \prod_{i=1}^{2} A(f_i, \eta_1 t) A(f_4, -(1 + \eta_3)t)^* \times A(f_3, (1 + \eta_2)t) \prod_{i=5}^{6} A(f_i, -\eta_1 t)^* \right\rangle_0^T, \quad (2.19)$$

where a factor $\exp[-i(q_1^0 + q_2^0 - q_4^0 - \omega)t]$ has been dropped, since

$$A(f_3, (1 + \eta_2)t)A(f_5, -\eta_1 t)^* A(f_6, -\eta_1 t)^* \Omega$$

is a one-particle state with a t-dependent wave-function $\hat{f}_{356}(t) \in \mathfrak{D}(R^3)$. One sees easily that

$$\|A(f_4, -(1 + \eta_3)t)^* |\hat{f}_{356}(t)\rangle - a_{\text{in}}(\hat{f}_4)^* |\hat{f}_{356}(t)\rangle\| \leq \int_{-\infty}^{-(1+\eta_3)t} ds \left\|\frac{d}{ds} A(f_4, s)^* |\hat{f}_{356}(t)\rangle\right\| = o(|t|^{-\infty}) \quad \text{for} \quad t \to +\infty. \quad (2.20)$$

Then up to $o(|t|^{-\infty})$, one can replace in (2.19) $A(f_4, -(1+\eta_3)t)^*$ by $a_{\text{in}}(\hat{f}_4)^*$ and $A(f_1, \eta_1 t)A(f_2, \eta_1 t)$ by $a_{\text{out}}(\hat{f}_1)a_{\text{out}}(\hat{f}_2)$. Since $a_{\text{in}}(\hat{f}_4)a_{\text{out}}(\hat{f}_2)^*a_{\text{out}}(\hat{f}_1)^*\Omega$ is a one-particle state with $\hat{f}_{421}$ being C^∞ and of compact support around $\mathbf{0}$, $\langle \hat{f}_{421} \mid \hat{f}_{356}(t)\rangle_0$ converges faster than any power of t to

$$\left\langle \prod_{i=1}^{2} a_{\text{out}}(\hat{f}_i)a_{\text{in}}(\hat{f}_4)^*a_{\text{out}}(\hat{f}_3) \prod_{i=5}^{6} a_{\text{in}}(\hat{f}_i)^* \right\rangle_0^{\mathrm{T}}$$

$$= \int \frac{d\mathbf{q}}{2\omega} \langle \hat{f}_1 \hat{f}_2^{\text{out}} \mid \hat{f}_4 \mathbf{q}^{\text{in}}\rangle^{\mathrm{T}} \langle \hat{f}_3 \mathbf{q}^{\text{out}} \mid \hat{f}_5 \hat{f}_6^{\text{in}}\rangle^{\mathrm{T}}, \qquad (2.21)$$

using

$$E_1 = \int \frac{d\mathbf{q}}{2\omega} |\mathbf{q}\rangle\langle\mathbf{q}|$$

for the projector on $\mathfrak{H}_1$ and the restrictions on the supports of the wavefunctions.

One remarks that only the weaker assumption $\lambda, \mu \geq 1$ in the nonoverlap condition (a) has been used to derive (2.2). For the proof of $T(t) = o(|t|^{-\infty})$ for $t \to -\infty$ and of the regularity of the one-particle reduced amplitude the slightly stronger assumption (a) has been made.

For $t \leq 0$ we consider

$$G(s, t) = \alpha^6 \int dq \prod_{i=1}^{3} \tilde{f}_i^*(q_i)$$

$$\times \exp[-i(q_i^0 - \omega_i)s] \prod_{i=4}^{6} \tilde{f}_i(q_i) \exp[-i(q_i^0 - \omega_i)s]$$

$$\times \exp[-i(\omega_1 + \omega_2 - \omega_4 - \omega)t]\langle \tilde{A}(q_1) \cdots \tilde{A}(-q_6)\rangle_0^{\mathrm{T}}, \qquad (2.22)$$

which gives $T(t)$ in the limit $s \to +\infty$. As before, one can show that for any $\eta_4 > 0$ there exists an $\epsilon > 0$ such that for all $\tilde{f}_i \in \mathfrak{D}(U_\epsilon(p_i))$

$$|G(-\eta_4 t, t) - T(t)| = o(|t|^{-\infty}) \text{ for } t \to -\infty. \qquad (2.23)$$

For sufficiently small ϵ, $\eta_4 > 0$ the essential supports of the wavefunctions of particles 1, 2, 4 in $G(-\eta_4 t, t)$ are spacelike to those of 3, 5, 6 separating linearly in $|t|$. Again, by almost locality the VEV in $G(-\eta_4 t, t)$ can be replaced by $\langle \tilde{A}(q_3)\tilde{A}(-q_5)\cdot \tilde{A}(-q_6)\tilde{A}(q_1)\tilde{A}(q_2)\tilde{A}(-q_4)\rangle_0^T$, which vanishes by the support conditions on the $\{\tilde{f}_i\}$. Therefore $T(t)$ is $o(|t|^{-\infty})$ for $t \to -\infty$.

It follows from these considerations that

$$\frac{d}{dt} T(t) = -i \int \prod_{i=1}^{6} \frac{d\mathbf{q}_i}{2\omega_i} f_i^{(*)}(\mathbf{q}_i)$$

$$\times \frac{\exp[-i(\omega_1 + \omega_2 - \omega_4 - \omega)t]}{\omega_1 + \omega_2 - \omega_4 + \omega}$$

$$\times [(q_1 + q_2 - q_4)^2 - m^2]\langle \mathbf{q}_1\mathbf{q}_2\mathbf{q}_3^{\text{out}} \mid \mathbf{q}_4\mathbf{q}_5\mathbf{q}_6^{\text{in}}\rangle^{\mathrm{T}} \qquad (2.24)$$

belongs to $\mathcal{S}(R^1)$ in the variable t. By the kinematical assumptions $\partial(\omega_1 + \omega_2 - \omega_4 - \omega)/\partial\mathbf{q}_i \neq 0$ for at least one $\mathbf{q}_i$ in the support of $\hat{f}_1^* \otimes \cdots \otimes \hat{f}_6$. Introducing $\omega_1 + \omega_2 - \omega_4 - \omega$ as a new variable (2.24) implies[17] that $[(q_1 + q_2 - q_4)^2 - m^2] \times \langle \mathbf{q}_1\mathbf{q}_2\mathbf{q}_3^{\text{out}} \mid \mathbf{q}_4\mathbf{q}_5\mathbf{q}_6^{\text{in}}\rangle^{\mathrm{T}}$ is C^∞ in $\omega_1 + \omega_2 - \omega_4 - \omega$, when integrated over the remaining variables with test functions satisfying the conditions of the theorem. Finally the regularity of the one-particle irreducible amplitude (2.3) follows in the same way from the strong decrease of the piecewise C^∞ function $T(t) - \theta(t)T(+\infty)$ at $t \to \pm\infty$.

The theorem can be generalized to more complicated mass spectra and spins, if the one-particle space of the real intermediate particle lies nondegenerated outside of the mass continuum in the corresponding sector of the total Hilbert space. Furthermore, one-particle singularities can be exhibited in any connected many-body amplitude for scattering configurations which are uniformly nonoverlapping and where the incoming particles, which do not interact in the first collision, are causally independent of the outgoing particles not taking part in the second interaction.

III. CONCLUSION

The majorizations in the last section give a rigorous asymptotic meaning to space–time diagrams for certain many-body processes in almost local quantum field theory. Similar to the fact that the spatial cluster decomposition properties[18] of the S matrix display an $o(|\mathbf{a}|^{-\infty})$ law for large spacelike translations $|\mathbf{a}|$ of uniformly nonoverlapping wave packets, the rescattering limit is attained as $o(|t|^{-\infty})$ for scattering configurations, which involve dominant large spacelike separations.

Goldberger and Watson[15] have discussed the notion of a "time interval" in S-matrix theory. They postulate as a general property of relativistic quantum mechanics the factorization

$$S \to \prod_{i=1}^{n} S_i \qquad (3.1)$$

of the scattering amplitude describing n successive interactions if all the time intervals between the collisions tend to infinity. In the spirit of the theorem in Sec. 2 one can prove that (3.1) holds for causally

[18] K. Hepp, Helv. Phys. Acta **37**, 659 (1964).

independent scattering configurations, e.g., as graphically shown in Fig. 2 .The limit

$$\int \frac{d\mathbf{p}}{2\omega_p}\frac{d\mathbf{q}}{2\omega_q}\langle \hat{f}_1\hat{f}_2^{\text{out}} \mid \hat{f}_6\mathbf{p}^{\text{in}}\rangle^T \times \langle \hat{f}_3\hat{f}_4\mathbf{p}^{\text{out}} \mid \hat{f}_7\mathbf{q}^{\text{in}}\rangle^T\langle \hat{f}_5\mathbf{q}^{\text{out}} \mid \hat{f}_8\hat{f}_9^{\text{in}}\rangle^T$$

is attained faster than any power of t for $t \to +\infty$.

Certain timelike cluster decomposition properties[14] connected with the vacuum structure of the S matrix can also be derived, e.g., for the process characterized in Fig. 3. One chooses wave packets $\{\hat{f}_i\}$ centered around $\mathbf{p}_i$ with $p_1 + p_2 = p_5 + p_6$, $p_3 + p_4 = p_7 + p_8$, such that the two independent two-body scatterings in Fig. 3 are kinematically possible. If for all $\mathbf{q}_i \in \text{supp } \hat{f}_i$ $q_1 + q_2 - q_5 - q_6 \in U_\epsilon(o)$, $\epsilon > 0$ sufficiently small, $q_i^0 = \omega_i$, then by the spectral condition no real intermediate particle can be exchanged. If the wave packets $\{\hat{f}_i\}$ are uniformly nonoverlapping for all time translations

$$\hat{f}_i^t(\mathbf{q}) = \hat{f}_i(\mathbf{q}) \exp(i\omega t), \qquad i = 1, 2, 5, 6, \; t \geq 0,$$

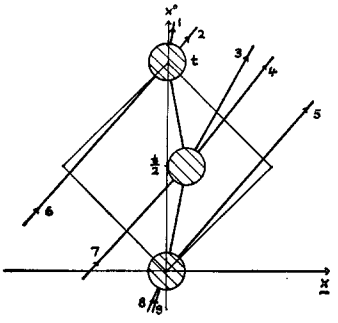

FIG. 2. Multiple Scattering.

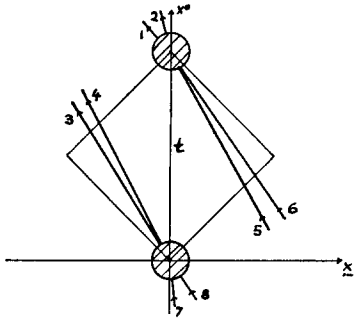

FIG. 3. Timelike Vacuum Structure.

and if the particles 3, 4 are causally independent of 5, 6, then one can show as before that

$$\lim_{t\to\infty}\langle \hat{f}_1^t\hat{f}_2^t\hat{f}_3\hat{f}_4^{\text{out}} \mid \hat{f}_5^t\hat{f}_6^t\hat{f}_7\hat{f}_8^{\text{in}}\rangle = \langle \hat{f}_1\hat{f}_2^{\text{out}} \mid \hat{f}_5\hat{f}_6^{\text{in}}\rangle\langle \hat{f}_3\hat{f}_4^{\text{out}} \mid \hat{f}_7\hat{f}_8^{\text{in}}\rangle \qquad (3.2)$$

is reached faster than any power of t.

These results illustrate that the S matrix in a relativistic almost local quantum field theory or in the Haag–Araki framework of local observables[19] displays much of the vacuum and one-particle structure, which one expects from physical common sense.

ACKNOWLEDGMENTS

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[19] H. Araki, *Einfuehrung in die axiomatische Quantenfeldtheorie* (Zürich, 1961/62).

Remarks on the Geometric Nature of Quantum Phase Space*

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Several geometric remarks on the foundations of quantum mechanics are presented. For example, quantum phase space is the tangent bundle to quantum configuration space.

1. INTRODUCTION

HERE I wish to point out several curious facts concerning the geometric properties of classical and quantum phase space. The first remark is that there is a way to prolong a classical observable to a quantum one. (However, this does not resolve the difficulties, pointed out most clearly by Van Hove,[1] concerning the quantization of classical systems whose Lagrangian is not of the simple type occurring in Newtonian particle dynamics.) The second remark is that the quantum phase space may be considered as the cotangent bundle to the quantum configuration space, just as the classical phase space may be identified with the cotangent bundle of configuration space, and that there is a 2-differential form on quantum phase space that plays the same role as the form $dp \wedge dq$ (p = momentum coordinate, q = position coordinate) does in classical mechanics.

2. QUANTUM AND CLASSICAL PHASE SPACE AND OBSERVABLES

We will work with the Hamiltonian viewpoint. For notational simplicity, we will consider a one-dimensional configuration space. Configuration and momentum space will be assigned to the variables q and p, respectively. Classical phase space Π is then the space of variables p, q. A classical observable is a real-valued function on Π. We will denote the ring of C^∞ real-valued functions on Π by $F(\Pi)$, and again merely for the sake of notational simplicity, will deal with observables that are in $F(\Pi)$. The Poisson bracket

$$(f, g) \to \{f, g\} = \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial g}{\partial p}$$

makes $F(\Pi)$ into a Lie algebra. Let ω be the 2-differential form $dq \wedge dp$. For fixed $f \in F(\Pi)$, the map $g \to X_f(g) = \{f, g\}$ is a *derivation* of the ring of functions, i.e. $X_f(g_1g_2) = X_f(G_1)g_2 + g_1X_f(g_2)$. By the general principles of differential geometry, X_f then defines a vector field on P, which generates (modulo certain global problems that we will ignore) a one-parameter transformation group on Π whose orbits are the integral curves of X_f. Alternately, the orbits of this group are the solutions of the Hamilton equations with Hamiltonian f, namely:

$$dq/dt = \partial f/\partial p; \qquad dp/dt = -\partial f/\partial q.$$

This one-parameter transformation group consists of *canonical transformations*, i.e., transformations of Π that preserve the form ω. Conversely, any one-parameter group of canonical transformations arises in this way from a function on Π. (If Π is a general manifold, one must specify that the first Betti number of Π be zero for this to be true.) The Lie algebras of the group of canonical transformations may be considered as the subalgebras of the Lie algebra of all vector fields on Π consisting of those for which the Lie derivative of ω is zero. The set of all vector fields is an (infinite-dimensional) Lie algebra with respect to the Jacobi bracket operation $(X, Y) \to [X, Y]$. Thus, the map $f \to X_f$ is a homomorphism of the Lie algebra defined by Poisson bracket onto the Lie algebra of the canonical group, with kernel the constant functions. As Van Hove points out,[1] quantum mechanics is concerned with representations of various subalgebras of the Lie algebra structure on $F(\Pi)$ in which the constant functions are *not* in the kernel.

Turn to the quantum mechanical system based on the classical one. According to the standard ideas, we construct the Hilbert space H of all square-integrable functions, say $q \to \psi(q)$, on configuration space, with the inner product

$$\langle \psi_1, \psi_2 \rangle = \int \psi_1(q)\bar{\psi}_2(q)\, dq.$$

Let $\mathbf{S}$ be the unit sphere in H, i.e., the set of $\psi \in H$ with $||\psi|| = 1$. $||\psi||$ is the associated norm, namely $\langle \psi, \psi \rangle^{\frac{1}{2}}$. The multiplicative group $\theta \to e^{i\theta}$ of complex

* Work performed in part under the auspices of the U. S. Atomic Energy Commission.
[1] L. Van Hove, Acad. Roy. Belg. Classe Sci. Mem. 261 1 (1951).

numbers of absolute value one acts on $\mathbf{S}$ (i.e., ψ goes into $e^{i\theta}\psi$), and the quantum phase space $\tilde{\Pi}$ is the "quotient" of $\mathbf{S}$ by this group, i.e., the space of orbits. Alternately, of course, one may consider $\tilde{\Pi}$ is the projective space of H, namely the set of all one-dimensional linear subspaces.

A given $\psi \in \mathbf{S}$ that is, let us say, continuous, may be given by its polar decomposition

$$\psi(q) = [P(q)]^{\frac{1}{2}} e^{iS(q)/\hbar}.$$

$P(q)$ is the density for a probability measure on configuration space, namely $P(q)dq$. Then, we may also consider $\tilde{\Pi}$ as the set of all pairs (P, S) of real-valued functions on configuration space, with $P(q) \geq 0$; $\int P(q)dq = 1$. Strictly speaking, two S's that differ by a constant must be identified, and this only gives a dense subset of the phase space defined from the entire Hilbert space, but we will not make this distinction in our notations. (This material is discussed in more detail in the recent book by G. W. Mackey[2].)

Now, a *classical* observable is just a real-valued function on Π. We have seen how the functions, modulo the constants, may be associated with the infinitesimal generators, i.e., the Lie algebra, of the basic group of classical mechanics, namely the canonical group. From the standard point of view, the basic group of quantum mechanics is the group of all unitary transformations of H. An infinitesimal generator of a one-parameter group of unitary transformations is a self-adjoint linear operator, say A, defined on a dense dimension $D(A)$ in H.

A self-adjoint operator A defines a real-valued function on $\tilde{\Pi}$, or at least on a dense subset, namely

$$f_A: \psi \to \langle A(\psi), \psi \rangle = f_A(\psi)$$

is real-valued, and, for $\psi \in \mathbf{S}$, is invariant under the group action on $\mathbf{S}$, hence passes to the quotient to define a real-valued function on $\tilde{\Pi}$. This suggests that we consider the "quantum observables" to be the set of real-valued functions on $\tilde{\Pi}$. Notice, however, that the functions f_A defined by self-adjoint operators do not exhaust all such functions, for example, the product $f_A f_B$ will not necessarily be an adjoint operator.

This has all been review; now we come to the point, namely asking whether a classical observable may be considered as a quantum one, i.e., as a real-valued function on $\tilde{\Pi}$. Suppose then that $f \in F(\Pi)$. We can now extend f to give a function $\tilde{f}$ on $\tilde{\Pi}$ by the formula

$$\tilde{f}(P, S) = \int f(q, \partial S/\partial q)P(q)\, dq.$$

We can now *embed* Π in $\tilde{\Pi}$ so that $\tilde{f}$ appears as an *extension* of f. Namely, associate with each point $(q_0, P_0) \in \Pi$ the element $(P, S) \in \tilde{\Pi}$, where:

$$P(q) = \delta_{q_0}(q),$$

i.e., P is the Dirac delta function concentrated at q_0;

$$S(q) = p_0 q,$$

i.e., S is "plane wave" in configuration space with "momentum" P_0.
With this choice of P and S,

$$\tilde{f}(P, S) = \int f(q, p_0)\delta_{q_0}\, dq = f(p_0, q_0),$$

i.e., $\tilde{f}$ restricted to Π is just f. Of course, this way of identifying Π with a subset of $\tilde{\Pi}$ is not strictly consistent with the Hilbert-space definition of $\tilde{\Pi}$ since $\delta_{q_0}^{\frac{1}{2}} \exp(ip_0 q/h)$ cannot, in any reasonable way, be identified with an element of the Hilbert space. However, we shall not go into this point, beyond remarking that this fits in with other indications that the standard Hilbert-space framework is not really adequate for quantum mechanics.

We may ask: For which $f \in F(\Pi)$ is there a self-adjoint operator A such that $\tilde{f} = f_A$? We do not have a definitive answer for this, but shall proceed to certain examples.

(a) f is a function of q alone. A be the operator $\psi \to f\psi$, i.e., multiplication by f. Then, for $\psi = (P^{\frac{1}{2}}e^{iS/\hbar})$

$$\int A(\psi)\bar{\psi}\, dq = \int f(q)P(q)\, dq = \tilde{f}(P, S),$$

i.e., $\tilde{f} = f_A$.

(b) Let $A = ci(\partial/\partial q)$, with c a real constant, defined as usual as a self-adjoint operator

$$\begin{aligned}\langle A(\psi), \psi \rangle &= ci \int \frac{\partial}{\partial q}(Pe^{iS/\hbar})^{\frac{1}{2}}(Pe^{-iS/\hbar})^{\frac{1}{2}}\, dq \\ &= ci \int \left[\frac{1}{2}\frac{\partial p}{\partial q} + P\frac{i}{\hbar}\frac{\partial S}{\partial q}\right] dq \\ &= -\frac{c}{\hbar}\int \frac{\partial S}{\partial q}P(q)\, dq.\end{aligned}$$

If $c = -h$, $f = p$, then $f_A = \tilde{f}$, i.e., momentum p corresponds to $-hi\,\partial/\partial q$.

Thus, (a) and (b) give the usual quantitization rules for the position and momentum observables.

(c) Let $A = \partial^2/\partial q^2$.

[2] G. W. Mackey, *The Mathematical Foundations of Quantum Mechanics* (W. A. Benjamin, Inc., New York, 1963).

$$f_A(\psi) = \langle A(\psi), \psi\rangle = \int \frac{\partial^2}{\partial q^2}(\psi), \bar{\psi}\, dq$$

$$= -\int \frac{\partial}{\partial q}(\psi)\frac{\partial}{\partial q}(\bar{\psi})\, dq$$

$$= -\int \left(\frac{1}{2(P)^{\frac{1}{2}}}\frac{\partial P}{\partial q}e^{iS/\hbar} + \tfrac{1}{4}\psi\frac{\partial S}{\partial q}\right) \times \left(\frac{1}{2(P)^{\frac{1}{2}}}\frac{\partial P}{\partial q}e^{-iS/\hbar} - \frac{i}{\hbar}\bar{\psi}\frac{\partial S}{\partial q}\right) dq$$

$$= -\int \left[\frac{1}{4P}\left(\frac{\partial P}{\partial q}\right)^2 + \frac{1}{\hbar^2}\left(\frac{\partial S}{\partial q}\right)^2 P(q)\right] dq.$$

Put $f(p, q) = p^2$, i.e., f is the Hamiltonian for a free particle. Then

$$f_A(\psi) = -\hbar^{-2}\bar{f}(P, q) - \frac{1}{4}\int \frac{\partial}{\partial q}(\log P)\frac{\partial}{\partial q}(\log P)P(q)\, dq.$$

Thus, when we take the classical observable to be quadratic in momentum, we see the usual difficulties in "quantizing" a classical system reappear. However, it might be interesting to investigate the physical meaning of the deviation term, which can also be written as

$$\frac{1}{4}\int \frac{\partial^2}{\partial q^2}(\log P)P \log P(q)\, dq.$$

Here we make contact with certain well-known speculations by Bohm[3] into a possible "causal" approach to quantum mechanics. An additional point of interest is that

$$\int P(q) \log P(q)\, dq$$

is the entropy of the probability distribution. If P is a Gaussian distribution, then $(\partial^2/\partial q^2)(\log P)$ is a constant, hence the deviation is essentially the entropy.

3. QUANTUM PHASE SPACE AS THE COTANGENT BUNDLE OF CONFIGURATION SPACE.

If the configuration space of a classical problem is a manifold M, then (from the Hamiltonian point of view) "phase space" is its cotangent bundle.[2] (From the Lagrangian viewpoint, the tangent bundle is the phase space.) If q is a point of M, a tangent vector is an eigenvalence class of curves passing through q, with two curves identified if they have a first-order contact at q. M_q, the tangent space at q, is the set of tangent vectors. It can be made into a vector space; the cotangent space, M_q^*, is the dual space of M_q. The cotangent bundle is then the union of the M_q^*, where q ranges over M. We denote the cotangent bundle by $T^*(M)$. Quantum mechanics involves configuration spaces that are infinite-dimensional manifolds. Now, the intensive mathematical study of this subject has just begun. For example, one can find a treatment of those manifolds that are "modeled" on a Banach space in a recent book by Lang.[4] While these are too restrictive for the purposes of quantum mechanics (for example, the space of probability-measures is not of this type) it can serve as a guide to further development.

Now, the quantum configuration space corresponding to a classical problem is just the space of all probability distributions on the classical configuration space. We want to show how its cotangent bundle can be identified with the space $\tilde{\Pi}$ constructed in the last section.

Again, for simplicity we will only consider a one-dimensional classical configuration space, with variable q. If $t \to P^t(q)$ is a curve in the space of probability distributions, with $P^0(q) = P(q)$, then the function

$$q \to (\partial/\partial t)P^t(q)|_{t=0} = Q(q)$$

should represent its "tangent vector." Now

$$\int Q(q)\, dq = \frac{d}{dt}\int P^t(q)\, dq|_{t=0} = 0. \qquad (3.1)$$

Hence, the space of all functions Q satisfying (3.1) should be the "tangent space" to a point of quantum configuration space. A linear form on this tangent space is the form $Q \to \int Q(q)S(q)dq$, for a function $q \to S(q)$. If $S(q)$ is constant, this linear form is zero. Then, we should identify a point in the cotangent bundle within a pair (P, S), with the such pairs identified if their S's differ by a constant. We then see how the cotangent bundle can be identified with the space $\tilde{\Pi}$ considered in Sec. 2.

Now, in classical mechanics, a fundamental role is played by the two-differential form $\omega = dp \wedge dq$. This form is just a skew-symmetric bilinear form on the tangent space to the cotangent bundle. We should look for the corresponding object for quantum phase space. For a linear space, the tangent bundle to the cotangent bundle may be regarded as a direct sum of the tangent bundle and cotangent bundle. Then, a "tangent vector" to a "point" (P, S) of the cotangent bundle $\tilde{\Pi}$ should be regarded as pair (Q, S'), with Q satisfying (3.1). The two-differential

[3] D. Bohm, Phys. Rev. 65 166 (1952).

[4] S. Lang, *Introduction to Differentiable Manifolds*, Interscience Publishers, Inc., New York, 1962).

form on $\tilde{\Pi}$ corresponding to ω is that which assigns to the pair (Q, S') and (Q_1, S_1') of tangent vectors to the cotangent bundle the number

$$\int QS_1'(q), -Q_1S'(q)\, dq. \tag{3.2}$$

Let us check that this gives a result compatible with the embedding of Π into $\tilde{\Pi}$. Let $t \to (q(t), p(t))$ be a curve in Π. It goes over into the curve $t \to (\delta_{q(t)}, p(t)q)$ in $\tilde{\Pi}$. Now the tangent vector to the curve $t \to \delta_{q(t)}$ is not really a function, but functional assigning the value $(\partial f/\partial q)(q(t))(dq/dt)$ to a function f on q-space. Then, if $t \to (q_1(t), p_1(t))$ is another such curve in Π, the value of the form 3.2 on the tangent vectors to the image curves in $\tilde{\Pi}$ is

$$\frac{dq(t)}{dt}\frac{dp_1(t)}{dt} - \frac{dp(t)}{dt}\frac{dq_1(t)}{dt},$$

i.e., just the number that the form $\omega = dq \wedge dp$ assigns to the tangent vectors to these curves in Π. So, we may say that the differential form on $\tilde{\Pi}$ defined by (3.2) is, when restricted to the subset Π, just the form ω on Π. Finally, give such a 2-form on $\tilde{\Pi}$ enables us to calculate the "Hamilton equations" corresponding to any in real-valued function on $\tilde{\Pi}$. The result for a function of the form

$$\tilde{f}(P, S) = \int f(q, \partial S/\partial q)P(q)\, dq$$

is readily found to be

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial q}\left(\frac{\partial f}{\partial p}\left(q, \frac{\partial S}{\partial q}\right)P(q)\right) = 0,$$

$$\frac{\partial S}{\partial t} + f\left(q, \frac{\partial S}{\partial q}\right) = 0.$$

The second equation is just the Hamilton–Jacobi partial differential equation. A solution generates a flow on q-space whose orbits are the solutions of

$$dq/dt = \partial f/\partial p(q, \partial S/\partial q).$$

The first equation then says that $P(q,t)\, dq$ is just the probability measure obtained by transforming the initial one under this flow. Then, the dynamics on $\tilde{\Pi}$ generated by $\tilde{f}$ is the extension of the dynamics on Π generated by f. In this geometric picture, the dynamics associated with quantum mechanics is generated by a different sort of function than one merely obtained by extending a classical observable in the way we have explained. It would be interesting to give a characterization of the type of functions on $\tilde{\Pi}$ that do give rise to quantum dynamics in terms of the intrinsic geometric structure of $\tilde{\Pi}$, but we have as yet no answer to this.

Solution of an Integral Equation in $V-\theta$ Scattering

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The Muskhelishvili method is used to obtain the off-the-mass- shell $V-\theta$ scattering amplitude.

I. INTRODUCTION

RECENTLY a complete solution of the Lee model[1] in the $V-\theta$ sector has been given,[2,3] thus completely determining the $V-\theta$ scattering state in terms of bare states. We present a solution of the integral equation that is central to this problem by using the Muskhelishvili[4] method thereby settling the question of uniqueness, while at the same time providing a systematic approach to a new class of integral equations.

II.

The bare $V-\theta$ scattering wavefunction obeys the integral equation

$$\psi(\omega,\omega_0) = -\frac{1}{\omega}-\frac{1}{\pi}\int_\mu^\infty \frac{\operatorname{Im} h^+(\omega')\,d\omega'}{\omega'+\omega-\omega_0-i\epsilon}\frac{\psi(\omega',\omega_0)}{h^-(\omega_0-\omega')}, \quad (1)$$

where

$$h(z) = z+\frac{z^2}{\pi}\int_\mu^\infty \frac{U(\omega')\,d\omega'}{\omega'(\omega'-z)} \quad (2)$$

$$h^+(\omega) = h(\omega+i\epsilon)$$

$$h^-(\omega_0-\omega) = h(\omega_0-\omega+i\epsilon).$$

It will be assumed that

$$\lim_{\omega\to\infty}(h(\omega)/\omega) = Z, \qquad 0<Z<1. \quad (4)$$

The integral equation above is conveniently transformed to

$$M(\omega) = \frac{\omega-\omega_0}{h^-(\omega_0-\omega)} \times\left[C+\frac{1}{\pi}\int_\mu^\infty \frac{\operatorname{Im} h^+(\omega')\,d\omega'}{\omega'+\omega-\omega_0-i\epsilon}\frac{M(\omega')}{\omega'}\right], \quad (5)$$

where

$$M(\omega) = \frac{\omega(\omega-\omega_0)\psi(\omega,\omega_0)}{h^-(\omega_0-\omega)} \quad (6)$$

$$C = -1-\frac{1}{\pi}\int_\mu^\infty \frac{\operatorname{Im} h^+(\omega')}{\omega'-\omega_0+i\epsilon}\frac{M(\omega')}{\omega'}\,d\omega'.$$

Let

$$\mathfrak{M}(z) \equiv \frac{z-\omega_0}{h(\omega_0-z)} \times\left[C+\frac{1}{\pi}\int_\mu^\infty \frac{\operatorname{Im} h^+(\omega')\,d\omega'}{\omega'+z-\omega_0}\frac{M(\omega')}{\omega'}\right]; \quad (7)$$

it follows by comparison of Eqs. (5) and (7) that

$$\mathfrak{M}(\omega-i\epsilon) \equiv \mathfrak{M}^-(\omega) = M(\omega). \quad (8)$$

Replacing Eq. (8) in (7) it becomes

$$\mathfrak{M}(z) = \frac{z-\omega_0}{h(\omega_0-z)} \times\left[C+\frac{1}{\pi}\int_\mu^\infty \frac{\operatorname{Im} h^+(\omega')\,d\omega'}{\omega'+z-\omega_0}\frac{\mathfrak{M}^-(\omega')}{\omega'}\right]. \quad (9)$$

Defining

$$H(z) \equiv h(\omega_0-z)/(z-\omega_0) \quad (10)$$

and using Eq. (9) it follows that

$$\mathfrak{M}^+(\omega)-\mathfrak{M}^-(\omega) = 2i[\operatorname{Im} H^-(\omega)/H^+(\omega)] \times(\mathfrak{M}^-(\omega)+\mathfrak{M}^+(\omega_0-\omega)). \quad (11)$$

It is clear from Eq. (9) or (11) that $\mathfrak{M}(z)$ has a cut for all real z such that

$$\omega_0-\mu > z. \quad (12)$$

We first restrict ω_0 so that, for all real z satisfying Eq. (12), $\mathfrak{M}(\omega_0-z)$ has no cut. This is satisfied for all $\omega_0<2\mu$. The solution that is obtained under this restriction can further be analytically continued to complex ω_0 at the end.

Letting

$$\mathfrak{N}(z) \equiv \mathfrak{M}(z)+\mathfrak{M}(\omega_0-z) \quad (13)$$

[1] T. D. Lee, Phys. Rev. **95**, 1329 (1954); G. Källén and W. Pauli, Kgl. Danske Videnskab. Selskab Mat.-Fys. Medd. **30**, No. 7 (1955).
[2] R. P. Kenschaft and R. D. Amado, J. Math. Phys. **5**, 1340 (1964).
[3] A. Pagnamenta, $V\theta$-Bound State and Uniqueness in the three Particle Sector of the Lee Model (preprint)
[4] N. I. Muskhelishvili, Singular Integral Equations (P. Noordhoff Ltd. Groningen, The Netherlands, 1953).

and $\omega < \omega_0 - \mu$, it follows from Eq. (11) that

$$\mathfrak{N}^+(\omega) - \mathfrak{N}^-(\omega) = 2i[\text{Im } H^-(\omega)/H^+(\omega)]\mathfrak{N}^-(\omega). \quad (14)$$

For $\omega > \omega_0 - \mu$ using Eqs. (9), (10), and (13) gives

$$\mathfrak{N}^+(\omega) - \mathfrak{N}^-(\omega) = -2i[\text{Im } H^+(\omega_0 - \omega)/H^-(\omega_0 - \omega)] \times (\mathfrak{M}^+(\omega_0 - \omega) + \mathfrak{M}^-(\omega)), \quad (15)$$

since in this interval $\mathfrak{M}^-(\omega) = \mathfrak{M}^+(\omega)$, Eq. (15) becomes

$$\mathfrak{N}^+(\omega) - \mathfrak{N}^-(\omega) = -2i[\text{Im } H^+(\omega_0 - \omega)/H^-(\omega_0 - \omega)]\mathfrak{N}^+(\omega). \quad (16)$$

Equations (14) and (16) define a homogeneous Muskhelishvili problem such that

$$\mathfrak{N}^+(\omega) = g(\omega)\mathfrak{N}^-(\omega), \quad (17)$$

where

$$g(\omega) = H^-(\omega)/H^+(\omega) \quad \text{if} \quad \omega < \omega_0 - \mu$$
$$g(\omega) = H^-(\omega_0 - \omega)/H^+(\omega_0 - \omega) \text{ if } \omega > \omega_0 - \mu. \quad (18)$$

The solution of Eq. (17) is

$$\ln \mathfrak{N}(z) = \text{Pn}(z) + \frac{1}{2\pi i}\int_{-\infty}^{+\infty} \frac{\ln g(\omega)}{\omega - z}\, d\omega, \quad (19)$$

where $\text{Pn}(z)$ is a polynomial of degree n. After substitution from (18) into Eq. (19)

$$\ln \mathfrak{N}(z) = \text{Pn}(z) - \ln (H(\omega_0 - z)H(z)). \quad (20)$$

Equation (4) has been used in going from Eq. (19) to (20). Since $\mathfrak{M}(z) \to \text{const}$ as $z \to \infty$, it follows that Pn (z) must be a constant, hence

$$\mathfrak{N}(z) = \beta/H(\omega_0 - z)H(z). \quad (21)$$

To determine $\mathfrak{M}(z)$ it is convenient to rewrite Eq. (11) as

$$\mathfrak{M}^+(\omega) - \mathfrak{M}^-(\omega) = 2i[\text{Im } H^-(\omega)/H^+(\omega)]\mathfrak{N}^-(\omega).$$

It should be emphasized that $\mathfrak{M}(z)$ has a cut only for $\omega < \omega_0 - \mu$. The function $\mathfrak{M}(z)$ satisfying these conditions is

$$\mathfrak{M}(z) = \text{Pn}'(z) - \frac{1}{\pi}\int_{\mu}^{\infty} \frac{d\omega'}{\omega' + z - \omega_0} \times \frac{\text{Im } H^+(\omega_0 - \omega')}{H^-(\omega_0 - \omega')}\, \mathfrak{N}^+(\omega_0 - \omega'). \quad (22)$$

The polynomial Pn′ (z) is seen to be a constant by the argument following Eq. (20). Substitution of Eq. (21) into (22) yields

$$\mathfrak{M}(z) = \alpha - \frac{\beta}{\pi}\int_{\mu}^{\infty} \frac{d\omega'}{\omega' + z - \omega_0} \frac{1}{H^+(\omega')} \times \text{Im } \frac{1}{H^-(\omega_0 - \omega')}. \quad (23)$$

From Eqs. (4) and (5) it follows that

$$\lim_{z\to\infty} \mathfrak{N}(z) = \beta/Z^2,$$

and comparing this with Eqs. (13) and (23) shows that

$$2\alpha = \beta/Z^2. \quad (24)$$

We now turn to the determination of α. From Eq. (1) it follows that

$$\lim_{\omega\to 0} \omega\psi(\omega, \omega_0) = -1,$$

which is combined with Eqs. (6) and (8) to give

$$\mathfrak{M}^-(0) = \omega_0/h^+(\omega_0). \quad (25)$$

Substituting Eqs. (10) and (24) into (23) yields

$$\mathfrak{M}(z) = \alpha\left[1 + \frac{2Z^2}{\pi}\int_{\mu}^{\infty} \omega'\, d\omega' \frac{1}{h^+(\omega_0 - \omega')} \text{Im } \frac{1}{h^-(\omega')} - 2z\frac{Z^2}{\pi}\int_{\mu}^{\infty} \frac{\omega'\, d\omega'}{\omega' + z - \omega_0} \frac{1}{h^+(\omega_0 - \omega')} \text{Im } \frac{1}{h^-(\omega')}\right];$$

this is simplified further by comparison with (25) to become

$$\mathfrak{M}(z) = \omega_0/h^+(\omega_0) + 2zZ^2\alpha A(z, \omega_0), \quad (26)$$

where

$$A(z, \omega_0) = -\frac{1}{\pi}\int_{\mu}^{\infty} \frac{\omega'\, d\omega'}{\omega' + z - \omega_0} \frac{1}{h^+(\omega_0 - \omega')} \times \text{Im } \frac{1}{h^-(\omega')}.$$

To transform this to the form given in Ref. 2 we note that from Eqs. (13), (25), and (26)

$$\mathfrak{N}^+(\omega_0) = \mathfrak{M}^+(\omega_0) + \mathfrak{M}^-(0) = 2\omega_0/h^+(\omega_0) + 2Z^2\alpha\omega_0 A^+(\omega_0, \omega_0), \quad (27)$$

and that from Eq. (21) and (24)

$$\mathfrak{N}^+(\omega_0) = 2\alpha Z^2 \cdot \omega_0/h^+(\omega_0). \quad (28)$$

Eliminating αZ^2 between Eqs. (27) and (28) gives

$$\mathfrak{M}(z) = \frac{\omega_0}{h^+(\omega_0)} + \frac{2zA(z, \omega_0)}{1 - h^+(\omega_0)A^+(\omega_0, \omega_0)}.$$

This result agrees with that of Refs. 2 and 3.

On the Structure of the Finite Parts of the Generating Functional of Propagators in Quantumelectrodynamics

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Starting from their generating functional, we investigate the structure of the finite and divergent parts of propagators in quantum electrodynamics. A renormalizability condition is expressed by means of a set of recursion formulas between the finite parts of radiative corrections of the generating functional; this condition is the algebraic formulation of Salam's rule for the extraction of finite parts from divergent integrals. The former sets of equation should finally allow the actual computation of the radiative correction of higher orders.

1. INTRODUCTION

In the frame of the axiomatic formulation of quantum field theory, the vacuum expectation values of time-ordered products of field operators can be obtained as the coefficients of the expansion at the value $J = 0$ of a functional

$$u[J/g, m]$$

of the argument $J(x)$. This functional, called *generating functional*, depends also of numerical parameters g, m describing the particles of the field.[1] As a matter of fact, this is just a way of speaking, since in all cases of physical interest, expectation values of this type are expressed by integrals of products of Schwartz distributions and neither the generating functional nor its coefficients have any kind of meaning. Renormalization theory is a collection of rules sometimes heuristic, for the extraction and interpretation of meaningful results. In a former paper,[2] we studied the most general form of the divergent terms of a renormalizable field theory without specification of type of interaction.

In this paper, we are studying quantumelectrodynamics: it turns out that the most suitable formulation for the renormalization of a theory with a given interaction is the one known as functional formulation which leads to the expression of the generating functional $u[\cdots]$ of the propagators (see Ref. 1 and Appendix III). We recall in Sec. 2 the form and some of the properties of this generating functional. Section 3 deals with regularization methods and renormalization constants, the renormalization being introduced by means of formal series. Its main result is expressed by formula (3.7) which can be easily proved, if all concerned functions and functionals are supposed to be well defined and all series to be convergent. Its extension to formal series requires some intricate—but by no means difficult—considerations given in Appendix I. However, it is to be noted that the introduction of formal series, though important for a correct and rigorous formulation, is specially intended for a mathematically minded reader. An important consequence of formula (3.7) is examined in Sec. 4 where a renormalizability condition is expressed by the recursion formulas (4.8) between the finite parts of the unrenormalized radiative corrections of the generating functional of Quantumelectrodynamics. It is then verified in Sec. 5 that this condition is identical with Salam's extraction rule of finite parts, from divergent integrals. Returning to the recursion formulas (4.8), in Sec. 5, we solve them and obtain explicitly the general form of the divergent terms in Quantumelectrodynamics.

We finally give in Appendices I and II, some methods of calculations and some formulas which may be useful for the understanding of this paper.

2. FORMAL EXPRESSIONS FOR THE GENERATING FUNCTIONAL

For quantumelectrodynamics, the generating functional u is a Lorentz-invariant functional (scalar)

$$u_0[\eta, \bar{\eta}, J/e, m]$$

of the arguments $\eta(x)$, $\bar{\eta}(x)$, and $J(x)$. The functions of x, η, and $\bar{\eta}$ are spinor-valued functions, whose components anticommute; they are called sources of the electron field. The function J is a vector-valued function, whose components $J_\mu(x)$ are c-

[1] H. Lehman, K. Symanzik, and W. Zimmerman, Nuovo Cimento **1**, 1425 (1955); K. Symanzik, Z. Naturforsch. **9**, 809 (1954); H. Umezawa and A. Visconti, Nuovo Cimento **1**, 1079 (1955).

[2] A. Visconti and Y. Le Gaillard, Nuovo Cimento **34**, 914 (1964). For a more rigorous foundation of this formalism (using formal series, regularization, etc.) and for application to the renormalization of two point propagators in general and for simple models, see J. Soffer and A. Visconti, *ibid.* **38**, 917 (1965).

numbers; it is the source of the photon field. {We adopt the metric: $x = (\mathbf{x}, x_4 = ix_0)$, the greek indices run from 1 to 4. Furthermore the $\eta_\alpha(x)$ are elements of a Grassman algebra and as functions of x, they belong to the $\mathfrak{D}$ space of indefinitely derivable functions with compact support [see discussion below after formulas (2.2)].} The functional u depends also on two parameters e and m which represent, respectively, the charge and mass of the electrons. Finally, the propagators are the functional derivatives of u for $\eta(x)$, $\bar{\eta}(x)$, $J(x) \equiv 0$.[3]

The generating functional $u_0[\eta, \bar{\eta}, J/m, \kappa]$ for the free fields has a particularly simple form,

$$u_0[\eta, \bar{\eta}, J/m, \kappa] \equiv \exp\left\{-\frac{1}{2}\int \bar{\eta}_\alpha(x) S^{(c)}_{\alpha\beta}(x - x')\eta_\beta(x') - \frac{1}{4}\int J_\mu(x)\Delta^{(c)}(x - x', \kappa)J_\mu(x')\right\} \equiv u_0[\eta, \bar{\eta}/m]u_0[J/\kappa], \tag{2.1}$$

where integrations and summations have to be preformed over all repeated variables or indices. It is a matter of straightforward calculation to show that the derivatives of $u_0[\eta, \bar{\eta}, J/m, \kappa]$ for $\eta, \bar{\eta}, J = 0$ give indeed the well-known propagators of the free fields.

We also remark that the photon propagator $\Delta^{(c)}(x, \kappa)$ satisfies the equation

$$(\Box_x - \kappa)\Delta^{(c)}(x, \kappa) = 2i\delta(x), \tag{2.2a}$$

i.e., the photon is supposed to be a particle of mass $\kappa^{\frac{1}{2}}$, we avoid in this way all discussions about infrared divergences. Note that

$$S^{(c)}(x, m) = (\gamma\partial - m)\Delta^{(c)}(x, m^2). \tag{2.2b}$$

Furthermore, it has to be remarked that $u_0[\cdots]$ is a well-defined functional of Fréchet–Volterra type, as one can see for $u_0[J/\kappa]$, provided that each $J_\rho(x)$ belongs to S space (i.e., is an indefinitely derivable function and its product and the products of its derivatives by any polynomial in x tend to 0 when the argument tends to ∞). The study of $u_0[\eta\bar{\eta}/m]$ requires some more intricate considerations since $\eta_\alpha(x)$ and $\bar{\eta}_\alpha(x)$ belong to a Grassman algebra.

Let us now come back to the generating functional $u[\cdots]$ of the interacting fields; a formal calculation shows that one obtains all the Feynman diagrams, as predicted by the conventional theory of quantumelectrodynamics, by defining $u[\cdots]$ as follows:

$$u[\eta, \bar{\eta}, J/e, m, \kappa] = \exp\left\{ie\int d\xi\, \Gamma(\xi)\right\}u_0[\eta, \bar{\eta}, J] \equiv \sum_{n=0}^{\infty}\frac{(ie)^n}{n!}\int d\xi_n \cdots d\xi_1\, \Gamma(\xi_n)\cdots\Gamma(\xi_1) \times u_0[\eta, \bar{\eta}, J/m, \kappa] \equiv u_0[\eta, \bar{\eta}, J] + \sum_{n\geq 1}\frac{e^n}{n!}u_n[\eta, \bar{\eta}, J/m, \kappa], \tag{2.3}$$

where $\Gamma(\xi)$ is the differential operator:

$$\Gamma(\xi) = \frac{\delta}{\delta\eta_\alpha(\xi)}\gamma^\mu_{\alpha\beta}\frac{\delta}{\delta\bar{\eta}_\beta(\xi)}\frac{\delta}{\delta J_\mu(\xi)}. \tag{2.4}$$

One has to take into account the anticommuting properties of the spinor sources in the evaluation of the functional derivatives.[4] The expansion (2.3), is, as is well known, only symbolic; for instance, the first perturbative term $u_1[\cdots]$ reads

$$u_1[\eta, \bar{\eta}, J/m, \kappa] = i\int d\xi\, \Gamma(\xi)u_0[\eta, \bar{\eta}, J/m, \kappa] = -\frac{i}{(2)^3} \times \int \bar{\eta}_\alpha(x)S^{(c)}_{\alpha\beta}(x - \xi, m)\gamma^\mu_{\beta\rho}S^{(c)}_{\rho\sigma}(\xi - y, m)\eta_\sigma(y) \times \Delta^{(c)}(\xi - \zeta, \kappa)J_\mu(\zeta)u_0[\eta, \bar{\eta}, J] + \frac{i}{(2)^2}\operatorname{Tr}(S^{(c)}(0)\gamma_\mu) \times \int d\xi\, d\zeta\, \Delta^{(c)}(\xi - \zeta)J_\mu(\zeta)u_0[\eta, \bar{\eta}, J], \tag{2.5}$$

where integrations and summations over repeated variables shall be performed. We note that even in this particularly simple case, there is a divergence since, in distribution theory, there is no way to define $S^{(c)}(0)$.

As a matter of fact, this type of divergence could be easily avoided, one needs only a redefinition of $\Gamma(\xi)$ such that no physical result is changed. In conventional quantum field theory, one reaches this result by using Wick's ordered products, in functional formalism, we shall simply replace $\Gamma(\xi)$ by $:\Gamma(\xi):$ defined as follows:

$$:\Gamma(\xi): = \lim_{\xi_2 = \xi_1 = \xi}\left\{\frac{\delta}{\delta\eta_\alpha(\xi_2)}\gamma^\mu_{\alpha\beta}\frac{\delta}{\delta\bar{\eta}_\beta(\xi_1)} + \tfrac{1}{2}\operatorname{Tr}[\gamma_\mu S^{(c)}(\xi_1 - \xi_2, m)]\right\}\frac{\delta}{\delta J_\mu(\xi)}. \tag{2.6}$$

It is now a matter of very simple algebra to verify

[3] For the definition of functional derivatives considered as distributions, see M. B. Donsker and J. L. Lions, Acta Math. **108**, 148 (1962).

[4] J. Schwinger, Proc. Natl. Acad. Sci. U. S. **37**, 452, 455 (1951); K. Symanzik, J. Math Phys. **1**, 249 (1960); A. Visconti and J. Carmona, Nuovo Cimento **29**, 742 (1963).

that the first approximation of the generating functional defined by

$$u[\eta, \bar{\eta}, J/e, m, \kappa] = \exp\left(ie \int d\xi \, :\Gamma(\xi):\right) u_0[\eta, \bar{\eta}, J/m, \kappa] \quad (2.7)$$

becomes

$$u_1[\eta, \bar{\eta}, J/m, \kappa] = i \int d\xi : \Gamma(\xi) : u_0[\eta, \bar{\eta}, J/m, \kappa] \quad (2.8)$$

and is a "well-defined" functional (see Appendix III), since the subtracted term in (2.6) eliminates the term which degenerates into $S^{(c)}(0)$ at the limit $\xi_1 = \xi_2 = \xi$. We may also remark that the former difficulty does not really occur in quantumelectrodynamics, since through Furry's theorem Tr $\{\gamma_\mu S^{(c)}(0)\} = 0$. Consider now divergences of higher-order approximations, their interpretation and elimination become rapidly an overhelming task. Renormalization theory tries to state in a precise form the rules for the extraction and calculation of finite parts from divergent integrals and their physical interpretations.

3. REGULARIZATION, RENORMALIZATION, AND FORMAL SERIES FOR THE GENERATING FUNCTIONAL

We want now to give a meaning to the symbolical quantity $u[\eta, \bar{\eta}, J/e, m, \kappa]$: our first step will consist in the regularization of each of its perturbative approximations $u_n[\eta, \bar{\eta}, J/m, \kappa]$. Then, since each of its terms is supposed to be meaningful, we shall be able to consider $u[\cdots]$ as the sum of the *formal* series (2.3), i.e., the functional $u[\cdots]$ will represent the set of Fréchet–Volterra functionals $\{u_n^{(\mathrm{reg})}[\eta, \bar{\eta}, J/m, \kappa]\}$ and we shall apply to $u[\cdots]$ the known rules about the calculations of formal series (product of formal series, inverse of a formal series, substitution of a formal series into another, etc ...).[5] The rules for the regularization of divergent integrals can be developed within the frame of distribution theory.[6] They can be most easily formulated as follows: F being a meaningless integral of a well-defined function $f(x)$ (a rational function for instance), we consider the integral

$$F(\lambda) = \int f(x, \lambda)\, dx, \quad (3.1)$$

where $f(x, \lambda)$ is substituted to $f(x)$ and is defined in such a way that $F(\lambda)$ is meaningful and that for $\lambda = \lambda_0$, $f(x, \lambda)$ becomes identical (converges uniformly for instance) to $f(x)$:

$$f(x, \lambda_0) \equiv f(x). \quad (3.2)$$

The choice of $f(x, \lambda)$ contains, of course, a large part of arbitrariness and the same happens to the next step when one defines another function of λ, say $\mathfrak{D}F(\lambda)$ such that

$$\lim_{\lambda=\lambda_0} [F(\lambda) - \mathfrak{D}F(\lambda)] \equiv \mathcal{P}F \quad (3.3)$$

becomes now a well defined quantity, generally, a distribution. $\mathfrak{D}F(\lambda)$ is called the *divergent part* of $F(\lambda)$ (since it is divergent indeed for $\lambda = \lambda_0$) and $\mathcal{P}F$ is the *finite* part of F and is indeed a well defined quantity for $\lambda = \lambda_0$. Coming back to quantum-electrodynamics, it is known that the Pauli–Villars regularization method is a realization of the first step of the mathematical techniques we just alluded to. We do not want to examine in detail the possible regularization methods, but shall rather focus our attention on the step following the regularization, namely the determination of the finite and divergent parts of the radiative corrections, i.e., $\mathcal{P}u_n[\eta, \bar{\eta}, J/m, \kappa]$ and $\mathfrak{D}u_n^{(\mathrm{reg})}[\eta, \bar{\eta}, J/m, \kappa]$, as prescribed by renormalization theory. In order to state precisely the content of this theory, we need to introduce a few definitions. Let us note, first of all, that since we are going to work with regularized quantities in the remaining of this paper, we shall avoid most of the time, for simplicity's sake, the index (reg).

As a provisional hypothesis, suppose then $u[\eta, \bar{\eta}, J/e, m, \kappa]$ to be a well-defined Fréchet–Volterra functional and consider the following c-number quantities called renormalization constants

$$\mathfrak{N}(e, m, \kappa), \quad Z_2(e, m, \kappa), \quad Z_3(e, m, \kappa), \quad e_0(e, m, \kappa),$$
$$m_0(e, m, \kappa), \quad \kappa_0(e, m, \kappa), \quad \text{and} \quad Z_1(e, m, \kappa) \quad (3.4)$$

defining respectively a normalization factor of the generating functional; a change of scale of the spinor sources (defined by Z_2); a change of scale of the boson source (defined by Z_3); the replacement of the observed charge e, the observed masses m of the electrons and $\kappa^{\frac{1}{2}}$ of the boson by the bare charge e_0 and the bare masses m_0 and κ_0. It will

[5] For a general definition of formal series, see N. Bourbaki, *Algèbre* (Hermann & Cie, Paris, 1962), Vol. 2, Chap. IV, Sec. 5. The less mathematically minded reader may consult H. Cartan, *Théorie élémentaire des fonctions analytiques d'une ou plusieurs variables complexes* (Hermann & Cie., Paris, 1961), p. 9, where all rules are clearly stated. Formal series have been already considered by S. Wightman, Proc. Int. Congr. Math., Amsterdam 1962, 587.

[6] L. Schwartz, *Theorie des Distributions* (Hermann & Cie., Paris, 1957) Vol. I, p. 38.

also be convenient to introduce the last constant Z_1 by the relation

$$Z_2 Z_3^{\frac{1}{2}} e_0 = Z_1 e. \tag{3.5}$$

We now build up the functional

$$u_Z[\eta, \bar{\eta}, J/e, m, \kappa] \equiv (1/\mathfrak{N}) u[Z_2^{-\frac{1}{2}}\eta, Z_2^{-\frac{1}{2}}\bar{\eta}, Z_3^{-\frac{1}{2}} J/e_0, m_0, \kappa_0], \tag{3.6}$$

which will lead to the definition of the *renormalized* generating functional (cf end of this section). But, before studying this point and its consequences, we need to prove first an important formula.

It is a matter of a rather lengthy computation [see Appendix I formula (13)] to show that the total derivative du_Z/de is given by

$$(d/de)u_Z[\eta, \bar{\eta}, J/e, m, \kappa] = Du_Z[\eta, \bar{\eta}, J/e, m, \kappa], \tag{3.7}$$

where the operator D

$$\begin{aligned} D \equiv & -\frac{d \log \mathfrak{N}}{de} \\ & - \frac{1}{2}\frac{d \log Z_2}{de}\left(\int \bar{\eta}_\alpha(\xi)\frac{\delta}{\delta\eta_\alpha(\xi)} + \eta_\alpha(\xi)\frac{\delta}{\delta\eta_\alpha(\xi)}\right) \\ & - \frac{1}{2}\frac{d \log Z_3}{de}\int J_\mu(\xi)\frac{\delta}{\delta J_\mu(\xi)} + Z_2 Z_3^{\frac{1}{2}}\frac{de_0}{de} i\int d\xi\, \Gamma(\xi) \\ & + Z_2\frac{dm_0}{de}\int d\xi\, \mathfrak{M}_{e1}(\xi) + Z_3\frac{d\kappa_0}{de}\int d\xi\, \mathfrak{M}_{ph}(\xi) \end{aligned} \tag{3.8}$$

is an differential operator which acts on functionals, and

$$\mathfrak{M}_{e1}(\xi) = i\lim_{\xi'=\xi}\left[\frac{\delta^2}{\delta\eta_\alpha(\xi)\delta\bar{\eta}_\alpha(\xi')} + \tfrac{1}{2}Z_2^{-1}\,\mathrm{Tr}\, S^{(c)}(\xi' - \xi, m_0)\right], \tag{3.9}$$

$$\mathfrak{M}_{ph}(\xi) = \frac{i}{2}\lim_{\xi'=\xi}\left[\frac{\delta^2}{\delta J_\mu(\xi)\delta J_\mu(\xi')} + \tfrac{1}{2}Z_3^{-1}\Delta^{(c)}(\xi - \xi', \kappa_0)\right]. \tag{3.10}$$

{Eq. (3.7) can be compared with the equation

$$\frac{du}{de}[\eta, \bar{\eta}, J/e, m, \kappa] = i\int d\xi\, \Gamma(\xi) u[\eta, \bar{\eta}, J/e, m, \kappa]$$

which is a straightforward consequence of (2.3). This kind of equations have been introduced by Caianiello under the name of "branching equations."[7]}

The formula (3.8) *is valid under the assumption* (cf. *preceding paragraph*): $\mathrm{Tr}\,\{\gamma_\mu S^{(c)}(0)\} = 0$, *and it should be also remarked that the two last* terms in the previous formulas (3.9) and (3.10) can be amalgamated with the term $d \log \mathfrak{N}/de$ in (3.8) and contribute only to vacuum effects.

All these considerations are valid as far as the series (2.3) is a convergent one and has $u^{(\mathrm{reg})}[\cdots]$ as a sum. We shall see now that all previous formulas, from (3.7) to (3.10), remain valid when $u^{(\mathrm{reg})}[\cdots]$ represents a formal series: we shall get rid, in this way, of the provisional hypothesis upon which was based (3.7). Let us, therefore, consider the following formal series in the associated variables ϵ, α, β, X, Y:

$$\begin{aligned} & \frac{1}{\mathfrak{N}}\sum_n \frac{(i\epsilon)^n}{n!}\int d\xi_n \cdots d\xi_1\, \Gamma(\xi_n)\cdots\Gamma(\xi_1) \\ & \times \sum_i \frac{X^i}{i!}\int \bar{\eta}(x_i)\cdots\bar{\eta}(x_1)\frac{\delta^i}{\delta\bar{\eta}(x_i)\cdots\delta\bar{\eta}(x_1)} \\ & \times \sum_k \frac{X^k}{k!}\int \eta(y_k)\cdots\eta(y_1)\frac{\delta^k}{\delta\bar{\eta}(y_k)\cdots\delta\eta(y_1)} \\ & \times \sum_l \frac{Y^l}{l!}\int J(\zeta_l)\cdots J(\zeta_1)\frac{\delta^l}{\delta J(\zeta_l)\cdots\delta J(\zeta_1)} \\ & \times \sum_p \frac{\alpha^p}{p!}\frac{\partial^p}{\partial m^p}\sum_q \frac{\beta^q}{q!}\frac{\partial^q}{\partial\kappa^q} u_0[\eta, \bar{\eta}, J/m, \kappa]. \end{aligned} \tag{3.11}$$

We first remark that if all required analyticity and convergence conditions are satisfied, then (3.11) defines the functional[8]

$$(1/\mathfrak{N})u[\eta(1+X), \bar{\eta}(1+X), J(1+Y)/(1+X)^2(1+Y)\epsilon, m+\alpha, \kappa+\beta]. \tag{3.12}$$

Suppose now that the scalars defined by (3.4) are once more formal series in the associated variable e, with coefficients functions of m and κ. Perform in (3.11) the following substitutions

$$\begin{aligned} & X \to Z_2^{-\frac{1}{2}} - 1, \quad Y \to Z_3^{-\frac{1}{2}} - 1, \quad \epsilon \to Z_2 Z_3^{\frac{1}{2}} e_0, \\ & \alpha \to m_0 - m = -\delta m, \quad \beta \to \kappa_0 - \kappa = -\delta\kappa, \end{aligned} \tag{3.13}$$

and divide the result by the formal series $\mathfrak{N}$. All previous operations are supposed to be allowed, in other terms, the series $\mathfrak{N}$ has a constant term equal to 1, and all the substituted series are at last of order 1 (i.e., there is no constant term in these series). This last condition means that the constant terms are 1 in the series Z_2 and Z_3, and respectively m, κ in the series m_0, κ_0. It will be verified later on (see below Sec. 4) that all these requirements are physically meaningful. In accordance with (3.6) and (3.12) we shall continue to denote the formal sum of (3.11) after the substitutions (3.13) by

$$u_Z[\eta, \bar{\eta}, J/e, m, \kappa],$$

[7] E. Caianiello, Nuovo Cimento **13**, 637 (1959).

[8] Note that the order of fermions sources in the series (3.11) is important: any modification introduces sign changes due to the anticommuting character of this kind of sources.

indeed, if all analyticity and convergence conditions were satisfied, the result would be expressed by (3.6).

Our final contention is that, in the meaning of formal series, Eq. (3.7) remains true: this point, which requires some lengthy, but by no means difficult, calculations will be proved in Appendix I.

We are now ready to state precisely the main assumption of renormalization theory: *we shall suppose that there is a special choice of the constants (3.4) such that all the results calculated from the expression of* $u_Z[\cdots]$, *which will be denoted by* $u^{(\mathrm{ren})}[\eta, \bar{\eta}, J/e, m, \kappa]$ *once this choice has been made, are in complete agreement with the experimental data. We shall furthermore assume that there exists a certain regularization method giving rise to a finite part (see 3.1) such that*

$$u^{(\mathrm{ren})}[\eta, \bar{\eta}, J/e, m, \kappa] = \mathcal{P}u[\eta, \bar{\eta}, J/e, m, \kappa]. \quad (3.14)$$

4. RENORMALIZABILITY CONDITIONS AND CONNECTION BETWEEN FINITE AND DIVERGENT PARTS

We are now able to study the further consequences of our former assumption. Suppose that one works within the frame of a given regularization method which is compatible with the renormalization program defined in the previous section and leading to formula (3.14): then there exists a choice of renormalization constants such that Eq. (3.7) can be written as:

$$(d/de)\mathcal{P}u[\eta, \bar{\eta}, J/e, m, \kappa] = D\mathcal{P}u[\eta, \bar{\eta}, J/e, m, \kappa], \quad (4.1)$$

where D represents now the differential operator (3.8) with the right choice of renormalization constants; this is to be understood once again as an equation for the formal series,

$$\mathcal{P}u[\eta, \bar{\eta}, J/e, m, \kappa] = \sum_{n=0} \frac{e^n}{n!} \mathcal{P}u_n[\eta, \bar{\eta}, J/m, \kappa]. \quad (4.2)$$

The integrodifferential operator D has been introduced in (3.8). Since D does not involve at all the differentiation symbol d/de, it can be thus defined by a formal series[9]

$$D = \sum_{k=0} \frac{e^k}{k!} D^{(k)}, \quad (4.3a)$$

$$\begin{aligned} D^{(k)} = \frac{d^k D}{de^k}\Big]_{e=0} = \lim_{e=0} - \Big\{ & \frac{d^{k+1}}{de^{k+1}} \log \mathfrak{N} \\ & + \frac{1}{2} \frac{d^{k+1}}{de^{k+1}} \log Z_2 \int \left(\bar{\eta} \frac{\delta}{\delta \bar{\eta}} + \eta \frac{\delta}{\delta \eta} \right) \\ & + \frac{1}{2} \frac{d^{k+1}}{de^{k+1}} \log Z_3 \int J \frac{\delta}{\delta J} \\ & - \frac{d^k}{de^k} \left(Z_2 Z_3^{\frac{1}{2}} \frac{de_0}{de} \right) i \int d\xi\, \Gamma(\xi) \\ & - \frac{d^k}{de^k} \left(Z_2 \frac{dm_0}{de} \int d\xi\, \mathfrak{M}_{\mathrm{el}}(\xi) \right) \\ & - \frac{d^k}{de^k} \left[Z_2 \frac{d\kappa_0}{de} \int d\xi\, \mathfrak{M}_{\mathrm{ph}}(\xi) \right] \Big\}. \end{aligned} \quad (4.3b)$$

In other terms, one deduces $D^{(k)}$ from D by replacing the coefficients of D by their kth derivatives at the value $e = 0$. The handling of the subtracted terms in formulas (3.9) and (3.10) (especially when one takes derivatives) requires some caution, but in both of these formulas, these terms, being independent of the sources, can be added to the term $d \log \mathfrak{N}/de$ of (3.8). Therefore, in the applications of Sec. 5, we shall simply omit in the calculations of $\mathfrak{M}_{\mathrm{el}}$ and $\mathfrak{M}_{\mathrm{ph}}$ all terms which are independant of the sources, i.e. all terms expressed only by vacuum diagrams.

Bringing now (4.3a) and (4.3b) into (4.1) we deduce the following set of recursion formulas:

$$\mathcal{P}u_n[\eta, \bar{\eta}, J/m, \kappa] = \sum_{k=0}^{n-1} \binom{n-1}{k} D^{(k)} \mathcal{P}u_{n-1-k}[\eta, \bar{\eta}, J/m, \kappa] \quad (4.4)$$

valid for $n \geq 1$.

Consider now the two terms $\mathcal{P}u_0[\cdots]$ and $\mathcal{P}u_1[\cdots]$ which represent the finite part of $u_0[\cdots]$ and $u_1[\cdots]$ as given by (2.1), (2.3), and (2.5). Since $u_0[\cdots]$ is a Fréchet–Volterra functional, we may identify $\mathcal{P}u_0[\cdots]$ with $u_0[\cdots]$. We then look into the structure of $\mathcal{P}u_1[\cdots]$ as defined by (4.4). Calling

$$\mathfrak{N}^{(n)}, z_1^{(n)}, z_2^{(n)}, z_3^{(n)}, e_0^{(n)}, \delta m^{(n)}, \delta\kappa^{(n)}, \quad (4.5)$$

the nth respective coefficients (functions of m and κ) of the formal series in e which are symbolized by $\mathfrak{N}$, Z_1, Z_2, Z_3, e_0, δm, $\delta\kappa$, one sees that Eq. (4.4) takes the form

$$\begin{aligned} \mathcal{P}u_1[\cdots] = \Big\{ & -\mathfrak{N}^{(1)} - \frac{1}{2} z_2^{(1)} \int \left(\bar{\eta}_\alpha(\xi) \frac{\delta}{\delta \bar{\eta}_\alpha(\xi)} \right. \\ & \left. + \eta_\alpha(\xi) \frac{\delta}{\delta \eta_\alpha(\xi)} \right) - \frac{1}{2} z_3^{(1)} \int J_\mu(\xi) \frac{\delta}{\delta J_\mu(\xi)} \\ & + i e_0^{(1)} \int d\xi\, :\Gamma(\xi): - \delta m^{(1)} \int d\xi\, \mathfrak{M}_{\mathrm{el}}(\xi) \\ & - \delta\kappa^{(1)} \int d\xi\, \mathfrak{M}_{\mathrm{ph}}(\xi) \Big\} u_0[\eta, \bar{\eta}, J/m, \kappa]. \end{aligned} \quad (4.6)$$

On the other hand, the $u_1[\cdots]$ as given by (2.8), i.e., the $u_1[\cdots]$ which results from the replacement in (2.7) of $\Gamma(\xi)$ by $:\Gamma(\xi):$ is also a "well-defined"

[9] Note that the differentiation is a well defined operation in the theory of formal series.

functional. Hence, we may identify once again $\mathcal{P}u_1[\cdots]$ with the expression (2.8) of $u_1[\cdots]$ and get

$$\mathfrak{M}^{(1)} = z_2^{(1)} = z_3^{(1)} = \delta m^{(1)} = \delta\kappa^{(1)} = 0, \quad (4.7a)$$

$$e_0^{(1)} = 1, \quad (4.7b)$$

and

$$D^{(0)} = i \int d\xi \, :\Gamma(\xi): . \quad (4.7c)$$

Let us single out the term $k = 0$ in the recurrent system (4.4); it is finally transformed into

$$\mathcal{P}u_n[\cdots] = i \int d\xi \, :\Gamma(\xi): \mathcal{P}u_{n-1}[\cdots] + \sum_{k=1}^{n-1} \binom{n-1}{k} D^{(k)} \mathcal{P}u_{n-1-k}[\cdots]. \quad (4.8)$$

These equations (4.8) represent a necessary condition to be verified by any kind of regularization method acting as a renormalization, in other terms, supposing that one works within the frame of a given regularization method, we are able to decide the following question: does Eq. (3.14) hold or not? It is proven in the last section of this paper that (4.8) is also a sufficient condition. But, for the time being, we want to point out some important practical consequences of this formula: we show in the next section that Salam's prescriptions[10] for removing divergences in quantumelectrodynamics (in particular) verifies (4.8): hence, one may assert that this formula represents an algebraical formulation of Salam's rules. This is the point we are now going to study.

5. RENORMALIZATION CONSTANTS AND SALAM'S RULES

In his fundamental work on renormalization theory, Salam stated in an unambiguous way the rules following which, given a divergent integral in quantum field theory, one shall form the terms to be subtracted. This is indeed what is expressed by the recurrent system (4.8), but since these equations involve perturbative approximations of the generating functional instead of the propagators and their corresponding diagrams, simple transformations of these formulas will first be needed. Indeed going over from (4.8) to relations between finite parts of propagators, we shall show, by an actual computation of radiative corrections up to the fourth order that one is led to the same corrections as the ones arising in quantumelectrodynamics and it is well known that such corrections are, in their turn, in complete agreement with Salam's rules. It is also to be noted that these calculations will determine the renormalization constants in terms of the "infinite constants" of field theory.

We are thus led to take derivatives of (4.8) with respect to the sources for η, $\bar{\eta}$, $J = 0$. As a shorthand notation for propagators, let us use the one introduced by Caianiello[7] and denote the nth radiative approximation of a propagator $K\binom{x_1 \cdots x_p}{y_1 \cdots y_p}/t_1 \cdots t_q)$ by

$$K^{(n)}\binom{x_1 \cdots x_p}{y_1 \cdots y_p}/t_1 \cdots t_q) = (-1)^{\frac{1}{2}p(p-1)}(-i)^n \lim_{\eta,\bar{\eta},J=0} \frac{\delta^{2p+q} u_n[\eta, \bar{\eta}, J]}{\delta\bar{\eta}(x_p) \cdots \delta\bar{\eta}(x_1)\delta\eta(y_p) \cdots \delta\eta(y_1)\delta J(t_1) \cdots \delta J(t_q)}, \quad (5.1)$$

where x and y represent the insertion of, respectively, outgoing and incoming fermion lines and t the insertion of photon lines.

We recall too that the renormalization constants have been defined by formal series with coefficients given by (4.5) which depend of course on the regularization parameter λ. Furthermore, they have been determined in Sec. 4, in such a way that the following conditions are verified:

$$\mathcal{P}u_0[\cdots] = u_0[\eta, \bar{\eta}, J/m, \kappa] \quad (5.2)$$

and

$$\mathcal{P}u_1[\cdots] = u_1 = i \int d\xi \, :\Gamma(\xi): u_0[\cdots]. \quad (5.3)$$

After these preliminaries, we consider the second radiative approximation of the functional $u[\cdots]$, it follows from formulas (4.8) and (4.3b) that

$$\mathcal{P}u_2[\cdots] = u_2 + D^{(1)}u_0, \quad (5.4)$$

with

$$D^{(1)} = -\Big[\mathfrak{M}^{(2)} + \frac{1}{2} z_2^{(2)} \Big(\int \bar{\eta} \frac{\delta}{\delta\bar{\eta}} + \eta \frac{\delta}{\delta\eta} \Big) + \frac{1}{2} z_3^{(2)} \int J \frac{\delta}{\delta J} - 2z_1^{(1)} \int d\xi \, \Gamma(\xi) + \delta m^{(2)} \int d\xi \, \mathfrak{M}_{e1}(\xi) + \delta\kappa^{(2)} \int d\xi \, \mathfrak{M}_{ph}(\xi) \Big]. \quad (5.5)$$

It is clear that the two last terms of $D^{(1)}$ when acting on $u_0[\cdots]$ are respectively identical to

[10] A. Salam, Phys. Rev. 82, 226 (1951).

$\delta m^{(2)}(\partial/\partial m)u_0[\dots]$ and $\delta\kappa^{(2)}(\partial/\partial\kappa)u_0[\dots]$; on the other hand, the interpretation of $\mathfrak{N}^{(2)}$ is obvious: it corresponds to vacuum effects.

Computing the second-order derivatives of (5.4) with respect of the fermion sources and taking $\eta, \bar{\eta}, J = 0$, denoting in the usual way by $S_2'(x-y)$ the propagator $K^{(2)}(^x_y/0)$ of (5.1), one has

$$-\mathcal{P}S_2'(x-y) = -S_2'(x-y) + \left(z_2^{(2)} + \delta m^{(2)}\frac{\partial}{\partial m}\right)\tfrac{1}{2}S^{(c)}(x-y, m), \quad (5.6)$$

where we agreed to neglect both disconnected radiative corrections in $S_2(x-y)$ and the term $\mathfrak{N}^{(2)}S^{(c)}(x-y)$ which compensates them exactly.

The last term in (5.6) corresponds to the divergent part of the second approximation of the self-energy of an electron, indeed it is well known from conventional quantumelectrodynamics that in p-space this self-energy takes the following form:

$$S_2'(p) = S^{(c)}(p)\Sigma^{*(2)}(p)S^{(c)}(p) = S^{(c)}(p)(A + BS^{-1(c)}(p) + \Sigma_f^{(2)}(p))S^{(c)}(p), \quad (5.7a)$$

where

$$S^{-1(c)}(p) = -i(i\gamma p + m). \quad (5.7b)$$

Note that we have chosen for the fermion-free propagator the expression

$$\tfrac{1}{2}S^{(c)}(x-y, m) = -\frac{i}{(2\pi)^4}\lim_{\epsilon=0}\int d^4p\,\frac{e^{ipx}(i\gamma p - m)}{p^2 + m^2 - i\epsilon} = \frac{1}{(2\pi)^4}\int d^4p\, e^{ipx}S^{(c)}(p).$$

A and B are two divergent constants and $\Sigma_f^{(2)}(p)$ is a temperate distribution in p.[11] From known properties of $S^{(c)}(p)$ formula (5.7a) can also be brought into the form

$$S_2'(p) = -iA(\partial/\partial m)S^{(c)}(p) + BS^{(c)}(p) + S^{(c)}(p)\Sigma_f^{(2)}(p)S^{(c)}(p). \quad (5.8)$$

Let us now take the Fourier transform of (5.5) and bring (5.8) in it, one gets the second-order correction of the mass of the electron and the change of scale of electron field quantity:

$$\delta m^{(2)} = -iA, \qquad z_2^{(2)} = B. \quad (5.9)$$

The same considerations apply to the finite part of the second-order correction to the boson line, and equations entirely analogous to (5.7) with introduction of two new divergent constants C and C' may be used for the identification of $z_3^{(2)}$ and $\delta\kappa^{(2)}$.

We now remark that nothing has been said about the corrections of Z_1, as a matter of fact their study requires some considerations about the vertex part. We will choose for the boson free propagator, the expression

$$\Delta^{(c)}(x-y, \kappa) = -\frac{2i}{(2\pi)^4}\lim_{\epsilon=0}\int d^4k\,\frac{e^{ikx}}{k^2 + \kappa - i\epsilon},$$

which reduces for the limiting case of quantum-electrodynamics to Dyson's gauge. It is then well known—and it results from a general formula given in Appendix II—that the vertex part $K(^z_y/t)$ has no approximations of even order, i.e., all its even-order radiative corrections are 0.

We shall *assume* that this holds for its finite part,

$$\mathcal{P}K^{(2)}(^x_y/t) = 0; \quad (5.10)$$

the left-hand side of (5.10) can be expressed through formula (5.4) which, in its turn reduces to

$$\mathcal{P}K^{(2)}(^x_y/t) = -iz_1^{(1)}K^{(1)}(^x_y/t) \quad (5.11a)$$

with

$$K^1(^z_y/t) = \frac{1}{(2)^3} \times \int S^{(c)}(x-\xi)\gamma S^{(c)}(\xi - y)\Delta^{(c)}(\xi - t)\,d^4\xi. \quad (5.11b)$$

We therefore have

$$z_1^{(1)} = 0 \quad (5.12)$$

and

$$D^{(1)} = -\left[\frac{1}{2}z_2^{(2)}\int d\xi\left(\bar{\eta}(\xi)\frac{\delta}{\delta\bar{\eta}(\xi)} + \eta(\xi)\frac{\delta}{\delta\eta(\xi)}\right) + \frac{1}{2}z_3^{(2)}\int d\xi\, J(\xi)\frac{\delta}{\delta J(\xi)} + \delta m^{(2)}\int d\xi\,\mathfrak{M}_{el}(\xi) + \delta\kappa^{(2)}\int d\xi\,\mathfrak{M}_{ph}(\xi)\right]. \quad (5.13)$$

Let us now examine the third radiative correction of the generating functional. Equation (4.8) leads to the formula

$$\mathcal{P}u_3 = i\int d\xi\,\Gamma(\xi)\mathcal{P}u_2 + 2D^{(1)}u_1 + D^{(2)}u_0, \quad (5.14)$$

which, according to (5.4) can be brought into the form

$$\mathcal{P}u_3 = u_3 - (z_2^{(2)} + z_3^{(2)})u_1 + 3D^{(1)}u_1 + D^{(2)}u_0 \quad (5.15)$$

with

$$D^{(2)} = -\left[\frac{1}{2}z_2^{(3)}\left(\int\bar{\eta}\frac{\delta}{\delta\bar{\eta}} + \eta\frac{\delta}{\delta\eta}\right) + \frac{1}{2}z_3^{(3)}\int J\frac{\delta}{\delta J} - (3z_1^{(2)} - 2z_2^{(2)} - z_3^{(2)})i\int d\xi\,\Gamma(\xi) + \delta m^{(3)}\int\mathfrak{M}_{el}(\xi) + \delta\kappa^{(3)}\int\mathfrak{M}_{ph}(\xi)\right]. \quad (5.16)$$

[11] In the published expressions of $\Sigma_f^{(2)}$, there is an infrared divergency which should be disregarded.

We neglected again all disconnected radiative corrections and the subtracted terms in the expressions of $\mathfrak{M}_{el}$ and $\mathfrak{M}_{ph}$ given by (3.9) and (3.10).

It is now once more well known (cf. Appendix II) that, in the special Dyson gauge, propagators having an even number of external lines contain no radiative corrections of odd order; we assume as previously that this property holds for their finite parts. Thus

$$z_2^{(3)} = z_3^{(3)} = \delta m^{(3)} = \delta\kappa^{(3)} = 0, \tag{5.17}$$

and $D^{(2)}$ reduces to the simpler expression

$$D^{(2)} = (3z_1^{(2)} - 2z_2^{(2)} - z_3^{(2)})i\int d\xi\,\Gamma(\xi). \tag{5.18}$$

Bringing (5.18) into (5.15), it turns out that $\mathcal{P}u_3$ takes its final form:

$$\mathcal{P}u_3 = u_3 + 3D^{(1)}u_1 + 3(z_1^{(2)} - z_2^{(2)} - \tfrac{1}{2}z_3^{(2)})u_1. \tag{5.19}$$

Consider now this last expression and take derivatives with respect to $\bar\eta(x),\eta(y)$, and $J(t)$ (and for the value of sources $\bar\eta,\ \eta,\ J = 0$) of both of its sides; then

$$\mathcal{P}K^{(3)}\binom{x}{y}/t) = K^{(3)}\binom{x}{y}/t) + 3\left[\left(2z_2^{(2)} + \delta m^{(2)}\frac{\partial}{\partial m}\right) + \left(z_3^{(2)} + \delta\kappa^{(2)}\frac{\partial}{\partial\kappa}\right) - z_1^{(2)}\right]K^{(1)}\binom{x}{y}/t) \tag{5.20}$$

and $K^{(1)}$ is given by (5.11b). Decomposing $K^{(3)}$ into its finite and divergent parts,

$$K^{(3)}\binom{x}{y}/t) = \mathcal{P}K^{(3)}\binom{x}{y}/t) + \mathfrak{D}K^{(3)}\binom{x}{y}/t), \tag{5.21a}$$

one may cast Eq. (5.20) into the form

$$\mathfrak{D}K^{(3)}\binom{x}{y}/t) = -3\left[\left(2z_2^{(2)} + \delta m^{(2)}\frac{\partial}{\partial m}\right) + \left(z_3^{(2)} + \delta\kappa^{(2)}\frac{\partial}{\partial\kappa}\right) - z_1^{(2)}\right]K^{(1)}\binom{x}{y}/t). \tag{5.21b}$$

It can now be seen, from the expression of the second-order radiative corrections of the vertex in conventional quantumelectrodynamics, that the first term of the right-hand side of (5.21b) is the divergence introduced by the corrections of the electron lines $x - \xi$ and $y - \xi$ in $K^{(1)}$ and that the second term is the divergence introduced by the correction of the single boson line in the same $K^{(1)}$.

The last term of (5.21b) is thus the proper vertex graph (in e^3) whose divergent part is

$$LK^{(1)}\binom{x}{y}/t), \tag{5.22a}$$

where L is one of the "infinite constants" of field theory. One may therefore infer that

$$z_1^{(2)} = L. \tag{5.22b}$$

Let us turn our attention to the more complicated case of the fourth-order approximation of $u[\cdots]$. According to formula (4.8), its finite part takes the form

$$\mathcal{P}u_4 = i\int d\xi\,\Gamma(\xi)\mathcal{P}u_3 + 3D^{(1)}\mathcal{P}u_2 + 3D^{(2)}u_1 + D^{(3)}u_0. \tag{5.23}$$

From (5.4) and (5.19), it follows that

$$\mathcal{P}u_4 = u_4 - 6(2z_2^{(2)} + z_3^{(2)} - D^{(1)})u_2 + 12z_1^{(2)}u_2 + (D^{(3)} + 3D^{(1)}D^{(1)})u_0 \tag{5.24}$$

with

$$D^{(3)} = -\left[\frac{1}{2}(z_2^{(4)} - 3z_2^{(2)}z_2^{(2)})\int\left(\bar\eta\frac{\delta}{\delta\bar\eta} + \eta\frac{\delta}{\delta\eta}\right) + \frac{1}{2}(z_3^{(4)} - 3z_3^{(2)}z_3^{(2)})\int J\frac{\delta}{\delta J} + (\delta m^{(4)} + 3z_2^{(2)}\delta m^{(2)})\int d\xi\,\mathfrak{M}_{el}(\xi) + (\delta\kappa^{(4)} + 3z_3^{(2)}\delta\kappa^{(2)})\int d\xi\,\mathfrak{M}_{ph}(\xi)\right]. \tag{5.25}$$

In order to be more definite, we examine especially the finite part of the fourth-order radiative corrections to the two-point fermion propagator. From (5.24) and (5.1), it follows that

$$\mathcal{P}K^{(4)}\binom{x}{y}/0) = K^{(4)}\binom{x}{y}/0) - 6\left(3z_2^{(2)} + \delta m^{(2)}\frac{\partial}{\partial m} + z_3^{(2)} + \delta\kappa^{(2)}\frac{\partial}{\partial\kappa}\right)S_2'(x-y) + 12z_1^{(2)}S_2'(x-y) + (z_2^{(4)} + \delta m^{(4)}\,\partial/\partial m)\tfrac{1}{2}S^{(c)}(x-y) - 6\left(z_2^{(2)}z_2^{(2)} + \tfrac{1}{2}\delta m^{(2)}\delta m^{(2)}\frac{\partial^2}{\partial m^2} + 2z_2^{(2)}\delta m^{(2)}\frac{\partial}{\partial m}\right)\tfrac{1}{2}S^{(c)}(x-y). \tag{5.26}$$

Let us now compare (5.26) with the expressions obtained in conventional quantumelectrodynamics, it is known that the only connected fourth-order divergent graphs which contribute to the self-energy of an electron are the following ones.

(I) the improper sum of the graphs built up by the corrections of the external lines of a divergent, irreducible, self-energy graph.

(II) and (III) the proper graphs one gets by the correction of the internal lines of the irreducible self-energy graph: (II) corresponds to the correction of the fermion line, and (III) to the correction of the photon line.

(IV) the well-known overlapping divergence of fourth order, obtained by the correction of the vertex. Their respective contributions can be easily computed as functions of the divergent constants A and B introduced in the expression (5.7) of the self-energy of the electron, the divergent constants C and C' which play an analogous role for the boson and six other constants $\alpha, \beta, \alpha', \beta', \alpha'', \beta''$ introduced by the *skeleton* divergences in the proper graphs denoted by I, II, III, IV. It must be also noted that in contradistinction to the constants A, B, C, C' typical of the second-order divergences, the constants $\alpha \cdots \beta''$ are typical of the fourth-order corrections of self-energy graphs.

Elementary calculations show that the divergences $\mathfrak{D}S_4^{\mathrm{I}}(x-y), \cdots \mathfrak{D}S_4^{\mathrm{IV}}(x-y)$ of the graphs denoted by I, $\cdots$ IV can be brought into the following form, after Fourier transformation:

$$\begin{aligned}
\mathfrak{D}S_4^{\mathrm{I}}(p) &= \tfrac{1}{2}(AS^{(c)}(p)+B)S_2'(p) \\
&\quad + \tfrac{1}{2}S_2'(p)(AS^{(c)}(p)+B) \\
&\quad - S^{(c)}(p)(\tfrac{1}{2}AS^{(c)}(p)+\tfrac{1}{2}B)^2, \\
\mathfrak{D}S_4^{\mathrm{II}}(p) &= \tfrac{1}{2}S^{(c)}(p)(B\Sigma^{*(2)}(p) - Ai(\partial/\partial m)\Sigma^{*(2)}(p)) \\
&\quad \times S^{(c)}(p) + \alpha_4 S^{(c)}(p)^2 + \beta_4 S^{(c)}(p), \qquad (5.27) \\
\mathfrak{D}S_4^{\mathrm{III}}(p) &= \tfrac{1}{2}S^{(c)}(p)(C - C'i\,\partial/\partial\kappa)\Sigma^{*(2)}(p) \\
&\quad \times S^{(c)}(p) + \alpha_4' S^{(c)}(p)^2 + \beta_4' S^{(c)}(p), \\
\mathfrak{D}S_4^{\mathrm{IV}}(p) &= -z_1^{(2)} S_2'(p).
\end{aligned}$$

Take now the Fourier transform of (5.26) [an operation which presents no difficulty since there are no differential operators with respect to x or y in (5.26)], after having replaced $K^{(4)}(\substack{x\\y}/0)$, first term of the right-hand side of (5.26), by the sum of its finite and divergent parts:

$$\begin{aligned}
\mathfrak{D}K^{(4)}(p) &= 6(3z_2^{(2)} + \delta m^{(2)}\,\partial/\partial m + z_3^{(2)} \\
&\quad + \delta\kappa^{(2)}\,\partial/\partial\kappa)K^{(2)}(p) - 12z_1^{(2)}K^{(2)}(p) \\
&\quad - (z_2^{(4)} + \delta m^{(4)}\,\partial/\partial m)S^{(c)}(p) \\
&\quad + 6(z_2^{(2)}z_2^{(2)} + 2z_2^{(2)}\delta m^{(2)}\,\partial/\partial m \\
&\quad + \tfrac{1}{2}\delta m^{(2)}\delta m^{(2)}\,\partial^2/\partial m^2)S^{(c)}(p), \qquad (5.28)
\end{aligned}$$

where $K^{(4)}(p) = S_4'(p)$ and $K^{(2)}(p) = S_2'(p)$ are Fourier transform of $K^{(4)}(\substack{x\\y}/0)$ and $K^{(2)}(\substack{x\\y}/0)$.

We now remark that bringing the relations (5.9) into (5.28), one gets the following four equalities:

$$\begin{aligned}
&(3z_2^{(2)} + \delta m^{(2)}\,\partial/\partial m)K^{(2)}(p) \\
&\quad = +(AS^{(c)}(p)+B)S_2'(p) + S_2'(p)(AS^{(c)}(p)+B) \\
&\quad + S^{(c)}(p)(B\Sigma^{*(2)}(p) - Ai(\partial/\partial m)\Sigma^{*(2)}(p)S^{(c)}(p)), \\
&(z_3^{(2)} + \delta\kappa^{(2)}\,\partial/\partial\kappa)K^{(2)}(p) \\
&\quad = +S^{(c)}(p)(C - C'i\,\partial/\partial\kappa)\Sigma^{*(2)}(p)S^{(c)}(p) \\
&\quad - z_1^{(2)}K^{(2)}(p) = -z_1^{(2)}S_2'(p), \\
&(z_2^{(2)}z_2^{(2)} + \tfrac{1}{2}\delta m^{(2)}\delta m^{(2)}\,\partial^2/\partial m^2 \\
&+ 2z_2^{(2)}\delta m^{(2)}\,\partial/\partial m)S^{(c)}(p) = (AS^{(c)}(p)+B)^2 S^{(c)}(p).
\end{aligned}$$

If furthermore, one chooses $z_2^{(4)}$ and $\delta m^{(4)}$ such that

$$\begin{aligned}
&z_2^{(4)} + \delta m^{(4)}(\partial/\partial m)S^{(c)}(p) \\
&= 24[(\alpha_4+\alpha_4'+\alpha_4'')S^{(c)}(p)^2 + (\beta_4+\beta_4'+\beta_4'')S^{(c)}(p)],
\end{aligned}$$

one has

$$\begin{aligned}
\mathfrak{D}S_4'(p) &= 4!(\mathfrak{D}S_4^{\mathrm{I}}(p) + \mathfrak{D}S_4^{\mathrm{II}}(p) \\
&\quad + \mathfrak{D}S_4^{\mathrm{III}}(p) + \mathfrak{D}S^{\mathrm{IV}}(p)).
\end{aligned}$$

Again, as it was done for the second and third order of radiative corrections, the fourth-order renormalization constants have been identified with the "infinite" constants of quantumelectrodynamics.

6. AN EXPLICIT FORM OF THE FINITE AND DIVERGENT PARTS OF $u[\cdots]$

The proof that (4.8) is a sufficient condition for a regularized theory to be a renormalized one can be based on the uniqueness of the solution of the differential equation (3.7) which involves a first-order derivative with respect to the charge e.[12] But we shall prefer to use another argument, namely to exhibit an explicit form of the solution of (3.7) and solve the problem we have in mind by working directly with this solution. This is the harder way, but in doing so, we shall collect formulas important for further use.

The considerations of section 4 apply as well to $u_z[\cdots]$, and it turns out that the formal series solution of (3.7),

$$u_z[\eta, \bar\eta, J/e, m, \kappa] = \sum \frac{e^n}{n!} u_z^{(n)}[\eta, \bar\eta, J/m, \kappa] \qquad (6.1)$$

satisfy the recursion formulas

$$u_z^{(n)} = \sum_{k=0}^{n-1} \binom{n-1}{k} D^{(k)} u_{(z)}^{(n-1-k)} \quad \text{for} \quad n \geq 1. \qquad (6.2)$$

We shall also assume, as before,

$$u_z^{(0)}[\eta, \bar\eta, J/m, \kappa] \equiv u_0[\eta, \bar\eta, J/m, \kappa], \qquad (6.3a)$$

and

$$D^{(0)} = i \int d\xi\, :\Gamma(\xi):. \qquad (6.3b)$$

[12] This solution, in the frame of formal series, is indeed uniquely determined by $u_0[\cdots]$ and the recurrence formulas in $d^n u_Z[\cdots]/de^n$ expressed by (3.7).

The solution of the recurrent system (6.2) in terms of the $D^{(k)}$'s and $u_0[\cdots]$ can be obtained as follows: iterate (6.2) by bringing in the expression of $u_Z^{(n-1-k)}$ given by (6.2)

$$u_Z^{(n)}[\cdots] = \sum_{k_1=0}^{n-1} \sum_{k_2=0}^{n-1-k_1-1} \binom{n-1}{k_1}\binom{n-2-k_1}{k_2} \times D^{(k_1)} D^{(k_2)} u_Z^{(n-1-k_1-1-k_2)}; \quad (6.4)$$

after l iterations,

$$u_Z^{(n)}[\cdots] = \sum_{k_1=0}^{n-1} \sum_{k_2=0}^{n-2-k_1} \cdots \binom{n-1}{k_1} \times \binom{n-2-k_2}{k_2} \cdots \binom{n-l-\sum_{i=1}^{l-1} k_i}{k_l} \times D^{(k_1)} \cdots D^{(k_l)} u_Z^{(n-l-k_1\cdots k_l)}. \quad (6.5)$$

We now choose l such that $n - l = \sum_{i=1}^{l} k_i$; then

$$u_Z^{(n)}[\cdots] = \sum_{l=1}^{n} \sum_{k_1+k_2+\cdots k_l=n-l} C_{nk_1\cdots k_l} \times D^{(k_1)} \cdots D^{(k_l)} u_0[\cdots] \quad (6.6a)$$

with

$$C_{nk_1\cdots k_l} = \binom{n-1}{k_1} \cdots \binom{n-i-\sum_{i=1}^{i-1} k_i}{k_i} \cdots 1. \quad (6.6b)$$

Let us now single out the term $l = n$ in (6.6a); one gets

$$u_Z^{(n)}[\cdots] = u_n[\cdots] + \sum_{l=1}^{n-1} \sum_{k_1+\cdots k_l=n-l} C_{nk_1\cdots k_l} D^{(k_1)} \cdots D^{(k_l)} u_0[\cdots] \quad (6.7)$$

since $(D^0)^n u_0[\cdots] = u_n[\cdots]$ from (6.3b) and (2.7).

We express $u_n[\cdots]$ as a sum of its finite and divergent part,

$$u^{(n)}[\cdots] = \mathcal{P}u_n[\cdots] + \mathfrak{D}u_n[\cdots]; \quad (6.8)$$

if the theory is to be regularizable and renormalizable too, then there should exist a choice of renormalization constants such that

$$u_Z^{(n)}[\cdots] = u_n^{(\mathrm{ren})}[\cdots] = \mathcal{P}u_n[\cdots], \quad (6.9)$$

as it follows from (3.14). Bringing now (6.8) and (6.9) into (6.7), we obtain an expression of the divergent part,

$$\mathfrak{D}u_n[\cdots] = -\sum_{l=1}^{n-1} \sum_{k_1+\cdots k_l=n-l} C_{nk_1\cdots k_l} \times D^{(k_1)} \cdots D^{(k_l)} u_0[\cdots], \quad (6.10)$$

while the finite part is obtained by bringing (6.9) into (6.6a),

$$\mathcal{P}u_n[\cdots] = \sum_{l=1}^{n} \sum_{k_1+\cdots k_l=n-l} C_{nk_1\cdots k_l} \times D^{(k_1)} \cdots D^{(k_l)} u_0[\cdots]. \quad (6.11)$$

Formulas (6.10) and (6.11) play for the renormalized generating functional the same role which was played by (2.7) for the unrenormalized one; they emphasize also what kind of structure is allowed for the divergent and finite part of the generating functional when the regularization of a given theory acts as a renormalization.

Conversely, one could solve Eq. (3.7) explicitly, obtain the solution (6.6a) and deduce the recursion formulas (4.8); the calculations are rather involved and will be given elsewhere.

REMARK

We noted already that regularization is a necessary step for the coherence of renormalization theory, but for practical calculations finite results can be obtained by using only subtractions of divergent terms.

This assertion is well known for the second-order correction of the two-point electron propagator and can be checked starting from formula (5.26). The same applies to the fourth order: it requires some lengthy calculations using formula (5.26) which will be given elsewhere.

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APPENDIX I

Instead of using the heavy formalism of quantumelectrodynamics, let us limit ourselves to the consideration of a self-interacting scalar field with mass $\kappa^{\frac{1}{2}}$, the interaction being of the form

$$g \int (\Phi(x))^a \, d^4x, \quad a \text{ is a positive integer,}$$

to which corresponds an interaction operator

$$\int d\xi\ \Gamma(\xi) = \left(\frac{1}{i}\right)^a \int d^4x\ \frac{\delta^a}{\delta J(x)^a}. \qquad \text{(I1)}$$

The reader will be able to convince himself that all the following considerations apply as well to quantumelectrodynamics, the only difference being that the formulas one gets for a scalar field are far more simple than the ones obtained in quantumelectrodynamics.

We also shall assume that regularization occurs by the introduction of a single regularization parameter, namely that

$$\exp\left[ig \int d\xi\ \Gamma(\xi)\right] u_0^{(\mathrm{reg})}[J/\kappa] \qquad \text{(I2)}$$

represents the well-defined formal series[13]

$$\sum_{n=0}^{\infty} \frac{g^n}{n!} u_n[J/\kappa] = \sum_{n=0}^{\infty} \frac{(ig)^n}{n!} \times \int d\xi_n \cdots d\xi_1\ \Gamma(\xi_n) \cdots \Gamma(\xi_1) u_0^{(\mathrm{reg})}[J/\kappa]. \qquad \text{(I3)}$$

Our aim is to define the renormalization process through formal series and to show that these series become identical with the series (3.6) when all the existence and analyticity conditions are satisfied.

Consider as in (3.11) the formal series in the associated variables ϵ, μ, κ,

$$\exp\left(i\epsilon \int \Gamma(\xi)\, d\xi\right) B[X] \exp\left[\mu \frac{\partial}{\partial \kappa}\right] u_0^{(\mathrm{reg})}[J/\kappa] = \sum_{n=0}^{\infty} \frac{(i\epsilon)^n}{n!} \int d\xi_n \cdots d\xi_1\ \Gamma(\xi_n) \cdots \Gamma(\xi_1) \times \sum_{p=0}^{\infty} \frac{X^p}{p!} \int dx_p \cdots dx_1\ J(x_p) \cdots J(x_1) \times \frac{\delta^p}{\delta J(x_p) \cdots \delta J(x_1)} \sum_{q=0}^{\infty} \frac{\mu^q}{q!} \frac{\partial^q}{\partial \kappa^q} u_0^{(\mathrm{reg})}[J/\kappa]. \qquad \text{(I4)}$$

We first note that when all required analyticity and existence conditions are satisfied the former series reduces to

$$u^{(\mathrm{reg})}[(1 + X)J/Z^{a/2}\epsilon, \kappa + \mu]. \qquad \text{(I5)}$$

As we did in (3.12) for quantumelectrodynamics, perform then, in accordance with the rules of formal series, the following substitutions:

$$\epsilon \to Z^{a/2}G, \quad X \to Z^{-\frac{1}{2}} - 1, \quad \mu \to \kappa_0 - \kappa = -\delta\kappa, \qquad \text{(I6)}$$

where Z, G, κ_0 are formal series, the associated variable being the coupling constant g. We suppose furthermore that the constant term in Z is supposed to be 1 and there is no constant term in the expression of $\delta\kappa$.

The series (I4) takes then the form

$$u_Z = \frac{1}{\mathfrak{N}} \exp\left(iZ^{a/2}G \int d\xi\ \Gamma(\xi)\right) B[Z^{-\frac{1}{2}} - 1] \times \left\{\exp\left(\mu \frac{\partial}{\partial \kappa}\right) u_0^{(\mathrm{reg})}[J/\kappa]\right\}_{\mu = -\delta\kappa} = \frac{1}{\mathfrak{N}} \sum_n (iZ^{a/2}G)^n \int d\xi_n \cdots d\xi_1\ \Gamma(\xi_n) \cdots \Gamma(\xi_1) \times \sum_p \frac{(Z^{-\frac{1}{2}} - 1)^p}{p!} \int dx_p \cdots dx_1\ J(x_p) \cdots J(x_1) \times \frac{\delta^p}{\delta J(x_p) \cdots \delta J(x_1)} \sum_q \frac{(-\delta\kappa)^q}{q!} \frac{\partial^q}{\partial \kappa^q} u_0^{(\mathrm{reg})}[J/\kappa] \qquad \text{(I7)}$$

and will be represented by

$$u^{(\mathrm{reg})}[Z^{-\frac{1}{2}}J/G, \kappa - \delta\kappa] = u_Z$$

in accordance with (I5).

We want now to work out the total derivative du_Z/dg; the result is a straightforward consequence of the following formulas whose proofs can be easily established by the reader.

$$\frac{\partial}{\partial X} B[X] = (1 + X)^{-1} \int d\xi\ J(\xi) \frac{\delta}{\delta J(\xi)} B[X] \qquad \text{(I8)}$$

with

$$B[X] = \sum_n \frac{X^n}{n!} \times \int dx_n \cdots dx_1\ J(x_n) \cdots J(x_1) \frac{\delta^n}{\delta J(x_n) \cdots \delta J(x_1)};$$

$$\left[\exp\left(i\epsilon \int d\xi\ \Gamma(\xi)\right), \int dx\ J(x) \frac{\delta}{\delta J(x)}\right] = i\epsilon \int d\xi\ \Gamma(\xi) \exp\left(i\epsilon \int d\xi\ \Gamma(\xi)\right); \qquad \text{(I9)}$$

$$\frac{\partial}{\partial \mu} \exp\left[\mu \frac{\partial}{\partial \kappa}\right] u_0^{(\mathrm{reg})}[J/\kappa] = \frac{i}{2} \lim_{\xi_1 = \xi} \left\{\int d\xi \frac{\delta^2}{\delta J(\xi_1)\, \delta J(\xi)} + \tfrac{1}{2}\Delta_{\mathrm{reg}}^{(c)}(\xi_1 - \xi, \kappa + \mu)\right\} \exp\left[\mu\, \partial/\partial\kappa\right] u_0^{(\mathrm{reg})}[J/\kappa], \qquad \text{(I10)}$$

and

$$\frac{\delta^2}{\delta J(\xi)\, \delta J(\xi)} B[X] = (1 + X)^2 B[X] \frac{\delta^2}{\delta J(\xi)\, \delta J(\xi)}. \qquad \text{(I11)}$$

The formula (I10) requires a comment: although $\Delta_{\mathrm{reg}}^{(c)}(\xi_1 - \xi, \kappa)$ is a well-defined function as far as

[13] The assumption is certainly valid for $a = 3,4$ corresponding to renormalizable theories.

$\xi_1 - \xi \neq 0$, we mean by $\Delta^{(c)}_{reg}(\xi_1 - \xi, \kappa + \mu)$ the formal series

$$\sum_k \frac{\mu^k}{k!} \frac{\partial^k}{\partial \kappa^k} \Delta^{(c)}_{reg}(\xi_1 - \xi, \kappa). \tag{I12}$$

These preliminaries being understood, we want now to prove the following formula which is the analog of (3.7) and (3.8),

$$du_Z/dg = -\left\{ d \frac{\log \mathfrak{N}}{dg} + \frac{1}{2} \frac{d \log Z}{dg} \int dx\, J(x) \frac{\delta}{\delta J(x)} + Z \frac{d\delta\kappa}{dg} \int d\xi\, \mathfrak{M}_{ph}(\xi) - \sum_{r=0}^{a} \left(\frac{d}{dg} (Z^{a/2} G) - \frac{r}{2} \frac{d \log Z}{dg} Z^{a/2} G \right) i\alpha_r \int d\xi\, \Gamma_r(\xi) \right\} u_Z. \tag{I13}$$

{In order to take into account the fact that in conventional quantum theory the Lagrangian of interacting field is expressed in terms of Wick's products, we replaced $\Gamma_a(\xi)$ defined by (I1) by a polynomial interaction of the form

$$:\Gamma(\xi): = \Gamma_a(\xi) + \sum_{r=0}^{a-2} \alpha_r \Gamma_r(\xi) = \sum_{r=0}^{a} \alpha_r \Gamma_r(\xi),$$

where $\Gamma_r(\xi) = (1/i)^r [\delta^r / \delta J(\xi)^r]$ and the coefficients α_r must be determined for each kind of interaction.}

Performing the derivative with respect to g of formal series (I7), one gets

$$\begin{aligned} du_Z/dg = & -\frac{d \log \mathfrak{N}}{dg} u_Z + i \frac{d(Z^{a/2} G)}{dg} \int d\xi\, \Gamma(\xi) u_Z \\ & + \frac{dZ^{-\frac{1}{2}}}{dg} \exp\left[i z^{a/2} G \int d\xi\, \Gamma(\xi) \right] \\ & \times \frac{\partial B}{\partial Z^{-\frac{1}{2}}} [Z^{-\frac{1}{2}} - 1] \left\{ \exp\left(\mu \frac{\partial}{\partial \kappa} \right) u_0^{(reg)}[J/\kappa] \right\}_{\mu = -\delta\kappa} \\ & + \exp\left[i Z^{a/2} G \int d\xi\, \Gamma(\xi) \right] B[Z^{-\frac{1}{2}} - 1] \\ & \times \left\{ \frac{d(-\delta\kappa)}{dg} \right\} \frac{\partial}{\partial \kappa} \exp\left(\mu \frac{\partial}{\partial \kappa} \right) u_0^{(reg)}[J/\kappa]_{\mu = -\delta\kappa}. \end{aligned}$$

Taking into account (I8), (I9), and (I10), we finally have

$$\begin{aligned} du_Z/dg = & -\left[\frac{d \log \mathfrak{N}}{dg} + \frac{1}{2} \frac{d \log Z}{dg} \int J \frac{\delta}{\delta J} \right. \\ & + Z \frac{d\delta\kappa}{dg} \int d\xi\, \mathfrak{M}_{ph}(\xi) \\ & \left. - \left(\frac{d(Z^{a/2} G)}{dg} - \frac{a}{2} \frac{d \log Z}{dg} Z^{a/2} G \right) i \int d\xi\, \Gamma(\xi) \right] u_Z. \end{aligned}$$

APPENDIX II

One can prove that[14]

$$u\left[\eta, \bar{\eta}, \frac{J}{e}, m, \kappa \right] = \sum_{n=0}^{\infty} \frac{(ie)^n}{n!} \int d\xi_n \cdots d\xi_1 \frac{\delta^{2n} u_0[\eta, \bar{\eta}/m]}{\delta\eta_{\alpha_n}(\xi_n) \delta\bar{\eta}_{\beta_n}(\xi_n) \cdots \delta\eta_{\alpha_1}(\xi_1) \delta\bar{\eta}_{\beta_1}(\xi_1)} \gamma^{\mu_n}_{\alpha_n\beta_n} \cdots \gamma^{\mu_1}_{\alpha_1\beta_1} \frac{\delta^n u_0[J/\kappa]}{\delta J_{\mu_n}(\xi_n) \cdots \delta J_{\mu_1}(\xi_1)}; \tag{II1}$$

then the propagators are given by

$$\begin{aligned} & \lim_{\eta, \bar{\eta}, J = 0} \frac{\delta^{2p+q} u[\cdots]}{\delta\bar{\eta}(x_n) \cdots \delta\bar{\eta}(x_1) \delta\eta(y_p) \cdots \delta\eta(y_1) \delta J(t_q) \cdots \delta J(t_1)} \\ & = \sum_{n=0}^{\infty} \frac{(ie)^n}{n!} \int d\xi_n \cdots d\xi_1 \lim_{\eta, \bar{\eta} = 0} \frac{\delta^{2n+2p} u_0[\eta, \bar{\eta}/m] \gamma^{\mu_n}_{\alpha_n\beta_n} \cdots \gamma^{\mu_1}_{\alpha_1\beta_1}}{\delta\bar{\eta}(x_n) \cdots \delta\bar{\eta}(x_1) \delta\eta(y_p) \cdots \delta\eta(y_1) \delta\eta_{\alpha_n}(\xi_n) \delta\bar{\eta}_{\beta_n}(\xi_n) \cdots \delta\eta_{\alpha_1}(\xi_1) \delta\bar{\eta}_{\beta_1}(\xi_1)} \\ & \qquad \times \lim_{J = 0} \frac{\delta^{n+q} u_0[J/\kappa]}{\delta J(t_q) \cdots \delta J(t_1) \delta J_{\mu_n}(\xi_n) \cdots \delta J_{\mu_1}(\xi_1)}. \end{aligned} \tag{II2}$$

From the expression of $u_0[J/\kappa]$ it follows that the terms such that $n + q$ is an odd integer vanish at the limit $J = 0$. Therefore propagators with an odd (even) number of insertion of photon lines do not contain radiative corrections of even (odd) order.

APPENDIX III

By a "well-defined" functional, we mean any functional of the form

$$\int \prod_{i=1}^{N} \bar{\eta}_{\lambda_i}(x_i) S^{(c)}_{\lambda_i\mu_i}(x_i - \xi_i) F_{\mu_i\nu_j\sigma_k}(\xi_1 \cdots \xi_N, \xi'_1 \cdots \xi'_N, \zeta_1 \cdots \zeta_p) \prod_{j=1}^{N} S^{(c)}_{\nu_j\tau_j}(\xi'_j - x'_j) \eta_{\tau_j}(x_j) \prod_{k=1}^{p} \Delta^{(c)}(\zeta_k - z_k) J_{\sigma_k}(z_k),$$

with $F_{\mu_i\nu_j\sigma_k}(\cdots)$ a temperate distribution.

[14] See Y. Le Gaillard, these de 3ème Cycle Faculté des Sciences de Marseille.

Group Theory of Harmonic Oscillators in n-Dimensional Space*

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It is shown how the states of N particles which move in a common n-dimensional harmonic oscillator potential can be classified according to the irreducible representations of the unitary groups U_N or U_n. The complete set of Nn independent integrals of the motion is obtained, their simultaneous eigenvectors being generalized Gel'fand basis vectors which can be enumerated either as bases for irreducible representations of U_N or U_n. Explicit formulas are given for the linear transformations induced on the basis vectors by the infinitesimal operators of U_N and U_n. The relation of the present work for $n = 3$ to that of Bargmann and Moshinsky is noted.

I. INTRODUCTION

RECENTLY, Baird and Biedenharn[1] have given an explicit set of orthonormal vectors which is a basis for an irreducible representation of the unitary group U_n. They call these vectors Gel'fand basis vectors since Gel'fand and Zetlin[2,3] originated the notational scheme, and also gave the linear transformations of these basis vectors induced by the infinitesimal operators of U_n. In this paper, we show that a generalized set of Gel'fand basis vectors spans the state space of N identical particles in an n-dimensional Cartesian space, each particle moving in an n-dimensional simple harmonic oscillator potential. The Gel'fand basis vectors can be enumerated either as bases for irreducible representations of U_N or U_n. The structure of the state space, in its relation to these unitary groups, is thus revealed concisely.

Of particular importance is the classification of the states of N particles moving in a common three-dimensional harmonic oscillator potential. Here one is interested in the physical classification of states where the total orbital angular momentum and its z component are diagonal. Bargmann and Moshinsky[4] have already given the complete set of $3N$ integrals of the motion and their eigenvalues, the set including the square of the angular momentum and its z component. In Sec. VII, we set down the explicit results which are obtained from our general theory for $n = 3$, and also relate these results to those of Bargmann and Moshinsky.

The work of this paper is arranged in the following order. In Sec. II, we summarize the results from several papers which are required for our use. The simple, but important, case of one particle in n-dimensional space is presented in some detail in Sec. III. These results are generalized to n particles in Sec. IV, where the appropriate set of n^2 independent integrals of the motion is given for characterizing the particle states in the manner indicated in the first paragraph. The N-particle case is obtained in Sec. V by direct modification of the results of Sec. IV. Finally, in Sec. VI, the generalized Gel'fand basis vectors are defined, and the complete solution is presented to the problem of classifying the N-particle states according to the irreducible representations of U_N or U_n.

II. RÉSUMÉ

The n^2 Weyl infinitesimal generators $E_{ij}(i, j = 1, 2, \cdots, n)$ of the unitary group U_n obey the commutation relations

$$[E_{ij}, E_{kl}] = \delta_{jk}E_{il} - \delta_{il}E_{kj}. \tag{1}$$

From the infinitesimal point of view, a basic problem in the determination of the irreducible representations of U_n is to find explicitly all sets of n^2 matrices E_{ij} of finite dimension which satisfy Eq. (1). It is also required that E_{ji} be the Hermitian conjugate of E_{ij} and that the matrices be irreducible. The E_{ij} can also be regarded as operators defined on an appropriate finite-dimensional Hilbert space, and it is this view which is adopted here.

The solution to the preceding problem has been presented by Gel'fand and Zetlin,[2] a detailed derivation of their results being given recently by Baird and Biedenharn.[1] The results are summarized in this section. A more complete list of references relating to the method is given in Ref. 1.

The first step in the method is to find a complete

* Work performed under the auspices of the U. S. Atomic Energy Commission.
[1] G. E. Baird and L. C. Biedenharn, J. Math. Phys. 4, 1449 (1963).
[2] I. M. Gel'fand and M. L. Zetlin, Doklady Akad. Nauk. 71, 825 (1950).
[3] The author is indebted to Dr. Paul R. Stein for calling his attention to a number of Gel'fand's papers and to Helen J. Chick for the translations.
[4] V. Bargmann and M. Moshinsky, Nucl. Phys. 18, 697 (1960); 23, 127 (1961).

set of independent invariants (generalized Casimir operators) for U_n. Gel'fand[5] appears to be the first author to give an explicit listing of these invariants. Biedenharn[6] also finds a set of invariants for the unimodular group SU_n, and his list becomes a set of invariants for U_n when the first-order operator is included. The Gel'fand invariants are simpler in form than Biedenharn's, and these are the ones we list:

$$I_k^{(n)} \equiv \sum_{i_1 i_2 \cdots i_k}^{n} E_{i_1 i_2} E_{i_2 i_3} \cdots E_{i_k i_1}, \tag{2}$$

where $k = 1, 2, \cdots, n$. It is straightforward to verify that the operators (2) are Hermitian and satisfy

$$[I_k^{(n)}, E_{ij}] = 0 \quad (\text{all } i, j, k) \tag{3}$$

as required of an invariant. Gel'fand's proof that the invariants (2) are also independent is related in a simple way to the fact that the traces of the various powers $H^k (k = 1, 2, \cdots, n)$ of a general Hermitian matrix H of dimension n are independent.[7] It must, of course, be possible to express Biedenharn's invariants for SU_n in terms of the invariants (2).

The operators

$$I_k^{(j)} \equiv \sum_{i_1 i_2 \cdots i_k}^{j} E_{i_1 i_2} E_{i_2 i_3} \cdots E_{i_k i_1} \tag{4}$$

for $k = 1, 2, \cdots, j$ are invariants for U_j. Consider now the set (I) of $n(n+1)/2$ operators as follows:

$$(I) = \begin{pmatrix} I_1^{(n)} I_2^{(n)} & \cdots & I_n^{(n)} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ I_1^{(2)} & I_2^{(2)} & \\ I_1^{(1)} & & \end{pmatrix}. \tag{5}$$

Each operator in the set is Hermitian, commutes with every other operator in the set, and is independent[7] of the other operators in the set.

Gel'fand and Zetlin[2] label the simultaneous eigenvectors of the operators (I) by a symbol (m) where

$$(m) = \begin{pmatrix} m_{1n} m_{2n} & \cdots & m_{nn} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ m_{12} & m_{22} & \\ m_{11} & & \end{pmatrix}. \tag{6a}$$

The m_{in} are integers which satisfy

$$m_{1n} \geq m_{2n} \geq \cdots \geq m_{nn} \geq 0, \tag{6b}$$

and the remaining m_{ij} are arbitrary nonnegative integers satisfying the conditions

$$m_{i,j+1} \geq m_{ij} \geq m_{i+1,j+1}. \tag{6c}$$

Thus, in the triangular scheme (6a), the m_{ij} lie between the pair of integers directly above. Baird and Biedenharn[1] denote the Gel'fand basis vectors (6) by the symbol $|(m)\rangle$ and note that each vector is associated with the Weyl basis tableau which has the Young pattern defined by the partition

$$[\lambda] = [\lambda_1 \lambda_2 \cdots \lambda_n] = [m_{1n} m_{2n} \cdots m_{nn}]. \tag{7}$$

Conditions (6c) are a consequence of the requirement that the Weyl basis tableau be lexical.

We note the following properties of the Gel'fand basis vectors $|(m)\rangle$:

(a) The basis vectors corresponding to distinct arrays (6) are orthonormal

$$\langle (m') \mid (m) \rangle = \delta_{m'm}. \tag{8}$$

(b) For a given partition $[\lambda]$, the number of orthogonal vectors enumerated as the m_{ij} run over all their allowed values is

$${}^{n}D_{[\lambda]} \equiv \prod_{i<j}^{n} \frac{(\lambda_i - \lambda_j + j - i)}{1!2! \cdots (n-1)!}. \tag{9}$$

(c) The ${}^{n}D_{[\lambda]}$ vectors described in (b) are a basis for an irreducible representation of the E_{ij} operators, hence, for an irreducible representation ${}^{n}\Gamma_{[\lambda]}$ of U_n.

Let ${}^{n}V_{[\lambda]}$ denote the vector space spanned by the ${}^{n}D_{[\lambda]}$ Gel'fand basis vectors $|(m)\rangle$ corresponding to a given partition $[\lambda]$. The linear transformations induced on ${}^{n}V_{[\lambda]}$ by the E_{ij} operators are given explicitly by the following equations:

$$E_{ii} \, |(m)\rangle = \left(\sum_{i=1}^{i} m_{i,i} - \sum_{i=1}^{i-1} m_{i,i-1} \right) |(m)\rangle, \tag{10a}$$

$$E_{i,i+1} \, |(m)\rangle = \sum_{i=1}^{i} \langle (m)_{ii}^{+} | \, E_{i,i+1} \, |(m)\rangle \, |(m)_{ii}^{+}\rangle, \tag{10b}$$

$$E_{i+1,i} \, |(m)\rangle = \sum_{i=1}^{i} \langle (m)_{ii}^{-} | \, E_{i+1,i} \, |(m)\rangle \, |(m)_{ii}^{-}\rangle, \tag{10c}$$

where $(m)_{ij}^{+}$ and $(m)_{ij}^{-}$ denote the sets obtained from array (6a) by replacing m_{ij} with $m_{ij} + 1$ and $m_{ij} - 1$, respectively. Using the definition

$$\lambda_{ij} \equiv m_{ij} + j - i, \tag{10d}$$

[5] I. M. Gel'fand, Mat. Sb. **26**, 103 (1950).
[6] L. C. Biedenharn, J. Math. Phys. **4**, 436 (1963).
[7] If several of the eigenvalues of the Hermitian matrix are equal, then the n traces will no longer be independent. Thus, the proof of the independence of the invariants (2) assumes that the E_{ij} correspond to the elements of a general Hermitian matrix which has no relations among its elements other than the Hermiticity relations.

the coefficients in Eqs. (10b, c) are

$$\langle (m)_{ij}^{-}| E_{j+1,i} |(m)\rangle = \langle (m)| E_{i,j+1} |(m)_{ij}^{-}\rangle = \left[\frac{\prod_{k=1}^{i-1}(\lambda_{k,j-1} - \lambda_{ij} + 1)}{\prod_{\substack{k=1 \\ k\neq i}}^{j}(\lambda_{kj} - \lambda_{ij} + 1)}\right]^{\frac{1}{2}} \cdot \left[\frac{-\prod_{k=1}^{j+1}(\lambda_{k,j+1} - \lambda_{ij})}{\prod_{\substack{k=1 \\ k\neq i}}^{j}(\lambda_{kj} - \lambda_{ij})}\right]^{\frac{1}{2}}. \quad (10e)$$

The result of applying any of the remaining E_{ij} operators to $|(m)\rangle$ can now be calculated by use of the following equation and its Hermitian conjugate:

$$E_{ij} = [E_{i,i-1}, [E_{i-1,i-2}, [\cdots, [E_{j+2,j+1}, E_{j+1,j}]]\cdots] \quad (11)$$

for $i = j + 2, j + 3, \cdots, n$.

While each Gel'fand basis vector is associated with a lexical Weyl basis tableau, it is also characterized by being a simultaneous eigenvector of the operators (I):

$$I_k^{(j)} |(m)\rangle = \lambda_k^{(j)}(m_{1j}, m_{2j}, \cdots, m_{jj}) |(m)\rangle, \quad (12a)$$

$$I_1^{(j)} |(m)\rangle = \left(\sum_{i=1}^{j} m_{ij}\right) |(m)\rangle. \quad (12b)$$

We do not require the explicit evaluation of the eigenvalues in Eq. (12a), but merely note that the eigenvalues of $I_k^{(j)}$ depend only on the $m_{ij}(i = 1, 2, \cdots, j)$, and each $\lambda_k^{(j)}$ is a polynomial of degree k in each m_{ij}.

For a given partition $[\lambda]$, let $|(\bar{m})\rangle$ denote the Gel'fand vector which has the m_{ij} chosen as large as possible, i.e., $\bar{m}_{ij} = m_{in}$ $(i = 1, 2, \cdots, j; j = 1, 2, \cdots, n - 1)$. The state $|(\bar{m})\rangle$ is the state of highest weight of Cartan and satisfies

$$E_{ij} |(\bar{m})\rangle = 0, \qquad (i < j = 1, 2, \cdots, n). \quad (13)$$

By using property (13), the explicit calculation of the eigenvalues $\lambda_k^{(n)}$ can be effected in a direct manner. The eigenvalues $\lambda_k^{(j)}(j = 1, 2, \cdots)$ are just the eigenvalues $\lambda_k^{(n)}(n = 1, 2, \cdots)$.

Baird and Biedenharn[1] derived results (10) by introducing an explicit operator realization of the E_{ij} generators, these operators being defined on a finite-dimensional Hilbert space. This is also the procedure of the following sections.

III. SYMMETRIC BASIS

In this section, some explicit results for the symmetric basis (the basis on which is defined an irreducible representation of U_n and which corresponds to a Young pattern of one row) are noted in detail because of the important role this basis plays in the subsequent developments. It was pointed out long ago by Jauch and Hill[8] that the eigenvectors of the Hamiltonian for a single particle in an n-dimensional isotropic harmonic oscillator potential present a basis for an irreducible representation of U_n. We now review these results in relation to the Gel'fand basis vectors.

The Hamiltonian in question is

$$H = \tfrac{1}{2}\sum_{i=1}^{n}(p_i^2 + x_i^2), \quad (14)$$

where $\mathbf{x} = (x_1, x_2, \cdots, x_n)$ and $\mathbf{p} = (p_1, p_2, \cdots, p_n)$ denote the position and linear momentum of the particle, and the units are such that the mass, the frequency, and $\hbar$ are unity. In terms of the usual creation and annihilation operators,[9]

$$a_i = (x_i - ip_i)/\sqrt{2}, \qquad \bar{a}_i = (x_i + ip_i)/\sqrt{2}, \quad (15)$$

the Hamiltonian (14) becomes

$$H = \sum_{i=1}^{n} a_i\bar{a}_i, \quad (16)$$

except for an unimportant additive constant. The a_i, $\bar{a}_i$ obey the commutation relations

$$[\bar{a}_i, a_j] = \delta_{ij}. \quad (17)$$

The eigenvectors of H corresponding to a given eigenvalue $r(r = 0, 1, \cdots)$ are completely characterized by specifying that they be simultaneous eigenvectors of the commuting operators $a_i\bar{a}_i$ or, equivalently, of

$$I_1^{(j)} \equiv \sum_{i=1}^{j} a_i\bar{a}_i, \qquad (j = 1, 2, \cdots, n). \quad (18)$$

The eigenvectors are also completely characterized by the Young pattern $[\lambda_1\lambda_2 \cdots \lambda_n] = [r0 \cdots 0] \equiv [r]$ and the lexical Weyl basis tableau which has $m_{11}1$'s, $m_{12} - m_{11}2$'s, $\cdots$, $m_{1n} - m_{1,n-1}n$'s$(m_{1n} = r)$ in the one-rowed Young pattern. In this case, the Weyl basis vectors and the Gel'fand basis vectors coincide and have the explicit definition

$$|m_{11}m_{12} \cdots m_{1n}\rangle \equiv \left|\begin{array}{ccccc} m_{1n}0 & \cdots & 0 & & \\ \cdot & & \cdot & & \\ & \cdot & & \cdot & \\ m_{13}0 & 0 & & & \rangle \\ m_{12} & 0 & & & \\ m_{11} & & & & \end{array}\right| \equiv \prod_{i=1}^{n} \frac{(a_i)^{m_{in}-m_{i+1,n}}|0\rangle}{[(m_{in} - m_{i+1,n})!]^{\frac{1}{2}}}, \quad (19a)$$

[8] J. M. Jauch and E. L. Hill, Phys. Rev. 57, 641 (1940).

[9] To save parentheses the bar is used to denote the operator which is Hermitian conjugate to a_i.

where $m_{n+1,n} \equiv 0$ and $|0\rangle$ is the state defined by

$$\bar{a}_i |0\rangle = 0, \qquad (i = 1, 2, \cdots, n). \tag{19b}$$

Let ${}^nV_{[r]}$, where $[r]$ designates the partition $[r, 0, \cdots, 0]$ with $n - 1$ zeros, denote the Hilbert space of dimension

$${}^nD_{[r]} = (n + r - 1)!/(n - 1)!r! \tag{20}$$

spanned by the orthonormal vectors (19a). The dimension is, of course, just the well-known degeneracy of H for a given eigenvalue r.

With an arbitrary $n \times n$ unitary matrix $U = (u_{ij})$, we associate the unitary transformation

$$a_i' = \sum_{j=1}^{n} a_j u_{ji}. \tag{21}$$

If we write $U = \exp iG$, where G is the Hermitian matrix

$$G = \sum_{i,j}^{n} g_{ij} E_{ij} (g_{ij}^* = g_{ji}),$$

and E_{ij} is a Weyl generator, then the unitary operator $\mathbf{U}$ to which U corresponds is given by

$$\mathbf{U} = \exp i\left(\sum_{i,j}^{n} g_{ij} E_{ij}\right),$$

in which E_{ij} is now the operator

$$E_{ij} = a_i \bar{a}_j, \qquad (i, j = 1, 2, \cdots, n). \tag{22}$$

The following operator identity is easily established:

$$a_i' = \mathbf{U} a_i \mathbf{U}^{-1} = \sum_{j=1}^{n} a_j u_{ji}. \tag{23}$$

It follows from Eq. (23) that the commutation relations for the a_i', $\bar{a}_i'$ operators are the same as those for the a_i, $\bar{a}_i$; furthermore, H is invariant[10] under the unitary transformation (23). Accordingly, the vector obtained by operating on the basis vector (19a) with $\mathbf{U}$ is again a vector of ${}^nV_{[r]}$:

$$\mathbf{U} |m_{11} m_{12} \cdots m_{1n}\rangle = \prod_{i=1}^{n} \left[\frac{\left(\sum_{j=1}^{n} a_j u_{ji}\right)^{m_{in} - m_{i+1,n}}}{[(m_{in} - m_{i+1,n})]^{\frac{1}{2}}} \right] |0\rangle. \tag{24}$$

The matrix elements of $\mathbf{U}$,

$$\langle m_{11}' m_{12}' \cdots m_{1n}' | \mathbf{U} | m_{11} m_{12} \cdots m_{1n}\rangle, \tag{25}$$

can now be identified by expanding the right-hand side of Eq. (24). Let ${}^n\Gamma_{[r]}(U)$ denote the matrix of dimension ${}^nD_{[r]}$ with elements (25). We summarize these results with the statement that the ${}^nD_{[r]}$ vectors of Eq. (19a), corresponding to given $m_{1n} = r$, are a basis for the irreducible representation ${}^n\Gamma_{[r]}$ of the unitary group U_n.

We are more interested in the representations of the infinitesimal operators E_{ij} of Eq. (22). Explicitly, we find

$$E_{jj} |m_{11} m_{12} \cdots m_{1n}\rangle = (m_{1j} - m_{1,j-1}) |m_{11} m_{12} \cdots m_{1n}\rangle, \tag{26a}$$

$$E_{j,j+1} |m_{11} m_{12} \cdots m_{1n}\rangle = [(m_{1,j+1} - m_{1j}) \cdot (m_{1j} - m_{1,j-1} + 1)]^{\frac{1}{2}} |m_{11} \cdots m_{1j} + 1 \cdots m_{1n}\rangle, \tag{26b}$$

$$E_{j+1,j} |m_{11} m_{12} \cdots m_{1n}\rangle = [(m_{1,j+1} - m_{1j} + 1) \cdot (m_{1j} - m_{1,j-1})]^{\frac{1}{2}} |m_{11} \cdots m_{1j} - 1 \cdots m_{1n}\rangle, \tag{26c}$$

$$I_1^{(j)} |m_{11} m_{12} \cdots m_{1n}\rangle = m_{1j} |m_{11} m_{12} \cdots m_{1n}\rangle. \tag{26d}$$

These results can be observed to be the special cases of the general results of Sec. II which correspond to the Gel'fand vectors (19a).

It is also of interest to examine the general operator $I_k^{(j)}$ of the set (5). We find upon substituting the E_{ij} of Eq. (22) into definition (4) that

$$I_k^{(j)} = (I_1^{(j)} + j - 1)^{k-1} I_1^{(j)}. \tag{27}$$

Thus, the $n(n + 1)/2$ operators of set (I) become dependent upon the n operators $I_1^{(j)} (j = 1, 2, \cdots, n)$. This does not imply a fault with the proof that the operators (I) are independent,[7] but rather that the operator realization (22) of the Weyl generators is a very special one. Indeed, besides satisfying the commutation relation (1) and the Hermiticity requirement, the operators (22) also satisfy

$$E_{ij} E_{kl} = E_{il} E_{kj} - \delta_{kl} E_{ij} + \delta_{jk} E_{il}. \tag{28}$$

Equation (27) is a direct consequence of this additional relation.

IV. GENERALIZATION TO n PARTICLES

In this section, n particles in a common n-dimensional harmonic oscillator potential are considered. The reason for considering $N = n$ is that, once this problem is solved, it is easy to see what modifications are required for the case of arbitrary N. Furthermore, in order to connect the results with those of the preceding section, we first view the problem as one for a *single particle in an n^2-dimensional space.* Thus, let n be replaced by n^2 in all results of Sec. III. The basis vectors (19a) become a basis for the Hilbert space ${}^{n^2}V_{[r]}$ of dimension

$${}^{n^2}D_{[r]} = (n^2 + r - 1)!/(n^2 - 1)!r!, \tag{29}$$

[10] G. A. Baker, Jr., Phys. Rev. 103, 1119 (1956).

and are a basis for the irreducible representation ${}^{n^2}\Gamma_{[r]}$ of U_{n^2}. Here $[r]$ denotes the partition with $n^2 - 1$ zeros. It is our object to demonstrate eventually precisely how the space ${}^{n^2}V_{[r]}$ reduces into a direct sum of subspaces, the basis vectors of each subspace constituting a basis for an irreducible representation of U_n.

The n^2 creation operators for a single particle in n^2-dimensional space are $a_i (i = 1, 2, \cdots, n^2)$. We now define

$$a_i^\alpha \equiv a_{(\alpha-1)n+i}, \tag{30a}$$

where $i, \alpha = 1, 2, \cdots, n$, and interpret

$$\mathbf{a}^\alpha = (a_1^\alpha, a_2^\alpha, \cdots, a_n^\alpha) \tag{30b}$$

as the creation operators for particle α in an n-dimensional harmonic oscillator potential. Conversely, if we had started from this second interpretation, we would proceed to the other by defining the $a_i (i = 1, 2, \cdots, n^2)$ by Eq. (30a). The commutation relations for the a_i^α, $\bar{a}_i^\alpha$ take the form

$$[\bar{a}_i^\alpha, a_j^\beta] = \delta^{\alpha\beta}\delta_{ij}. \tag{31}$$

An explicit realization of the $\mathbf{a}^\alpha$ operators in terms of the position $\mathbf{x}^\alpha$ and momentum $\mathbf{p}^\alpha$ operators for particle α is

$$\mathbf{a}^\alpha = (\mathbf{x}^\alpha - i\mathbf{p}^\alpha)/\sqrt{2}, \qquad \bar{\mathbf{a}}^\alpha = (\mathbf{x}^\alpha + i\mathbf{p}^\alpha)/\sqrt{2}. \tag{32}$$

It is also convenient to introduce the notation

$$\mathbf{a}_i = (a_i^1, a_i^2, \cdots, a_i^n). \tag{33}$$

The n^4 infinitesimal operators of U_{n^2} of Sec. III now become

$$E_{(\alpha-1)n+i,(\beta-1)n+j} = E_{ij}^{\alpha\beta} \equiv a_i^\alpha \bar{a}_j^\beta \tag{34}$$

for $i, j, \alpha, \beta = 1, 2, \cdots, n$. In this section, all indices $\alpha, \beta, \gamma, \cdots, i, j, k, \cdots$ run from 1 to n unless otherwise noted.

The basis vectors (19a) of ${}^{n^2}V_{[r]}$ (for $n \to n^2$) will also be enumerated by a new notation:

$$\left|\begin{matrix} m_1^1 m_2^1 \cdots m_n^1 \\ m_1^2 m_2^2 \cdots m_n^2 \\ \vdots \\ m_1^n m_2^n \cdots m_n^n \end{matrix}\right\rangle \equiv \prod_{i,\alpha} \left[\frac{(a_i^\alpha)^{m_i{}^\alpha}}{[(m_i^\alpha)!]^{\frac{1}{2}}}\right] |0\rangle, \tag{35a}$$

where the m_i^α are any nonnegative integers such that

$$\sum_{i,\alpha} m_i^\alpha = r. \tag{35b}$$

The n^2 Gel'fand quantum numbers of Eq. (19a) are related to the m_i^α by

$$m_{1,(\alpha-1)n+i} = \sum_{\beta=1}^{\alpha-1}\sum_{j=1}^{n} m_j^\beta + \sum_{j=1}^{i} m_j^\alpha. \tag{36}$$

The basis vectors enumerated by Eq. (35a) for all values of the m_i^α consistent with condition (35b) are precisely the basis vectors enumerated by Eq. (19a) for all $m_{1,(\alpha-1)n+i}$ consistent with

$$m_{1,n^2} = r \geq m_{1,n^2-1} \geq \cdots \geq m_{12} \geq m_{11}. \tag{37}$$

We next consider a unitary transformation of the n^2 creation operators a_i^α. Let U denote the $n^2 \times n^2$ unitary matrix as follows:

$$U = \begin{bmatrix} U^{11} U^{12} \cdots U^{1n} \\ U^{21} U^{22} \cdots U^{2n} \\ \vdots \\ U^{n1} U^{n2} \cdots U^{nn} \end{bmatrix}, \tag{38}$$

where each $U^{\alpha\beta}$ is an $n \times n$ matrix, and $u_{ij}^{\alpha\beta}$ denotes the element in row i and column j of $U^{\alpha\beta}$. With the unitary matrix (38), we associate the unitary transformation

$$(a_i^\alpha)' = \sum_{j,\beta} a_j^\beta u_{ji}^{\beta\alpha}. \tag{39}$$

Next consider the special unitary matrix with elements

$$u_{ij}^{\alpha\beta} = \delta^{\alpha\beta} v_{ij}. \tag{40a}$$

U becomes the direct product $U = I \otimes V$, where $V = (v_{ij})$ is itself an $n \times n$ unitary matrix and I the $n \times n$ unit matrix. The transformation (39) becomes

$$(a_i^\alpha)' = \sum_j a_j^\alpha v_{ji}. \tag{40b}$$

Thus, the unitary transformation associated with $U = I \otimes V$ transforms the components of each of the vectors $\mathbf{a}^\alpha$ in the same way. Similarly, for

$$u_{ij}^{\alpha\beta} = w^{\alpha\beta}\delta_{ij}, \tag{41a}$$

U becomes $U = W \otimes I$, where $W = (w^{\alpha\beta})$ is unitary. The transformation (39) becomes

$$(a_i^\alpha)'' = \sum_\beta a_i^\beta w^{\beta\alpha}, \tag{41b}$$

which shows that the components of each of the vectors $\mathbf{a}_i$ undergo the same transformation.

Momentarily, in this paragraph, let $E_{ij}^{\alpha\beta}$ denote a Weyl generator *matrix*: It is the $n^2 \times n^2$ matrix with the block structure (38) in which all elements are zero except in the $\alpha\beta$ block and within the $\alpha\beta$ block all elements are zero except for the element in row i and column j which is 1. It is a straightforward task

to demonstrate that the Weyl generators for a unitary matrix of the type $U = I \otimes V$ are

$$E_{ij} = \sum_{\alpha} E_{ij}^{\alpha\alpha}; \tag{42a}$$

similarly, the Weyl generators for a unitary matrix of the type $U = W \otimes I$ are

$$E^{\alpha\beta} = \sum_{i} E_{ii}^{\alpha\beta}. \tag{42b}$$

From the above results, we see that the infinitesimal operators for transformations of the types (40b) and (41b) are, respectively,

$$E_{ij} = \sum_{\alpha} E_{ij}^{\alpha\alpha} = \sum_{\alpha} a_i^{\alpha} \bar{a}_j^{\alpha}, \tag{43a}$$

$$E^{\alpha\beta} = \sum_{i} E_{ii}^{\alpha\beta} = \sum_{i} a_i^{\alpha} \bar{a}_i^{\beta}. \tag{43b}$$

It can be directly verified that

$$[E_{ij}, E_{kl}] = \delta_{jk} E_{il} - \delta_{il} E_{kj}, \tag{44a}$$

$$[E^{\alpha\beta}, E^{\gamma\delta}] = \delta^{\beta\gamma} E^{\alpha\delta} - \delta^{\alpha\delta} E^{\gamma\beta}, \tag{44b}$$

$$[E_{ij}, E^{\alpha\beta}] = 0. \tag{44c}$$

Thus, either set of operators, the E_{ij} *or* $E^{\alpha\beta}$, is an operator realization of the generators of U_n. Furthermore, the operators of the first set commute with the operators of the second set, this result being consistent with

$$(I \otimes V)(W \otimes I) = (W \otimes I)(I \otimes V) = W \otimes V.$$

We can go further and demonstrate that $U_1 = I \otimes V$ corresponds to the unitary *operator*

$$\mathbf{U}_1 = \exp i(\sum_{ij} g_{ij} E_{ij}), \tag{45a}$$

where $V = e^{iG}$, $G = (g_{ij})$ with $g_{ij}^* = g_{ji}$. Similarly, $U_2 = W \otimes I$ corresponds to the unitary operator

$$\mathbf{U}_2 = \exp i(\sum_{\alpha\beta} f^{\alpha\beta} E^{\alpha\beta}), \tag{45b}$$

where $W = e^{iF}$, $F = (f^{\alpha\beta})$ with $(f^{\alpha\beta})^* = f^{\beta\alpha}$. Also, from

$$[E_{ij}, a_k^{\alpha}] = a_i^{\alpha} \delta_{jk}, \tag{46a}$$

$$[E^{\alpha\beta}, a_i^{\gamma}] = a_i^{\alpha} \delta^{\beta\gamma}, \tag{46b}$$

the explicit operator transformations as follows can be verified:

$$(a_i^{\alpha})' = \mathbf{U}_1 a_i^{\alpha} \mathbf{U}_1^{-1} = \sum_{j} a_j^{\alpha} v_{ji}, \tag{47a}$$

$$(a_i^{\alpha})'' = \mathbf{U}_2 a_i^{\alpha} \mathbf{U}_2^{-1} = \sum_{\beta} a_i^{\beta} w^{\beta\alpha}. \tag{47b}$$

We are interested in several general features of the linear transformations induced on ${}^{n^2}V_{[r]}$ upon applying the operators E_{ij} and $E^{\alpha\beta}$ to the basis vectors (35). Consider the subspace of ${}^{n^2}V_{[r]}$ which is spanned by the basis vectors (35) which have the sums of the quantum numbers in the rows fixed, i.e., $\sum_i m_i^{\alpha} = \lambda^{\alpha}$, where $\lambda^1, \lambda^2, \cdots, \lambda^n$ are any set of fixed nonnegative integers satisfying $\sum_{\alpha} \lambda^{\alpha} = r$. It can be verified that when E_{ij} is applied to any vector in this subspace it yields a vector in the subspace. Similar results hold for the operators $E^{\alpha\beta}$ with respect to the subspace defined by

$$\sum_{\alpha} m_i^{\alpha} = \lambda_i, \quad \sum_{i} \lambda_i = r.$$

These considerations show that the representations of the E_{ij} and $E^{\alpha\beta}$ operators which are obtained from ${}^{n^2}V_{[r]}$ are reducible. We are not interested in the explicit linear transformations induced on ${}^{n^2}V_{[r]}$ by the E_{ij} and $E^{\alpha\beta}$ because the work of Baird and Biedenharn[1] shows us how to proceed directly to the irreducible subspaces. Before proceeding to this point, we wish to examine the role of the commuting operators given in Sec. II.

With respect to the infinitesimal operators $E_{ij}^{\alpha\beta}$ of U_{n^2}, we have already seen that there is only *one* independent invariant, namely, the harmonic oscillator Hamiltonian

$$H = I_1^{(n^2)} = \sum_{i,\alpha} E_{ii}^{\alpha\alpha}. \tag{48}$$

The entire set of $n^2(n^2 + 1)/2$ operators (I) (for $n \to n^2$) of Eq. (5) was shown to be dependent on the n^2 first-order operators

$$I_1^{(\alpha-1)n+i} = \sum_{\beta=1}^{\alpha-1} \sum_{j=1}^{n} E_{jj}^{\beta\beta} + \sum_{j=1}^{i} E_{jj}^{\alpha\alpha}. \tag{49}$$

It is, of course, just the set of simultaneous eigenvectors (35) of these operators, for a given eigenvalue r of H, which is the basis of the space ${}^{n^2}V_{[r]}$.

We now have the possibility of constructing a second set of commuting operators, namely, the set made up of the two sets analogous to set (5), constructed from the E_{ij} and $E^{\alpha\beta}$ operators. Thus, let (K) and (L) denote the operator sets as follows:

$$(K) = \begin{bmatrix} K_1^{(n)} K_2^{(n)} \cdots K_n^{(n)} \\ \cdot \qquad\qquad \cdot \\ \cdot \qquad\qquad \cdot \\ K_1^{(2)} \quad K_2^{(2)} \\ K_1^{(1)} \end{bmatrix}, \tag{50a}$$

where

$$K_k^{(j)} \equiv \sum_{i_1 i_2 \cdots i_k}^{j} E_{i_1 i_1} E_{i_2 i_2} \cdots E_{i_k i_k}, \tag{50b}$$

and E_{ij} is given by Eq. (43a). Similarly, let

$$(L) = \begin{bmatrix} L_1^{(n)} L_2^{(n)} \cdots L_n^{(n)} \\ \cdot \quad \cdot \quad \cdot \\ L_1^{(2)} \quad L_2^{(2)} \\ L_1^{(1)} \end{bmatrix}, \tag{51a}$$

where

$$L_k^{(\beta)} \equiv \sum_{\alpha_1 \alpha_2 \cdots \alpha_k}^{\beta} E^{\alpha_1 \alpha_2} E^{\alpha_2 \alpha_3} \cdots E^{\alpha_k \alpha_1}, \tag{51b}$$

and $E^{\alpha\beta}$ is given by Eq. (43b). Note that the $K_k^{(n)} (k = 1, 2, \cdots, n)$ are invariants with respect to unitary transformations of the type (40b), while the $L_k^{(n)} (k = 1, 2, \cdots, n)$ are invariants with respect to unitary transformations of the type (41b). We turn next to the investigation of the relations between the operators of sets (K) and (L) and between the operators of a given set.

It is evident that

$$H = I_1^{(n^2)} = K_1^{(n)} = L_1^{(n)}. \tag{52a}$$

The general result (also proved directly for $k = 2$)

$$K_k^{(n)} = L_k^{(n)} (k = 1, 2, \cdots, n) \tag{52b}$$

is also correct and can be established as follows: The identity

$$\sum_{i_1 i_2 \cdots i_k}^{n} E_{i_1 i_2} E_{i_2 i_3} \cdots E_{i_k i_{k+1}} = \sum_{\alpha_1 \alpha_2 \cdots \alpha_k}^{n} E^{\alpha_1 \alpha_2} a_{i_1}^{\alpha_2} \bar{a}_{i_{k+1}}^{\alpha_2} E^{\alpha_2 \alpha_4} \cdots E^{\alpha_k \alpha_1} \tag{53}$$

is easily proved for $k = 3$. Assume it to be correct for k and multiply by $E_{i_{k+1} i_{k+2}}$ from the right and sum on i_{k+1}. $E_{i_{k+1} i_{k+2}}$ can be moved to the position adjacent to $\bar{a}_{i_{k+1}}^{\alpha_2}$ on the right-hand side. If we now use the identity

$$\sum_{i=1}^{n} \bar{a}_i^{\alpha} E_{ij} = \sum_{\beta=1}^{n} \bar{a}_j^{\beta} E^{\beta\alpha}, \tag{54}$$

and rename the summation symbols appropriately on the right-hand side, Eq. (53) is seen to be correct for $k + 1$. Thus, its general validity follows by induction. In Eq. (53), we set $i_{k+1} = i_1$ and sum on i_1 to prove Eq. (52b).

Let (K') and (L') denote, respectively, the sets (50a) and (51a) which have the top row deleted. Assume there is a functional relation between the members of the set (K) and of set (L'), $F(L') = G(K)$. Then it follows that $[E^{\alpha\beta}, F(L')] = 0$ for all α, β. But this implies that $F(L')$ is a function of the invariants $L_k^{(n)} (k = 1, 2, \cdots, n)$ contrary to fact. Thus, the operators (L') are independent of the operators (K). Similarly, the operators (K') are shown to be independent of the operators (L).

We saw in Sec. III that a particular operator realization of the generators E_{ij} of U_n can satisfy auxiliary equations which cause some of the operators in set (K) to become dependent. Does this happen for the operators (43a, b)? We will now show that it does not, but more important is that the method of proof will show how, when we consider N particles in n-space, some of the operators in (K) or (L) do become dependent.

Gel'fand's[5] work shows that in determining the independence or dependence of the operators (K) or (L) we can treat the E_{ij} (or $E^{\alpha\beta}$) as commuting quantities. In terms of the a_i^{α} operators, this implies that $\mathbf{a}^{\alpha}$ and $\mathbf{a}_k$ can be considered to be ordinary vectors $\mathbf{z}^{\alpha}$ and $\mathbf{z}_k$ in an n-dimensional complex space. $\bar{\mathbf{a}}^{\alpha}$ and $\bar{\mathbf{a}}_k$ then correspond to the complex conjugate vectors $(\mathbf{z}^{\alpha})^*$ and $\mathbf{z}_k^*$. Thus,

$$E_{ij} \to \mathbf{z}_i \cdot \mathbf{z}_j \equiv \sum_{\alpha} z_i^{\alpha} (z_j^{\alpha})^*, \tag{55a}$$

$$E^{\alpha\beta} \to \mathbf{z}^{\alpha} \cdot \mathbf{z}^{\beta} \equiv \sum_{i} z_i^{\alpha} (z_i^{\beta})^*. \tag{55b}$$

Let $Z_j (j = 1, 2, \cdots, n)$ and $Z^{\beta} (\beta = 1, 2, \cdots, n)$ denote $j \times j$ and $\beta \times \beta$ Hermitian matrices as follows:

$$Z_j \equiv \begin{bmatrix} \mathbf{z}_1 \cdot \mathbf{z}_1 & \mathbf{z}_1 \cdot \mathbf{z}_2 & \cdots & \mathbf{z}_1 \cdot \mathbf{z}_j \\ \mathbf{z}_2 \cdot \mathbf{z}_1 & \mathbf{z}_2 \cdot \mathbf{z}_2 & \cdots & \mathbf{z}_2 \cdot \mathbf{z}_j \\ \vdots & & & \\ \mathbf{z}_j \cdot \mathbf{z}_1 & \mathbf{z}_j \cdot \mathbf{z}_2 & \cdots & \mathbf{z}_j \cdot \mathbf{z}_j \end{bmatrix}, \tag{56a}$$

$$Z^{\beta} \equiv \begin{bmatrix} \mathbf{z}^1 \cdot \mathbf{z}^1 & \mathbf{z}^1 \cdot \mathbf{z}^2 & \cdots & \mathbf{z}^1 \cdot \mathbf{z}^{\beta} \\ \mathbf{z}^2 \cdot \mathbf{z}^1 & \mathbf{z}^2 \cdot \mathbf{z}^2 & \cdots & \mathbf{z}^2 \cdot \mathbf{z}^{\beta} \\ \vdots & & & \\ \mathbf{z}^{\beta} \cdot \mathbf{z}^1 & \mathbf{z}^{\beta} \cdot \mathbf{z}^2 & \cdots & \mathbf{z}^{\beta} \cdot \mathbf{z}^{\beta} \end{bmatrix}. \tag{56b}$$

The operators in the jth row of (K) correspond to $\mathrm{Tr}\,(Z_j)^k (k = 1, 2, \cdots, j)$; the operators in the βth row of (L) correspond to $\mathrm{Tr}\,(Z^{\beta})^k (k = 1, 2, \cdots, \beta)$. Thus, the independent operators in the jth row of (K) are just those which correspond to independent $\mathrm{Tr}\,(Z_j)^k (k = 1, 2, \cdots, j)$. A similar statement applies to the operators in the βth row of (L).

Let $f_k = f_k(\mathbf{z}_1 \mathbf{z}_2 \cdots \mathbf{z}_j) \equiv \mathrm{Tr}\,(Z_j)^k$. Then functional dependence of $f_1, f_2, \cdots, f_j$ implies the existence of a function F such that

$$F(f_1, f_2, \cdots, f_j) \equiv 0 (j \leq n) \tag{57}$$

for all vectors $\mathbf{z}_1 \mathbf{z}_2 \cdots \mathbf{z}_j$. Since $j \leq n$, we can consider a set of j orthogonal vectors of distinct, but

varying, lengths $l_i = (\mathbf{z}_i \cdot \mathbf{z}_i)^{\frac{1}{2}} (l_1 \neq l_2 \neq \cdots \neq l_j)$. Then

$$f_k = l_1^{2k} + l_2^{2k} + \cdots + l_j^{2k}, \quad (k = 1, 2, \cdots, j).$$

But these $f_1, f_2, \cdots, f_j$ are functionally independent, and there can exist no relation (57) which is valid for all vectors $\mathbf{z}_1, \mathbf{z}_2, \cdots, \mathbf{z}_j$. Hence, $f_1, f_2, \cdots, f_j$ are functionally independent; correspondingly, the operators in the jth row of (K) are independent. Since there are no relations between the traces of Hermitian matrices of different dimensions, we further conclude that all operators in set (K) are independent. Upon applying the same considerations to the matrix (56b), we conclude that all operators in set (L) are independent.

Let $(K) \cup (L)$ denote the union of the operator sets (K) and (L) so that $(K) \cup (L)$ has n^2 elements, these elements being the operators in the sets (K') and (L') together with $K_k^{(n)} = L_k^{(n)} (k = 1, 2, \cdots, n)$. The results of the preceding paragraphs can be summarized as follows: The n^2 Hermitian operators of $(K) \cup (L)$, which are constructed from the two sets of explicit operator realizations (43a, b) of the generators of U_n, are a set of n^2 independent commuting operators. It has already been demonstrated that one basis of the space ${}^{n}V_{[r]}$ is characterized by the fact that the basis vectors are the simultaneous eigenvectors of the n^2 operators of Eq. (49). We now see that it must be possible to find a second basis of ${}^{n}V_{[r]}$ which is completely determined by the requirement that the basis vectors be simultaneous eigenvectors of the n^2 operators of $(K) \cup (L)$. We will turn to the construction of this second basis in Sec. VI. Now we will show how to modify the results of this section, thus far obtained, for the problem of N particles in n-space.

V. MODIFICATION TO N PARTICLES

It is a simple procedure to modify the results of the preceding section such that they are applicable to the description of N identical particles in a common n-dimensional harmonic oscillator potential. It is only necessary to let the superscripts $\alpha, \beta, \gamma, \cdots$ have the range $1, 2, \cdots, N$. In particular, the basis vectors (35) of the space ${}^{Nn}V_{[r]}$ become

$$\left| \begin{matrix} m_1^1 & m_2^1 & \cdots & m_n^1 \\ m_1^2 & m_2^2 & \cdots & m_n^2 \\ \vdots & & & \\ m_1^N & m_2^N & \cdots & m_n^N \end{matrix} \right\rangle \equiv \prod_{\alpha=1}^{N} \prod_{i=1}^{n} \left[\frac{(a_i^\alpha)^{m_i{}^\alpha}}{[(m_i^\alpha)!]^{\frac{1}{2}}} \right] |0\rangle \tag{58a}$$

with

$$\sum_{i=1}^{n} \sum_{\alpha=1}^{N} m_i^\alpha = r. \tag{58b}$$

The dimension of this space is

$${}^{Nn}D_{[r]} = (Nn + r - 1)!/(Nn - 1)!r!. \tag{58c}$$

It is evident that all the results of the preceding section up through Eq. (51) become applicable to the N-particle problem by this simple change of the range of superscripts and subscripts. We note a few more explicit results of this change. The unitary matrix U of Eq. (38) has dimension Nn, each of the N^2 $U^{\alpha\beta}$ being $n \times n$. The direct product matrix (40a) becomes $U = I_N \otimes V$, where I_N is the $N \times N$ unit matrix and V is an $n \times n$ unitary matrix. Similarly, the direct product matrix (41a) becomes $U = W \otimes I_n$, where I_n is the $n \times n$ unit matrix and W is an $N \times N$ unitary matrix. The E_{ij} of Eq. (43a) become an operator realization of the generators of U_n, while the $E^{\alpha\beta}$ of Eq. (43b) become an operator realization of the generators of U_N. The commuting operators (49) become Nn in number, and the vectors (58) are the simultaneous eigenvectors of these Nn operators.

We now come to the discussion of the operator sets (50a) and (51a), which become

$$(K) = \begin{bmatrix} K_1^{(n)} & K_2^{(n)} & \cdots & K_n^{(n)} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ & K_1^{(2)} & & K_2^{(2)} \\ & & K_1^{(1)} & \end{bmatrix}, \tag{59a}$$

$$(L) = \begin{bmatrix} L_1^{(N)} & L_2^{(N)} & \cdots & L_N^{(N)} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ & L_1^{(2)} & & L_2^{(2)} \\ & & L_1^{(1)} & \end{bmatrix}. \tag{59b}$$

A more complicated version of Eq. (53) can now be used to establish the identity

$$K_k^{(n)} = \sum_{j=1}^{k} \binom{k-1}{j-1} (n - N)^{k-j} L_j^{(N)}, \tag{60a}$$

from which also follows

$$L_k^{(N)} = \sum_{j=1}^{k} \binom{k-1}{j-1} (N - n)^{k-j} K_j^{(n)}. \tag{60b}$$

The discussion is now divided into two parts corresponding to $N > n$ and $N < n$. First, consider $N > n$. In Eq. (60b), k runs from 1 to N. Note that $K_j^{(n)}$ is still defined for $j > n$, but all such $K_j^{(n)}$ are

dependent on the set which has $j \leq n$. Thus, all operators in the top row of (L) are dependent on those in the top row of (K). Let (K') and (L') denote the sets (59a, b) which have the top row deleted. Then it follows as before that (K') is independent of (L), and (L') is independent of (K). Consider the operators in set (K). In the discussion of Eq. (56a) relating to the independence of the operators (K), the $\mathbf{z}_j (j = 1, 2, \cdots, n)$ become vectors with $N > n$ components. Since the number of vectors is less than the dimension of the space, it still follows that the operators (K) are independent. However, in Eq. (56b), the $\mathbf{z}^\alpha (\alpha = 1, 2, \cdots, N)$ become vectors with n components, and the total number of vectors exceeds the dimension of the space. By examining the cases $\beta \leq n$, we are still able to conclude that the operators in the n bottom rows of (L) are independent. However, for $\beta > n$, the rank of Z^β is at most n, since every set of $\beta > n$ vectors in n-dimensional space is linearly dependent. Using this point, we are able to conclude that the independent quantities among $\mathrm{Tr}\,(Z^\beta)^k$ $(\beta > n)$ $(k = 1, 2, \cdots, N)$ are just the first n corresponding to $k = 1, 2, \cdots, n$. Thus, the independent operators in sets (K) and (L) individually are the nonzero operators in the following arrays:

$$(K) = \begin{bmatrix} K_1^{(n)} & K_2^{(n)} & \cdots & K_n^{(n)} \\ \cdot & & & \cdot \\ & \cdot & & \\ & K_1^{(2)} & & K_2^{(2)} \\ & & K_1^{(1)} & \end{bmatrix}, \tag{61a}$$

$$(L) = \begin{bmatrix} L_1^{(N)} & L_2^{(N)} & \cdots & L_n^{(N)} & 0 & \cdots & 0 \\ \cdot & & & \cdot & & & \cdot \\ & \cdot & & & \cdot & & \\ & L_1^{(n+1)} & L_2^{(n+1)} & \cdots & L_n^{(n+1)} & 0 & \\ & & L_1^{(n)} & L_2^{(n)} & \cdots & L_n^{(n)} & \\ & & \cdot & & & \cdot & \\ & & & \cdot & & & \\ & & L_1^{(2)} & & L_2^{(2)} & & \\ & & & L_1^{(1)} & & & \end{bmatrix}, \tag{61b}$$

where in the second set we have replaced the dependent operators by the null operator. The top row of operators in (L) is dependent on the top row of (K). $(K) \cup (L)$ now designates the operators (K) together with the $N - 1$ bottom rows of (L), and it contains Nn independent operators. The simultaneous eigenvectors of the Nn operators of $(K) \cup (L)$ must also be a set of basis vectors for the space ${}^{Nn}V_{[r]}$.

In the same way, we find for $N \leq n$ that the independent operators in sets (K) and (L) individually are

$$(K) = \begin{bmatrix} K_1^{(n)} & K_2^{(n)} & \cdots & K_N^{(n)} & 0 & \cdots & 0 \\ \cdot & & & \cdot & & & \cdot \\ & \cdot & & & \cdot & & \\ & K_1^{(N+1)} & K_2^{(N+1)} & \cdots & K_N^{(N+1)} & 0 & \\ & K_1^{(N)} & K_2^{(N)} & \cdots & K_N^{(N)} & & \\ & \cdot & & & \cdot & & \\ & & \cdot & & & & \\ & K_1^{(2)} & & & K_2^{(2)} & & \\ & & K_1^{(1)} & & & & \end{bmatrix}, \tag{62a}$$

$$(L) = \begin{bmatrix} L_1^{(N)} & L_2^{(N)} & \cdots & L_N^{(N)} \\ \cdot & & & \cdot \\ & \cdot & & \\ & L_1^{(2)} & & L_2^{(2)} \\ & & L_1^{(1)} & \end{bmatrix}. \tag{62b}$$

The top row of (K) is dependent on the top row of (L). $(K) \cup (L)$ now designates the operators (L) together with the $n - 1$ bottom rows of (K), and it contains Nn independent operators. The simultaneous eigenvectors of the Nn operators of $(K) \cup (L)$ must also be a set of basis vectors for the space ${}^{Nn}V_{[r]}$.

VI. GEL'FAND BASES

A complete set of mutually commuting operators (the so-called integrals of the motion) for N identical particles moving in a common n-dimensional harmonic oscillator potential has been given in Secs. IV and V. The simultaneous eigenvectors of these operators, when appropriately enumerated, present bases for irreducible representations of the unitary groups U_N and U_n. This structure is examined in detail in this section. We consider first the case $N = n$, and then give the modifications for general N.

The operator realization (43a) of the generators of U_n is just the one used by Baird and Biedenharn.[1] They give the following explicit vector for the normalized state of highest weight (13) corresponding to the partition (7):

$$|(\bar{m})\rangle \equiv N^{\frac{1}{2}} \prod_{k=1}^{n} (a_{12\ldots k})^{m_{kn} - m_{k+1,n}} |0\rangle, \tag{63a}$$

where

$$a_{12\ldots k} \equiv \det \begin{bmatrix} a_1^1 & a_1^2 & \cdots & a_1^k \\ a_2^1 & a_2^2 & \cdots & a_k^k \\ \vdots & & & \\ a_k^1 & a_k^2 & \cdots & a_k^k \end{bmatrix}, \tag{63b}$$

$$N = \prod_{j=1}^{n} \left[\frac{\prod_{k=1}^{j-1} (m_{kn} - m_{jn} + j - k)!}{\prod_{k=1}^{j} (m_{kn} - m_{j+1,n} + j - k)!} \right]. \tag{63c}$$

The general Gel'fand basis vector corresponding to the array (m) of Eq. (6a) is obtained from the vector (63a) by the application of a suitable lowering operator

$$\mathcal{O}_{(m)}(E_{ij}) \tag{64}$$

which depends on all the m_{ij} in the set (m). $\mathcal{O}$ is also a polynomial in certain of the operators E_{ij} $(i, j = 1, 2, \cdots, n)$, and the notation (64) is intended to indicate only this general feature. Then

$$|(m)\rangle = \mathcal{O}_{(m)}(E_{ij})\ |(\bar{m})\rangle, \tag{65a}$$

$$\mathcal{O}_{(\bar{m})}(E_{ij}) = 1. \tag{65b}$$

The explicit form of $\mathcal{O}$ for $n = 2, 3$ is given below, but we never make explicit use of these results, and the general form of $\mathcal{O}$ is not required:

(a) $n = 2$,

$$\mathcal{O}_{(m)} = \left[\frac{(m_{11} - m_{22})!}{(m_{12} - m_{22})!(m_{12} - m_{11})!} \right]^{\frac{1}{2}} E_{21}^{m_{12} - m_{11}}; \tag{66}$$

(b) $n = 3$,

$$\mathcal{O}_{(m)} = A^{\frac{1}{2}} E_{21}^{m_{12} - m_{11}} E_{32}^{m_{23} - m_{33}} \cdot [E_{31}(E_{11} - E_{22}) + E_{32}E_{21}]^{m_{13} - m_{12}}, \tag{67a}$$

where

$$A = \left[\frac{(m_{11} - m_{22})!(m_{22} - m_{33})!}{(m_{12} - m_{11})!(m_{12} - m_{22})!(m_{23} - m_{22})!(m_{23} - m_{33})!} \right] \times \left[\frac{(m_{12} - m_{22} + 1)!(m_{12} - m_{23})!(m_{12} - m_{33} + 1)!}{(m_{13} - m_{22} + 1)!(m_{13} - m_{12})!(m_{13} - m_{23})!(m_{13} - m_{33} + 1)!} \right]. \tag{67b}$$

These forms of $\mathcal{O}$ for $n = 2, 3$ can be obtained from the explicit results of Baird and Biedenharn.[1]

The verification that $|(\bar{m})\rangle$ of Eq. (63a) satisfies)

$$E_{ij}|(\bar{m})\rangle = 0 \qquad (i < j = 1, 2, \cdots, n) \tag{68}$$

follows from

$$[E_{ij}, a_{12\cdots k}] = 0 \qquad (i < j = 1, 2, \cdots, n) \tag{69}$$

for $k = 1, 2, \cdots, n$. This second result is obtained from property (46a). But now we also see that

$$E^{\alpha\beta}\ |(\bar{m})\rangle = 0, \qquad (\alpha < \beta = 1, 2, \cdots, n). \tag{70}$$

Thus, $|(\bar{m})\rangle$ is also a state of highest weight with respect to the operators $E^{\alpha\beta}$ of U_n. Indeed, a study of the tableau technique whereby the state $|(\bar{m})\rangle$ is written down shows that $|(\bar{m})\rangle$ is the *unique* vector (for the given partition) of the space ${}^{n^2}V_{(r)}$ which has properties (68) and (70).

We can go much further. Because each $E^{\alpha\beta}$ commutes with each E_{ij}, every Gel'fand basis vector (65) also has the property

$$E^{\alpha\beta}\ |(m)\rangle = 0, \qquad (\alpha < \beta = 1, 2, \cdots, n). \tag{71}$$

Every Gel'fand basis vector (65) *is a state of highest weight with respect to the operators* $E^{\alpha\beta}$. But now the solution to our problem is evident. The simultaneous eigenvectors of the operators in the set $(K) \cup (L)$ are the generalized Gel'fand basis vectors defined as follows (We now require two arrays of type (6a), and we introduce the arrays (k) and (l), which refer, respectively, to the quantum numbers of operators (K) and (L).):

$$\left| \begin{array}{ccccccc} (k_{1n}, l^{1n}) & & (k_{2n}, l^{2n}) & \cdots & & (k_{nn}, l^{nn}) \\ (k_{1,n-1}, l^{1,n-1}) & & (k_{2,n-1}, l^{2,n-1}) & \cdots & (k_{n-1,n-1}, l^{n-1,n-1}) & & \\ \cdot & & & & & \cdot & \\ & \cdot & & & \cdot & & \\ & & (k_{13}, l^{13}) & (k_{23}, l^{23}) & (k_{33}, l^{33}) & & \\ & & & (k_{12}, l^{12}) & (k_{22}, l^{22}) & & \\ & & & & (k_{11}, l^{11}) & & \end{array} \right\rangle \equiv |(k, l)\rangle \equiv \mathcal{O}_{(k)}(E_{ij})\mathcal{O}_{(l)}(E^{\alpha\beta})\ |(\bar{k}, \bar{l})\rangle. \tag{72}$$

In this equation, (k) and (l) are the arrays obtained from (6) upon setting $m_{ij} = k_{ij}$ and $m_{\alpha\beta} = l^{\alpha\beta}$, respectively. Because of identity (52b), we also have $k_{in} = l^{in} (i = 1, 2, \cdots, n)$ in the top row of the generalized Gel'fand symbol (72), as well as in the top rows of (k) and (l) on the right-hand side of the equation. In referring to the arrays (k) and (l), we will always understand that the top rows are identified. We will sometimes employ the partition notation

$$[\lambda] = [\lambda_1 \lambda_2 \cdots \lambda_n] = [k_{1n} k_{2n} \cdots k_{nn}] = [l^{1n} l^{2n} \cdots l^{nn}], \tag{73}$$

and replace the double index top row of (72) by the single partition numbers $\lambda_1, \lambda_2, \cdots, \lambda_n$. $|(\bar{k}, \bar{l})\rangle$ now designates the highest weight vector (63a):

$$|(\bar{k}, \bar{l})\rangle \equiv N^{\frac{1}{2}} \prod_{k=1}^{n} (a_{12\cdots k})^{\lambda_k - \lambda_{k+1}} |0\rangle, \tag{74}$$

where N is the normalization factor (63c) with $m_{kn} = \lambda_k$. As an example, we have

$$\left| \begin{matrix} \lambda_1 & \lambda_2 \\ (k_{11}, & l^{11}) \end{matrix} \right\rangle = \left[\frac{(k_{11} - \lambda_2)!(l^{11} - \lambda_2)!}{(\lambda_1 - \lambda_2)!(\lambda_1 - k_{11})!(\lambda_1 - \lambda_2)!(\lambda_1 - l^{11})!} \right]^{\frac{1}{2}} \times E_{21}^{\lambda_1 - k_{11}} (E^{21})^{\lambda_1 - l^{11}} |(\bar{k}, \bar{l})\rangle. \tag{75}$$

Other than the equality of the numbers in the top rows of (k) and (l), there are no relations among the k_{ij} and $l^{\alpha\beta}$. These numbers assumed, for a given partition $[\lambda]$, exactly the values they assume in the single-index Gel'fand symbol, and they assume these values independently of one another:

$$k_{i,j+1} \geq k_{ij} \geq k_{i+1,j+1}, \tag{76a}$$

$$l^{\alpha,\beta+1} \geq l^{\alpha\beta} \geq l^{\alpha+1,\beta+1}. \tag{76b}$$

The results of Sec. II are immediately applicable to the generalized Gel'fand basis vectors. We note the following results explicitly:

(a) The generalized Gel'fand basis vectors which correspond to distinct partitions $[\lambda]$ and $[\lambda']$ are orthogonal. More generally,

$$\langle (k', l') \mid (k, l) \rangle = \delta_{(k')(k)} \delta_{(l')(l)}. \tag{77}$$

(b) The linear transformations induced on the $|(k, l)\rangle$ basis vectors by the E_{ij} and $E^{\alpha\beta}$ operators are *identical in structure*: the E_{ij} transformations involve only the numbers of array (k); the $E^{\alpha\beta}$ transformations those of (l). More precisely, the E_{ij} transformations are Eqs. (10) and (11) in which (k) replaces (m). In particular, in $E_{i+1,j}|(k, l)\rangle$, only the $k_{ij} (i = 1, 2, \cdots, j)$ are shifted, one at a time, to the values $k_{ij} - 1$.

(c) For a given partition $[\lambda]$ *and a given array* (l), let ${}^{n}V_{[\lambda]}^{(l)}$ denote the Hilbert space spanned by the Gel'fand basis vectors (72) which are enumerated as the $k_{ij} (i, j = 1, 2, \cdots, n - 1)$ run over all their allowed values. There are ${}^{n}D_{[\lambda]}$ [Eq. (9)] Gel'fand basis vectors of this space. Then the spaces ${}^{n}V_{[\lambda]}^{(l)}$ and ${}^{n}V_{[\lambda]}^{(l')}$, which correspond to distinct arrays (l) and (l'), are perpendicular:

$${}^{n}V_{[\lambda]}^{(l)} \perp {}^{n}V_{[\lambda]}^{(l')}, (l) \neq (l'). \tag{78a}$$

Similarly, for the given partition $[\lambda]$ and a given array (k), let ${}^{n}V_{[\lambda],(k)}$ denote the Hilbert space spanned by the ${}^{n}D_{[\lambda]}$ Gel'fand basis vectors (72) which are enumerated as the $l^{\alpha\beta} (\alpha, \beta = 1, 2, \cdots, n - 1)$ run over their allowed values. Then

$${}^{n}V_{[\lambda],(k)} \perp {}^{n}V_{[\lambda],(k')}, (k) \neq (k'). \tag{78b}$$

(d) For given $[\lambda]$ and given (l), the linear transformations induced on the basis vectors of ${}^{n}V_{[\lambda]}^{(l)}$ by the E_{ij} operators are an irreducible representation of dimension ${}^{n}D_{[\lambda]}$ of these operators. Since there are ${}^{n}D_{[\lambda]}$ distinct ways of selecting (l), there are ${}^{n}D_{[\lambda]}$ such perpendicular spaces. Since the linear transformations do not depend on which array (l) we select, the *same* representation of E_{ij} is found on each of the spaces ${}^{n}V_{[\lambda]}^{(l)}$, i.e., it is found a number of times equal to its dimension. Similarly, each of the ${}^{n}D_{[\lambda]}$ perpendicular spaces ${}^{n}V_{[\lambda],(k)}$, corresponding to the distinct ways of selecting array (k), yields an irreducible representation of $E^{\alpha\beta}$ of dimension ${}^{n}D_{[\lambda]}$.

(e) The set of all generalized Gel'fand basis vectors $|(k, l)\rangle$ which correspond to all partitions $[\lambda]$ of r must also be a new basis for the space ${}^{n^2}V_{[r]}$ introduced at the beginning of Sec. IV. Thus, the space ${}^{n^2}V_{[r]}$ can be reduced into either of the following direct sums:

$${}^{n^2}V_{[r]} = \sum_{[\lambda]} \sum_{(l)} \oplus {}^{n}V_{[\lambda]}^{(l)} = \sum_{[\lambda]} \sum_{(k)} \oplus {}^{n}V_{[\lambda],(k)}, \tag{79a}$$

where the sums are over all partitions $[\lambda]$ of r and over all distinct arrays (l) and (k). It follows from this result that

$${}^{n^2}\Gamma_{[r]} = \sum_{[\lambda]} \oplus {}^{n}D_{[\lambda]} {}^{n}\Gamma_{[\lambda]}, \tag{79b}$$

that is, the irreducible representation ${}^{n^2}\Gamma_{[r]}$ of U_{n^2} is reducible into a direct sum of irreducible representations ${}^{n}\Gamma_{[\lambda]}$ of U_n, and each representation ${}^{n}\Gamma_{[\lambda]}$ of U_n occurs as often as its dimension. Corresponding to the reduction (79a), we also have the

following sum formula relating the dimensions of the respective spaces:

$$^{n^2}D_{[r]} = \binom{n^2 + r - 1}{r} = \sum_{[\lambda]} (^nD_{[\lambda]})^2. \quad (79c)$$

Once again it is a simple procedure to modify the preceding results so that they are applicable to the problem of N particles in n-space. We give the results only for $N > n$, it being evident how to write down the corresponding results for $N < n$. The Gel'fand basis vectors [the simultaneous eigenvectors of the operators (61)] are

$$\left| \begin{array}{ccccccccc} (k_{1n}, l^{1N}) & (k_{2n}, l^{2N}) & \cdots & (k_{nn}, l^{nN}) & (0,0) & \cdots & (0,0) \\ (k_{1n}, l^{1,N-1}) & (k_{2n}, l^{2,N-1}) & \cdots & (k_{nn}, l^{n,N-1}) & (0,0) & \cdots & (0,0) \\ \cdot & & & \cdot & & & \\ \cdot & & & \cdot & & & \\ (k_{1n}, l^{1,n+1}) & (k_{2n}, l^{2,n+1}) & \cdots & (k_{nn}, l^{n,n+1}) & (0,0) & & \\ (k_{1n}, l^{1n}) & (k_{2n}, l^{2n}) & \cdots & (k_{nn}, l^{nn}) & & & \\ \cdot & & & \cdot & & & \\ \cdot & & & \cdot & & & \\ (k_{12}, l^{12}) & (k_{22}, l^{22}) & & & & & \end{array} \right\rangle \quad (k_{11}, l^{11})$$

$$= |(k, l)\rangle \equiv \mathcal{O}_{(k)}(E_{ij})\mathcal{O}_{(l)}(E^{\alpha\beta})\, |(\bar{k}, \bar{l})\rangle. \quad (80)$$

In this equation, (k) is the Gel'fand array (6) of n rows with $m_{ij} = k_{ij}$. (l) is a Gel'fand array (6) of N rows, which has $l^{\alpha\beta} = 0$ for $\alpha > n$. Again the non zero entries of the top rows of (k) and (l) are the same $k_{in} = l^{iN} (i = 1, 2, \cdots, n)$. We have chosen the notation in Eq. (80) to indicate that the vectors (80) *are indeed just those obtained from* Eq. (72) *for* $n \to N$ *by restricting the* $k_{ij} (i, j = 1, 2, \cdots, N)$ *and* $l^{\alpha\beta} (\alpha, \beta = 1, 2, \cdots, N)$ *to the particular values that appear on the left-hand side of* Eq. (80). If (k) is the n-rowed Gel'fand array which occurs on the right-hand side of Eq. (80) and $(k)_N$ is the modified N-rowed array

$$(k)_N \equiv \left[\begin{array}{ccccccc} k_{1n} & k_{2n} & \cdots & k_{nn} & 0 & \cdots & 0 \\ & k_{1n} & k_{2n} & \cdots & k_{nn} & 0 \cdots & 0 \\ & & \cdot & & & \cdot & \\ & & & \cdot & & \cdot & \\ & & & k_{1n} & k_{2n} & \cdots & k_{nn}\ 0 \\ & & & & (k) & & \end{array} \right],$$

then $\mathcal{O}_{(k)}(E_{ij}) = \mathcal{O}_{(k)_N}(E_{ij})$, an example, in point, being provided by Eqs. (66) and (67). This merely points out that the Gel'fand basis vectors for N particles in n-space ($N \geq n$) span a subspace of the space spanned by the Gel'fand basis vectors for N particles in N-space, indeed, for N particles in m-space ($m \geq n$). Finally, we note that the vector $|(\bar{k}, \bar{l})\rangle$ appearing in Eq. (80) is just the one of Eq. (74), where

$$[\lambda] = [k_{1n}k_{2n} \cdots k_{nn}] = [l^{1N}l^{2N} \cdots l^{nN}]. \quad (81)$$

It is evident from this discussion that the linear transformations induced on the basis vectors $|(k, l)\rangle$ of Eq. (80) by the $E_{ij} (i, j = 1, 2, \cdots, n)$ operators are those described in (b). Similarly, the $E^{\alpha\beta} (\alpha, \beta = 1, 2, \cdots, N)$ transformations are those described in (b), except that we set $n = N$ followed by $l^{\alpha\beta} = 0$ for $\alpha > n$.

The modifications of Eqs. (79) are also immediate. Let $[\lambda 0]$ denote the partition made up of $[\lambda]$ of Eq. (81) followed by $N - n$ zeros. The vector space $^nV^{(l)}_{[\lambda]}$ is of dimension $^nD_{[\lambda]}$, and there are $^ND_{[\lambda 0]}$ such perpendicular spaces which present a basis for the same irreducible representation of the E_{ij}. The vector space $^NV_{[\lambda 0],(k)}$ is of dimension $^ND_{[\lambda 0]}$, and there are $^nD_{[\lambda]}$ such perpendicular spaces which present a basis for the same irreducible representation of the $E^{\alpha\beta}$. The vector space $^{Nn}V_{[r]}$ with basis vectors (58) can be written as the following direct sums:

$$^{Nn}V_{[r]} = \sum_{[\lambda]} \sum_{(l)} \oplus\, ^nV^{(l)}_{[\lambda]} = \sum_{[\lambda]} \sum_{(k)} \oplus\, ^NV_{[\lambda 0],(k)}. \quad (82a)$$

Also, the representation $^{Nn}\Gamma_{[r]}$ of U_{Nn} is reducible in two ways as follows:

$$^{Nn}\Gamma_{[r]} = \sum_{[\lambda]} \oplus\, ^ND_{[\lambda 0]}\, ^n\Gamma_{[\lambda]} = \sum_{[\lambda]} \oplus\, ^nD_{[\lambda]}\, ^N\Gamma_{[\lambda 0]}. \quad (82b)$$

Equation (82a) also implies the sum formula relating the dimension of the respective spaces:

$$^{Nn}D_{[r]} = \binom{Nn + r - 1}{r} = \sum_{[\lambda]} {}^nD_{[\lambda]}\, ^ND_{[\lambda 0]}. \quad (82c)$$

VII. N PARTICLES IN 3-SPACE

The classification of the states of N particles, which move in a common three-dimensional har-

monic oscillator potential, in terms of irreducible bases for U_3 or U_N is a special case of the general theory. The eigenvalues of the $3N$ integrals of the motion, Eqs. (61a, b) for $n = 3$, are immediately available to us. Likewise, the linear transformations corresponding to the $E_{ij}(i, j = 1, 2, 3)$ and $E^{\alpha\beta}(\alpha, \beta = 1, 2, \cdots, N)$ are known explicitly. Thus, the complete solution to the problem is available, and it seems worthwhile to present it in detail.

In the second part of this section, we indicate how one proceeds from the Gel'fand basis to the Bargmann–Moshinsky basis where the total angular momentum is diagonal. We believe that the expression of these results in terms of the elegant Gel'fand notation does not unnecessarily duplicate the important work of Bargmann and Moshinsky.

The Gel'fand basis vectors (80) for $n = 3$ and $N \geq 3$ become

$$\left|\begin{matrix} (k_{13}, l^{1N}) & (k_{23}, l^{2N}) & (k_{33}, l^{3N}) & (0,0) & \cdots & (0,0) \\ (k_{13}, l^{1,N-1}) & (k_{23}, l^{2,N-1}) & (k_{33}, l^{3,N-1}) & (0,0) & \cdots & (0,0) \\ \ddots & & \ddots & & \ddots & \\ & (k_{13}, l^{14}) & (k_{23}, l^{24}) & (k_{33}, l^{34}) & (0,0) & \\ & (k_{13}, l^{13}) & (k_{23}, l^{23}) & (k_{33}, l^{33}) & & \\ & & (k_{12}, l^{12}) & (k_{22}, l^{22}) & & \\ & & & (k_{11}, l^{11}) & & \end{matrix}\right\rangle \equiv |(k, l)\rangle = \Theta_{(k)}(E_{ij})\Theta_{(l)}(E^{\alpha\beta})\,|(\bar{k}, \bar{l})\rangle, \tag{83a}$$

where

$$(k) = \begin{bmatrix} k_{13} & k_{23} & k_{33} \\ k_{12} & k_{22} & \\ k_{11} & & \end{bmatrix}, \tag{83b}$$

$$(l) = \begin{bmatrix} l^{1N} & l^{2N} & l^{3N} & 0 & \cdots & 0 \\ l^{1,N-1} & l^{2,N-1} & l^{3,N-1} & 0 & \cdots & 0 \\ \ddots & & & \ddots & \ddots & \\ & l^{13} & l^{23} & l^{33} & & \\ & & l^{12} & l^{22} & & \\ & & & l^{11} & & \end{bmatrix}, \tag{83c}$$

and $l^{1N} = k_{13}$, $l^{2N} = k_{23}$, $l^{3N} = k_{33}$. $\Theta_{(k)}$ is given by Eqs. (67). While we do not know $\Theta_{(l)}$ explicitly, we do not need it. The partition $[\lambda]$ is

$$[\lambda] = [k_{13}k_{23}k_{33}], \tag{83d}$$

and the vector $|(\bar{k}, \bar{l})\rangle$ is

$$|(\bar{k}, \bar{l})\rangle = N^{\frac{1}{2}}(a_{123})^{\lambda_3}(a_{12})^{\lambda_2-\lambda_3}(a_1)^{\lambda_1-\lambda_2}\,|0\rangle. \tag{83e}$$

The space ${}^3V^{(l)}_{[\lambda]}$ is of dimension

$${}^3D_{[\lambda]} = \tfrac{1}{2}(\lambda_1 - \lambda_2 + 1)\,(\lambda_1 - \lambda_3 + 2)(\lambda_2 - \lambda_3 + 1), \tag{84a}$$

and in ${}^{3N}V_{[r]}$ there are ${}^ND_{[\lambda 0]}$ such perpendicular spaces which present a basis for the same irreducible representation ${}^3\Gamma_{[\lambda]}$ of U_3. The space ${}^NV_{[\lambda 0],(k)}$ is of dimension

$${}^ND_{[\lambda 0]} = \left[\frac{2(\lambda_1 + N - 1)!(\lambda_2 + N - 2)!(\lambda_3 + N - 3)!}{(N-1)!(N-2)!(N-3)!(\lambda_1 + 2)!(\lambda_2 + 1)!\lambda_3!}\right]{}^3D_{[\lambda]}, \tag{84b}$$

and in ${}^{3N}V_{[\lambda]}$ there are ${}^3D_{[\lambda]}$ such perpendicular spaces which present a basis for the same irreducible representation ${}^N\Gamma_{[\lambda 0]}$ of U_N.

The following operators are diagonal on the basis (83a), and have the idicated eigenvalues

$$E_{11} \to k_{11}, \qquad E_{22} \to k_{12} + k_{22} - k_{11}, \qquad E_{33} \to k_{13} + k_{23} + k_{33} - k_{12} - k_{22},$$

$$K_1^{(j)} \to \sum_{i=1}^{j} k_{ij} (j = 1, 2, 3), \qquad K_2^{(2)} \to k_{12}^2 + k_{22}^2 + k_{12} - k_{22},$$

$$K_2^{(3)} \to k_{13}^2 + k_{23}^2 + k_{33}^2 + 2(k_{13} - k_{33}),$$

$$
\begin{aligned}
K_3^{(3)} &\to k_{13}^3 + k_{23}^3 + k_{33}^3 + 4k_{13}^2 + k_{23}^2 - 2k_{33}^2 \\
&\quad - (k_{13}k_{23} + k_{13}k_{33} + k_{23}k_{33}) \\
&\quad + 4k_{13} - 2k_{23} - 2k_{33}; \\
E^{11} &\to l^{11}, \qquad E^{22} \to l^{12} + l^{22} - l^{11}, \\
E^{33} &\to l^{13} + l^{23} + l^{33} - l^{12} - l^{22}, \qquad (85) \\
E^{\beta\beta} &\to \sum_{\alpha=1}^{3} (l^{\alpha\beta} - l^{\alpha,\beta-1}) \qquad (\beta = 4, 5, \cdots, N), \\
L_1^{(\beta)} &\to \sum_{\alpha=1}^{3} l^{\alpha\beta} \qquad (\beta = 1, 2, \cdots, N), \\
L_2^{(\beta)} &\to \sum_{\alpha=1}^{3} (l^{\alpha\beta})^2 + (\beta - 1)l^{1\beta} \\
&\quad + (\beta - 3)l^{2\beta} + (\beta - 5)l^{3\beta} \\
&\quad (\beta = 2, 3, \cdots, N), \\
L_3^{(\beta)} &\to [(l^{1\beta})^3 + (l^{2\beta})^3 + (l^{3\beta})^3 + 4(l^{1\beta})^2 \\
&\quad + (l^{2\beta})^2 - 2(l^{3\beta})^2 - (l^{1\beta}l^{2\beta} + l^{1\beta}l^{3\beta} + l^{2\beta}l^{3\beta}) \\
&\quad + 4l^{1\beta} - 2l^{2\beta} - 2l^{3\beta}] + 2(\beta - 3)[(l^{1\beta})^2 \\
&\quad + (l^{2\beta})^2 + (l^{3\beta})^2 + 2(l^{1\beta} - l^{3\beta})] \\
&\quad + (\beta - 3)^2(l^{1\beta} + l^{2\beta} + l^{3\beta}) \quad (\beta = 3, 4, \cdots, N).
\end{aligned}
$$

In these last equations, $l^{\alpha\beta} \equiv 0$ for $\alpha > \beta$. The calculation of the above eigenvalues is straightforward. For example, in calculating the eigenvalue of $L_3^{(\beta)}$, we first note that the eigenvalue depends only on $l^{1\beta}$, $l^{2\beta}$, $l^{3\beta}$. Accordingly, in Eq. (83a), we set $l^{1\alpha} = l^{1\beta}(\alpha = 1, 2, \cdots, N)$, $l^{2\alpha} = l^{2\beta}(\alpha = 2, 3, \cdots, N)$, $l^{3\alpha} = l^{3\beta}(\alpha = 3, 4, \cdots, N)$, $k_{11} = k_{12} = k_{13} = l^{1\beta}$, $k_{22} = k_{23} = l^{2\beta}$, and $k_{33} = l^{3\beta}$. The vector reduces to Eq. (83e) with $\lambda_\alpha = l^{\alpha\beta}(\alpha = 1, 2, 3)$ and $E^{\alpha\gamma}(\alpha < \gamma)$ annihilates it. Second, upon examining $L_3^{(\beta)}$ itself, we see that upon repeatedly commuting operators of the type $E^{\alpha\gamma}(\alpha < \gamma)$ to the right, we are eventually left with a third-order polynomial in the $E^{\alpha\alpha}$ as the only terms contributing to the eigenvalue. Finally, $E^{\alpha\alpha}$ is replaced by $l^{\alpha\beta}(\alpha = 1, 2, 3)$ and 0 $(\alpha = 4, 5, \cdots, N)$ when operating the vector described above. For checks on the calculation of the eigenvalue of $L_3^{(\beta)}$, we see that it agrees in form with the eigenvalue of $K_3^{(3)}$ for $\beta = 3$; it also agrees with the result obtained from Eq. (60b) for $n = 3$, $\beta = N$ upon using the eigenvalues of $K_i^{(3)}(j = 1, 2, 3)$.

The linear transformations for all the E_{ij} and $E^{\alpha\beta}$ operators can be obtained from the following ones (the transformations for E_{21} and E_{32} are obtained from the first two below by replacing l's by k's):

$$
E^{21}\,|(k, l)\rangle = [(l^{11} - l^{22})(l^{12} - l^{11} + 1)]^{\frac{1}{2}}\,|(k, l')\rangle, \qquad (86a)
$$

where (l') is the set (l) with l_{11} replaced by $l_{11} - 1$.

$$
\begin{aligned}
E^{32}\,|(k, l)\rangle &= \left[\frac{(l^{12} - l^{11})(l^{13} - l^{12} + 1)(l^{12} - l^{23})(l^{12} - l^{33} + 1)}{(l^{12} - l^{22})(l^{12} - l^{22} + 1)}\right]^{\frac{1}{2}} |(k, l')\rangle \\
&\quad + \left[\frac{(l^{11} - l^{22} + 1)(l^{13} - l^{22} + 2)(l^{23} - l^{22} + 1)(l^{22} - l^{33})}{(l^{12} - l^{22} + 1)(l^{12} - l^{22} + 2)}\right]^{\frac{1}{2}} |(k, l'')\rangle, \qquad (86b)
\end{aligned}
$$

where (l') and (l'') are the sets obtained from (l) by replacing l^{12} by $l^{12} - 1$ and l^{22} by $l^{22} - 1$, respectively.

$$
E^{43}\,|(k, l)\rangle = A_1^{\frac{1}{2}}\,|(k, l')\rangle + A_2^{\frac{1}{2}}\,|(k, l'')\rangle + A_3^{\frac{1}{2}}\,|(k, l''')\rangle, \qquad (86c)
$$

where

$$
\begin{aligned}
A_\alpha &= \left[(l^{\alpha 3} - \alpha + 3)\prod_{\gamma=1}^{2}(l^{\gamma 2} - l^{\alpha 3} + \alpha - \gamma)\prod_{\gamma=1}^{3}(l^{\gamma 4} - l^{\alpha 3} + \alpha - \gamma + 1)\right] \\
&\quad \times \left[\prod_{\substack{\gamma=1 \\ \gamma\neq\alpha}}^{3}(l^{\gamma 3} - l^{\alpha 3} + \alpha - \gamma + 1)\prod_{\substack{\gamma=1 \\ \gamma\neq\alpha}}^{3}(l^{\gamma 3} - l^{\alpha 3} + \alpha - \gamma)\right]^{-1}
\end{aligned}
$$

for $\alpha = 1, 2, 3$. (l'), (l''), (l''') are, respectively, the sets obtained from (l) by replacing l^{13} by $l^{13} - 1$, l^{23} by $l^{23} - 1$, and l^{33} by $l^{33} - 1$.

$$
E^{\beta+1,\beta}\,|(k, l)\rangle = B_1^{\frac{1}{2}}\,|(k, l')\rangle + B_2^{\frac{1}{2}}\,|(k, l'')\rangle + B_3^{\frac{1}{2}}\,|(k, l''')\rangle, \qquad (86d)
$$

where

$$
\begin{aligned}
B_\alpha &= \left[-\prod_{\gamma=1}^{3}(l^{\gamma,\beta-1} - l^{\alpha\beta} + \alpha - \gamma)\prod_{\gamma=1}^{3}(l^{\gamma,\beta+1} - l^{\alpha\beta} + \alpha - \gamma + 1)\right] \\
&\quad \times \left[\prod_{\substack{\gamma=1 \\ \gamma\neq\alpha}}^{3}(l^{\gamma\beta} - l^{\alpha\beta} + \alpha - \gamma + 1)\prod_{\substack{\gamma=1 \\ \gamma\neq\alpha}}^{3}(l^{\gamma\beta} - l^{\alpha\beta} + \alpha - \gamma)\right]^{-1}
\end{aligned}
$$

for $\alpha = 1, 2, 3$ and $\beta = 4, 5, \cdots, N-1$. (l'), (l''), (l''') are, respectively, the sets obtained from (l) by replacing $l^{1\beta}$ by $l^{1\beta} - 1$, $l^{2\beta}$ by $l^{2\beta} - 1$, and $l^{3\beta}$ by $l^{3\beta} - 1$.

Next, let $\mathbf{L} = (L_1, L_2, L_3)$ denote the total orbital angular momentum of the N particles:

$$L_i = \sum_{\alpha=1}^{N} (x_j^\alpha p_k^\alpha - x_k^\alpha p_j^\alpha), \qquad (i, j, k \text{ cyclic}), \qquad (87)$$

where $\mathbf{x}^\alpha$ and $\mathbf{p}^\alpha$ denote the position and momentum of particle α. We now wish to make a very important point. In Sec. III, Eq. (15), and Sec. IV, Eq. (32), we introduced an operator realization of the creation and annihilation operators $\mathbf{a}^\alpha$ and $\bar{\mathbf{a}}^\alpha$ in terms of $\mathbf{x}^\alpha$ and $\mathbf{p}^\alpha$. However, nowhere did we make explicit use of this definition, the entire development depending only on the basic commutation rule (31). All operators E_{ij} and $E^{\alpha\beta}$, hence, all integrals of the motion are expressed directly in terms of the a_i^α, $\bar{a}_i^\alpha$ operators. Thus, we are free to define the a_i^α, $\bar{a}_i^\alpha$ in terms of $\mathbf{x}^\alpha$ and $\mathbf{p}^\alpha$ in ways which differ from Eq. (32). In particular, for $n = 3$ and for the discussion of the angular momentum operators (87), it is convenient to make the definitions in the following way:

$$\mathbf{a}^\alpha \equiv [(b_1^\alpha + ib_2^\alpha)/\sqrt{2}, (ib_1^\alpha + b_2^\alpha)/\sqrt{2}, b_3^\alpha], \qquad (88a)$$

where

$$\mathbf{b}^\alpha \equiv (\mathbf{x}^\alpha - i\mathbf{p}^\alpha)/\sqrt{2}. \qquad (88b)$$

Then

$$\bar{\mathbf{a}}^\alpha = [(\bar{b}_1^\alpha - i\bar{b}_2^\alpha)/\sqrt{2}, (-i\bar{b}_1^\alpha + \bar{b}_2^\alpha)/\sqrt{2}, \bar{b}_3^\alpha], \qquad (88c)$$

$$\bar{\mathbf{b}}^\alpha = (\mathbf{x}^\alpha + i\mathbf{p}^\alpha)/\sqrt{2}. \qquad (88d)$$

Since the b's are just the previous a's, they satisfy the commutation relations (31). Since the present a_i^α are related to the b_i^α by a unitary transformation, they also satisfy Eq. (31). The a_i^α, $\bar{a}_i^\alpha$ of Eqs. (88a, c) can be expressed directly in terms of the x_i^α, p_i^α, and it is *this* explicit definition which we take for the a_i^α, $\bar{a}_i^\alpha$ of this section. Correspondingly, the E_{ij} and $E^{\alpha\beta}$ can be written out in terms of the x_i^α, p_i^α. The preceding results of this section, of course, remain valid.

It is now a straightforward task to verify the following equations:

$$L_1 = -(E_{13} + E_{31})/\sqrt{2} - i(E_{23} - E_{32})/\sqrt{2}, \qquad (89a)$$

$$L_2 = i(E_{13} - E_{31})/\sqrt{2} + (E_{23} + E_{32})/\sqrt{2}, \qquad (89b)$$

$$L_3 = E_{11} - E_{22}. \qquad (89c)$$

Thus, with the operator realizations (88a, c) of $\mathbf{a}^\alpha$, $\bar{\mathbf{a}}^\alpha$ in terms of $\mathbf{x}^\alpha$ and $\mathbf{p}^\alpha$, the right-hand sides of Eqs. (89) are just the angular momentum operators (87) in disguise. It is now apparent why the definitions (88) were made: L_3 of Eq. (89c) is *already diagonal* on the Gel'fand basis (83a).

The angular momentum components obey the commutation relations

$$[L_i, L_j] = iL_k, \qquad (i, j, k \text{ cyclic}), \qquad (90)$$

and are the generators of the single-valued representations of the rotation group R_3. We also introduce the ladder operators

$$L_+ \equiv L_1 + iL_2 = \sqrt{2}(-E_{13} + iE_{32}), \qquad (91a)$$

$$L_- \equiv L_1 - iL_2 = \sqrt{2}(-E_{31} - iE_{23}). \qquad (91b)$$

Then

$$[L_+, L_-] = 2L_3, \quad [L_3, L_\pm] = \pm L_\pm. \qquad (92)$$

The commutation relations (92) are the same as those for the generators E_{12}, E_{21}, $(E_{11} - E_{22})/2$ of SU_2. As noted by Dragt,[11] the operators $L_\pm$, L_3 form a subalgebra of the algebra of U_3 which is algebraically distinct from that of E_{12}, E_{21}, $(E_{11} - E_{22})/2$. This follows from the fact that $E_{11} + E_{22} + E_{33}$ is the only other independent element of the algebra of U_3 which commutes with $L_\pm$ and L_3, while both $E_{11} + E_{22} + E_{33}$ and $E_{11} + E_{22}$ commute with E_{12}, E_{21}, $(E_{11} - E_{22})/2$.

L_3 is diagonal on the Gel'fand basis (83a) and has eigenvalues

$$L_3 \to 2k_{11} - k_{12} - k_{22}. \qquad (93)$$

However, the square of the total angular momentum

$$L^2 \equiv L_3(L_3 + 1) + L_-L_+ = L_3(L_3 - 1) + L_+L_- \qquad (94)$$

is not diagonal. The angular momentum operators (89) do, of course, commute with all the operators $E^{\alpha\beta}$ of U_N. The problem of finding the simultaneous eigenvectors of L^2 and L_3 is thus seen to be the following one: We must find a new basis of the space ${}^3V_{[\lambda]}^{(l)}$, the basis vectors being also eigenvectors of L^2. Since the matrix elements of all E_{ij} are independent of which (l) set we choose, the unitary transformation from the Gel'fand basis of ${}^3V_{[\lambda]}^{(l)}$ to the new basis is also independent of (l). Accordingly, we set $(l) = (\bar{l})$ in Eq. (83a) and designate the basis vectors simply as

$$|(k)\rangle = \left| \begin{matrix} k_{13} & k_{23} & k_{33} \\ k_{12} & k_{22} & \\ k_{11} & & \end{matrix} \right\rangle = \mathcal{O}_{(k)}(E_{ij})\ |(\bar{k})\rangle, \qquad (95)$$

[11] A. J. Dragt, J. Math. Phys. 6, 533 (1965).

where $|(\bar{k})\rangle$ now denotes the state of highest weight (83e). These are, of course, just the Gel'fand basis vectors for U_3. The unitary transformation of the Gel'fand basis vectors (95) [for given partition (83d)] which diagonalizes L^2 is also the unitary transformation of the Gel'fand basis vectors (83a) which diagonalizes L^2. Thus, the basic problem is the same for all $N \geq 3$, namely, to reduce the space ${}^3V_{[\lambda]}$ into a direct sum of subspaces, the basis vectors of each of the subspaces presenting a basis for an irreducible representation of the operators L_i of R_3.

As already noted, L_3 is diagonal on the space ${}^3V_{[\lambda]}$ with basis (95). Indeed, it is only a question of studying the eigenvalue spectrum (93) of L_3 to determine which values of the angular momentum quantum number L will appear in the reduction of ${}^3V_{[\lambda]}$. The eigenvalues of L^2 must be of the form $L(L+1)$, where L is integral; for each value of L which occurs, one must also find $2L+1$ eigenvalues for L_3, namely,

$$L_3 \to M(M = L, L-1, \cdots, -L). \tag{96}$$

Thus, for given $[\lambda]$, we enumerate all the eigenvalues of L_3 from Eq. (93). From this enumeration, it is readily seen which values of L occur. They are tabulated in Tables I & II.

TABLE I. The allowed values of L
$[\mu \equiv k_{23} - k_{33}\ (\text{odd}),\ \nu = k_{13} - k_{23}]$.

1	3	5	$\cdots$	$\mu-2$	μ
2	4	6	$\cdots$	$\mu-1$	$\mu+1$
3	5	7	$\cdots$	μ	$\mu+2$
.					
.					
.					
ν	$\nu+2$	$\nu+4$	$\cdots$	$\nu+\mu-3$	$\nu+\mu-1$
$\nu+1$	$\nu+3$	$\nu+5$	$\cdots$	$\nu+\mu-2$	$\nu+\mu$.

TABLE II. The allowed values of L
$[\mu \equiv k_{23} - k_{33}\ (\text{even})]$.

ν(even)	0	2	4	$\cdots$	$\nu-2$	ν
ν(odd)	1	3	5	$\cdots$	$\nu-2$	ν
	2	4	6	$\cdots$	$\mu-2$	μ
	3	5	7	$\cdots$	$\mu-1$	$\mu+1$
	.					
	.					
	.					
	$\nu+1$	$\nu+3$	$\nu+5$	$\cdots$	$\nu+\mu-3$	$\nu+\mu-1$
	$\nu+2$	$\nu+4$	$\nu+6$	$\cdots$	$\nu+\mu-2$	$\nu+\mu$.

In Table II, the first *or* second row is included depending on whether $\nu = k_{13} - k_{23}$ is even or odd. If $\mu = 0$, only the top two rows remain in Table II.

Tables I & II solve the *eigenvalue* problem for L^2, and show which irreducible representations of R_3 will appear in this reduction of U_3. For $\mu \geq 2$, $\nu \geq 2$, we see from Tables I and II that the same irreducible representation of R_3 will appear a number of times—a given value of L is repeated, and there is still a degeneracy. But this was to be anticipated since the basis vectors (95) of ${}^3V_{[\lambda]}$ are enumerated by the three numbers k_{11}, k_{12}, k_{22} associated with the eigenvalues of the three operators $K_1^{(1)}, K_1^{(2)}, K_2^{(2)}$, and we do not expect to be able to enumerate a new basis of ${}^3V_{[\lambda]}$ by the two numbers L, M associated with the eigenvalues of L^2, L_3. We need a third operator and a third quantum number. This missing operator Ω should be built from the E_{ij} (so as to commute with the $E^{\alpha\beta}$ of U_N) and be the sixth independent member of the set

$$K_1^{(3)}, K_2^{(3)}, K_3^{(3)}, L^2, L_3, \Omega \tag{97}$$

so that the new basis vectors of ${}^3V_{[\lambda]}$ are uniquely labeled by L, M, ω, where ω denotes an eigenvalue of Ω.

Bargmann and Moshinsky[4] have given the explicit form of Ω and studied various of its properties. In order to make quite clear the relation of their results to the ones given here, we note the following relations between their notation and ours, the new symbols at the left referring to their notation:

$$\begin{aligned}
&\eta_{i\alpha} = b_i^\alpha,\ \xi_{i\alpha} = \bar{b}_i^\alpha,\ \mathfrak{n}_\alpha = \mathfrak{b}^\alpha,\ \xi_\alpha = \bar{\mathfrak{b}}^\alpha,\\
&\mathfrak{C}_{ij}^{(N)} = \sum_{\alpha=1}^{N} \eta_{i\alpha}\xi_{j\alpha} = \sum_{\alpha=1}^{N} b_i^\alpha \bar{b}_j^\alpha,\\
&\mathfrak{C}_{11}^{(N)} = [E_{11} + E_{22} + i(E_{12} - E_{21})]/2,\\
&\mathfrak{C}_{22}^{(N)} = [E_{11} + E_{22} - i(E_{12} - E_{21})]/2,\\
&\mathfrak{C}_{33}^{(N)} = E_{33},\\
&\mathfrak{C}_{12}^{(N)} = [i(E_{11} - E_{22}) + E_{12} + E_{21}]/2,\\
&\mathfrak{C}_{21}^{(N)} = [-i(E_{11} - E_{22}) + E_{12} + E_{21}]/2,\\
&\mathfrak{C}_{13}^{(N)} = (E_{13} - iE_{23})/\sqrt{2},\\
&\mathfrak{C}_{31}^{(N)} = (E_{31} + iE_{32})/\sqrt{2},\\
&\mathfrak{C}_{23}^{(N)} = (-iE_{13} + E_{23})/\sqrt{2},\\
&\mathfrak{C}_{32}^{(N)} = (iE_{31} + E_{32})/\sqrt{2},\\
&\mathfrak{C}_{\alpha\beta} = \mathfrak{n}_\alpha \cdot \xi_\beta = \sum_{i=1}^{3} b_i^\alpha \bar{b}_i^\beta = \sum_{i=1}^{3} a_i^\alpha \bar{a}_i^\beta = E^{\alpha\beta},\\
&Q_{ij} = (\mathfrak{C}_{ij}^{(N)} + \mathfrak{C}_{ji}^{(N)})/2 - \delta_{ij}K_1^{(3)}/3,\\
&\lambda_i = L_i = -i(\mathfrak{C}_{jk}^{(N)} - \mathfrak{C}_{kj}^{(N)}) \qquad (i, j, k \text{ cyclic}).
\end{aligned} \tag{98}$$

The symmetric Q_{ij} defined in the next to the last equation above are the significant quantities required for the definition of Ω. With respect to the angular momentum components L_i, we have the

commutation relations for a second-rank tensor:

$$[L_i, Q_{jk}] = i\epsilon_{ijl}Q_{lk} + i\epsilon_{ikl}Q_{jl}. \tag{99}$$

Q is also symmetric and traceless. The operator Ω is

$$\Omega = \sum_{i,j} Q_{ij}L_iL_j, \tag{100}$$

and can be shown by use of Eq. (99) to commute with all operators L_i of R_3. Let us also note that Q_{ij} takes the following form when expressed in terms of $\mathbf{x}^\alpha$, $\mathbf{p}^\alpha$:

$$Q_{ij} = \frac{1}{2}\sum_{\alpha=1}^{N}(x_i^\alpha x_j^\alpha + p_i^\alpha p_j^\alpha) - \tfrac{1}{3}\delta_{ij}H', \tag{101a}$$

where

$$H' = \frac{1}{2}\sum_{\alpha=1}^{N}(\mathbf{p}^\alpha\cdot\mathbf{p}^\alpha + \mathbf{x}^\alpha\cdot\mathbf{x}^\alpha) = K_1^{(3)} + \tfrac{3}{2}N \tag{101b}$$

is the true harmonic oscillator Hamiltonian.

The $3N$ integrals of the motion obtained by Bargmann and Moshinsky are

$$H^{(\beta)} = L_1^{(\beta)} \quad \text{or} \quad H_\beta = E^{\beta\beta} \qquad (\beta = 1, 2, \cdots, N), \tag{102a}$$

$$\Gamma^{(\beta)} = L_2^{(\beta)} - \tfrac{1}{3}(L_1^{(\beta)})^2 - (\beta - 3)L_1^{(\beta)} \qquad (\beta = 2, 3, \cdots, N), \tag{102b}$$

$$\Delta^{(\beta)} = P^{(\beta)}(L_1^{(\beta)}, L_2^{(\beta)}, L_3^{(\beta)}) \qquad (\beta = 3, 4, \cdots, N), \tag{102c}$$

$$\lambda^2 = L^2, \lambda_3 = L_3, \Omega, \tag{102d}$$

where H, Γ, Δ, and λ refer to their notation. We have not determined the explicit form of the polynomial function $P^{(\beta)}$, but since $\Delta^{(\beta)}$ is an invariant of U_β, it must be expressible in terms of the $L_k^{(\beta)}(k = 1, 2, 3)$. From Eq. (60a), we have the following relations among the invariants of U_3 and U_N:

$$\begin{aligned} K_1^{(3)} &= L_1^{(N)}, \\ K_2^{(3)} &= (3 - N)L_1^{(N)} + L_2^{(N)}, \\ K_3^{(3)} &= (3 - N)^2L_1^{(N)} + 2(3 - N)L_2^{(N)} + L_3^{(N)}. \end{aligned} \tag{103}$$

The Gel'fand basis vectors (83a) are the simultaneous eigenvectors of the $3N - 3$ operators (102a–c) together with $K_1^{(2)}$, $K_2^{(2)}$, L_3. The Bargmann and Moshinsky basis vectors are the simultaneous eigenvectors of all $3N$ operators (102). An appropriate notation for these basis vectors, which retains as much of the Gel'fand symbol (83a) as possible, is obtained by replacing the bottom two rows of (83a) by

$$\begin{bmatrix} l^{12} & & l^{22} \\ & l^{11} & \\ L & M & \omega \end{bmatrix}. \tag{104}$$

On this basis all the results of Eqs. (85) and (86) remain valid except for those equations which contain k_{11}, k_{12}, k_{22}. In addition, we gain the three eigenvalues

$$L^2 \to L(L + 1), L_3 \to M, \Omega \to \omega. \tag{105}$$

In general, there are several eigenvectors which have the same $L(L + 1)$ eigenvalue of operator L^2. Bargmann and Moshinsky[4] have determined a set of linearly independent eigenvectors which belongs to a given L, and also demonstrated that Ω is nondegenerate on this set. They obtained the eigenvectors by solving directly a number of differential equations. An alternative formulation of this problem can also be given: We select a *particular* L from Table I on II in accord with the given partition $[\lambda]$ of Eq. (83d) and form the linear combination of Gel'fand basis vectors (95) as follows:

$$|L\omega\rangle \equiv \sum_{\rho,\sigma} C(\rho\sigma\omega)\left|\begin{matrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \rho & \rho - L - 2\sigma & \\ & \rho - \sigma & \end{matrix}\right\rangle. \tag{106a}$$

The sum is over all ρ, σ consistent with

$$\begin{aligned} \lambda_1 \geq \rho \geq \lambda_2, \\ \lambda_2 + L \geq \rho - 2\sigma \geq \lambda_3 + L. \end{aligned} \tag{106b}$$

The vector $|L\omega\rangle$ already satisfies

$$L_3\,|L\omega\rangle = L\,|L\omega\rangle. \tag{107a}$$

We also impose the conditions

$$L_+\,|L\omega\rangle = 0, \tag{107b}$$

$$\Omega\,|L\omega\rangle = \omega\,|L\omega\rangle. \tag{107c}$$

The explicit linear transformations of the Gel'fand basis vectors in Eq. (106a) induced by L_+ and Ω can be obtained explicitly from Eqs. (86). These results and Eqs. (107b, c) uniquely determine the allowed values of ω and the coefficients $C(\rho\sigma\omega)$, except for normalization. We have not carried out these calculations, but are presently investigating the structure of the problem.

Once the normalized vectors $|L\omega\rangle$ have been determined, the normalized Bargmann–Moshinsky basis vectors are given by

$$\left|\begin{array}{c} \cdot\ \cdot\ \cdot\ \cdot\ \cdot \\ l^{12}\ \ l^{22} \\ l^{11} \\ L\ M\ \omega \end{array}\right\rangle = \mathcal{O}_{(l)}(E^{\alpha\beta})\ |[\lambda]; LM\omega\rangle, \qquad (108a)$$

where

$$|[\lambda]; LM\omega\rangle = \left[\frac{(L+M)!}{(2L)!(L-M)!}\right]^{\frac{1}{2}} L_-^{L-M}\ |L\omega\rangle. \qquad (108b)$$

The dots in the symbol on the left-hand side of Eq. (108a) indicate that the top $N-2$ rows from the Gel'fand symbol (83a) are to be provided.

The Gel'fand basis vectors for two particles in 3-space are given by

$$\left|\begin{array}{ccc} (k_{13}, l^{12}) & (k_{23}, l^{22}) & (0,0) \\ (k_{12}, l^{12}) & (k_{22}, l^{22}) & \\ (k_{11}, l^{11}) & & \end{array}\right\rangle = |(k, l)\rangle$$
$$= \mathcal{O}_{(k)}(E_{ij})\mathcal{O}_{(l)}(E^{\alpha\beta})\ |(\bar{k}, \bar{l})\rangle, \qquad (109a)$$

where

$$(k) = \begin{bmatrix} k_{13} & k_{23} & 0 \\ k_{12} & k_{22} & \\ k_{11} & & \end{bmatrix}, \qquad (l) = \begin{bmatrix} l^{12} & l^{22} \\ l^{11} & \end{bmatrix}, \qquad (109b)$$

$$[k_{13}k_{23}0] = [l^{12}l^{22}0] = [\lambda_1\lambda_20]. \qquad (109c)$$

The independent integrals of the motion are

$$K_1^{(1)}, K_1^{(2)}, K_2^{(2)}, K_1^{(3)}, K_2^{(3)}, L_1^{(1)}, \qquad (110a)$$

since we obtain from Eq. (60b) the relations

$$L_1^{(2)} = K_1^{(3)}, L_2^{(2)} = -K_1^{(3)} + K_2^{(3)}. \qquad (110b)$$

Thus, the problem of going to the Bargmann–Moshinsky basis is the same as before.

Our reason for noting these results for two particles is as follows: We can consider the $\mathbf{x}^\alpha$ and $\mathbf{p}^\alpha (\alpha = 1, 2)$ of Eq. (88b) to be the coordinates and momenta of a three-particle system relative to the center of mass, and Smith[12,13] and Dragt[11] have done a great deal of significant work on the classification of the states of such a system. Their classification treats all three particles on equal footing, and Dragt[11] notes that the classification of states is in one-to-one correspondence with the set of irreducible representations of U_3. The point we would like to make is that in the Smith–Dragt scheme U_3 enters the problem in an algebraically distinct manner from the way it enters the scheme (109), hence, also the Bargmann–Moshinsky scheme.

[12] F. T. Smith, Phys. Rev. **120**, 1058 (1960).
[13] F. T. Smith, J. Math. Phys. **3**, 735 (1962).

In order to establish the above statement, we consider the infinitesimal operators employed by Smith[12,13] and Dragt.[11] They first introduce the infinitesimal operators of the rotation group R_6:

$$\Lambda_{jk}^{\alpha\beta} \equiv x_j^\alpha p_k^\beta - x_k^\beta p_j^\alpha, \qquad (111a)$$

where $i, j = 1, 2, 3$; $\alpha, \beta = 1, 2$. The components of the total orbital angular momentum of the particles (relative to the center of mass) are then given by

$$J_i \equiv L_i = J_{jk} = \Lambda_{jk}^{11} + \Lambda_{jk}^{22}, (i, j, k \text{ cyclic}). \qquad (111b)$$

Next, a second-rank symmetric tensor is introduced:

$$K_{jk} = \Lambda_{jk}^{12} - \Lambda_{jk}^{21}. \qquad (111c)$$

Dragt then shows that the nine operators defined as follows obey the commutation relations (1) for the Weyl generators of U_3:

$$C_{jk} \equiv \tfrac{1}{2}(K_{jk} + iJ_{jk}). \qquad (112a)$$

In terms of the C_{jk}, we have

$$K_{jk} = C_{jk} + C_{kj}, \qquad (112b)$$

$$J_{jk} = -i(C_{jk} - C_{kj}). \qquad (112c)$$

The C_{jk} defined by Eq. (112a) can also be written in the form

$$C_{jk} = C_{jk}^{22} - C_{kj}^{11}, \qquad (113a)$$

where

$$C_{jk}^{\alpha\beta} = c_j^\alpha \bar{c}_k^\beta. \qquad (113b)$$

The c_i^α operators satisfy the commutation relations

$$[\bar{c}_i^\alpha, c_j^\beta] = \delta^{\alpha\beta}\delta_{ij}. \qquad (113c)$$

Furthermore, $\mathbf{c}^1$ and $\mathbf{c}^2$ are related to our $\mathbf{a}^1$, $\mathbf{a}^2$ given explicitly by Eqs. (88) by the following unitary transformation:

$$\begin{bmatrix} \bar{\mathbf{a}} \\ \bar{\mathbf{b}} \end{bmatrix} \equiv \begin{bmatrix} \mathbf{c}^1 \\ \mathbf{c}^2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} U & -iU \\ -U & -iU \end{bmatrix} \begin{bmatrix} \mathbf{a}^1 \\ \mathbf{a}^2 \end{bmatrix}, \qquad (114a)$$

where the first column to the left refers to Dragt's a's and b's, and U is the unitary matrix

$$U = \begin{bmatrix} i/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & i/\sqrt{2} & 0 \\ 0 & 0 & i \end{bmatrix}. \qquad (114b)$$

The C_{jk} of Eq. (112a) or (113) are the infinitesimal operators which generate the U_3 of the Smith–Dragt scheme.

We could express the C_{jk} directly in terms of the $E_{ij}^{\alpha\beta} = a_i^\alpha \bar{a}_j^\beta$ by use of Eqs. (113) and (114), but this is not necessary to prove our point. Let us recall

that the $E_{ij}^{\alpha\beta}(i, j = 1, 2, 3; \alpha, \beta = 1, 2)$ are a special operator realization of the generators of U_6. We found operator realizations of the algebra of U_3 and U_2, respectively, by considering the subalgebras of the algebra of U_6 defined by the operator sets

$$E_{ik} = \sum_{\alpha=1}^{2} E_{ik}^{\alpha\alpha}, \qquad E^{\alpha\beta} \equiv \sum_{i=1}^{3} E_{ii}^{\alpha\beta}. \tag{115a}$$

The C_{jk} are similarly just linear combinations of the $E_{jk}^{\alpha\beta}$ of U_6, and also define a subalgebra of the algebra of U_6, which is again recognized as an operator realization of the algebra of U_3. However, in this second instance, it is readily proved that the two operators[11]

$$\sum_{i=1}^{3} C_{ii}^{\alpha\alpha} \qquad (\alpha = 1, 2) \tag{115b}$$

are the *only other* elements of the algebra of U_6 which commute with all C_{jk}. Since the *four* $E^{\alpha\beta}(\alpha, \beta = 1, 2)$ commute with all of the E_{jk}, we must conclude that the U_3 subgroups of U_6 which are generated by E_{jk} and C_{jk}, respectively, are imbedded in U_6 in algebraically distinct ways.

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Note added in proof. The author wishes to thank Professor Moshinsky for bringing his attention to several additional publications[14-16] which relate directly to the present work. References (14) and (15) contain the derivation of the bases for the irreducible representations of the unitary groups, and are equivalent to the results obtained by Baird and Biedenharn.[1] Operators equivalent to the E_{ij} and $E^{\alpha\beta}$ of Eqs. (42a, b) were introduced in Ref. (16), and Theorem 3.14 of Ref. (15) is equivalent to the italicized statement following Eq. (71). Nagel and Moshinsky[17] have also now given the general form of the lowering operators of Eq. (65a). Finally, Brody, Moshinsky, and Renero[18] have utilized double-indexed Gel'fand basis vectors in their work on the Wigner coefficients of SU_n.

[14] M. Moshinsky, Rev. Mod. Phys. **34**, 813 (1962).
[15] M. Moshinsky, J. Math. Phys. **4**, 1128 (1963).
[16] M. Moshinsky, Nucl. Phys. **31**, 384 (1962).
[17] J. G. Nagel and M. Moshinsky, J. Math. Phys. **6**, 682 (1965).
[18] T. A. Brody, M. Moshinsky, and I. Renero, J. Math. Phys. **6**, 1540 (1965).

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New Variational Scheme for Finding the Excited States of One-Dimensional Systems

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A new relaxation–variation scheme for solving one-dimensional Schrödinger equations is described. The method approximates the nth eigenvalue and eigenfunction directly, without requiring approximations to the lower eigenfunctions. It is applicable to any one-dimensional Sturm–Liouville system.

IN this note we propose an apparently new scheme for finding the excited states of one-dimensional systems governed by the Schrödinger or other Sturm–Liouville equations. This method approximates the nth eigenvalue and eigenfunction directly without requiring the lower eigenfunctions, thus avoiding the main fault of the Ritz procedure.

For convenience, our discussion will be couched in terms of the Schrödinger equation in the interval $(0, L)$ with the boundary condition that the real eigenfunction $f(x)$ be zero at the end points. Then the following properties of the nth eigenfunction $f_n(x)$ are well known:

(a) $Hf_n(x) = E_n f_n(x)$ at each $x \in (0, L)$;

(b) $\delta \int_0^L f_n(x) H f_n(x)\, dx = 0$, for variations consistent with the boundary conditions;

(c) $\int_0^L f_n(x) f_m(x)\, dx = 0$ if $n > m$;

that the $E_{ij}^{\alpha\beta}(i, j = 1, 2, 3; \alpha, \beta = 1, 2)$ are a special operator realization of the generators of U_6. We found operator realizations of the algebra of U_3 and U_2, respectively, by considering the subalgebras of the algebra of U_6 defined by the operator sets

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For convenience, our discussion will be couched in terms of the Schrödinger equation in the interval $(0, L)$ with the boundary condition that the real eigenfunction $f(x)$ be zero at the end points. Then the following properties of the nth eigenfunction $f_n(x)$ are well known:

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(b) $\delta \int_0^L f_n(x) H f_n(x)\, dx = 0$, for variations consistent with the boundary conditions;

(c) $\int_0^L f_n(x) f_m(x)\, dx = 0$ if $n > m$;

(d) $f_n(x)$ has $n - 1$ nodes in $(0, L)$. Let us call these points $x_1, x_2, \cdots, x_{n-1}$ and set $x_0 = 0$ and $x_n = L$;

(e) On the subinterval $I_i = (x_{i-1}, x_i)$, the function $f_n(x)$ coincides (but for normalization) with the ground-state eigenfunction $\phi_i^0(x)$ of the same Schrödinger equation with boundary conditions that ϕ_i be zero at the end points of the *subinterval* I_i. Also, the ground-state eigenvalue E_i^0 going with ϕ_i^0 is in fact the same number E_n for all the subintervals I_i.

The usual (Ritz) procedure amounts to the theorem "(b) and (c) imply (a)", whereas our proposal is an application of the theorem "(d) and (e) imply (a)". The proof of this theorem is trivial. We now suggest a sequence of steps leading to a function which approximately satisfies (d) and (e):

1. Given a set of approximate node points $\{x_i\}$, we find the ground-state eigenvalue e_i on each subinterval I_i. This may be done variationally, normalizing the trial function ϕ_i on the subinterval. If, for example, the function ϕ_i is Fourier sine-analyzed on each subinterval, the minimization problem involves only computing integrals and finding the lowest eigenvalue of a quadratic form.

2. The approximate eigenvalues $\{e_i\}$ found in Step 1 will be unequal; the node points $\{x_i\}$ ought to be moved so as to equalize the e_i's. We have considered various schemes for moving the node points; in the examples we tried, the following method seemed to work best:

(i) Compute the differences $d_i = |e_{i+1} - e_i|$.

(ii) Move the node point x_i corresponding to the maximal d_i in the direction required to diminish d_i. Move it by the amount given by Newton's rule, so

$$\delta x_i = -d_i/d_i',$$

where d_i' is the derivative of d_i with respect to x_i. To estimate d_i', we have used only the kinetic energy part of e_i; for slowly varying potentials it leads to the dominant terms in d_i'.

This method only moves one node point per stage. It is possible to set up a similar Newton's-rule method to move the whole vector $(x_1, x_2, \cdots, x_{n-1})$ to find the zero of, say, $D = d_1^2 + d_2^2 + \cdots + d_{n-1}^2$, but this method didn't always work properly when our trial node points were far from the correct values.

By one of these methods, we derive a new set of node points $\{y_i\}$ and can continue recursively. At each step, the method provides both an upper and a lower bound for the eigenvalue, provided that the subinterval ground-state eigenvalues are found accurately enough. When the normalized eigenfunctions ϕ_i have been found for each subinterval I_i, they may be linked by demanding continuity of the derivative through each node.

We shall sketch a proof that the approximate subinterval eigenvalues $\{e_i\}$, for any choice of node points $\{x_i\}$, cannot all be greater (or less) than the exact nth eigenvalue E, so that the maximum of $\{e_i\}$ is an upper bound for E and the minimum, a lower bound. By e_i we mean the *exact* lowest eigenvalue on (x_{i-1}, x_i), which will never be known, so the method will in practice only provide *estimates* of bounds and not exact bounds.

The argument is based on the fact that (lowest) eigenvalues are ordered by inclusion of intervals; if interval I' is contained in I'', than the lowest eigenvalue $e(I')$ is certainly greater than $e(I'')$. This assumes finite potentials.

Let us try to construct a case for which each $e_i > E$. In order to have $e_1 > E$, we must choose $x_1 < x_1^0$, where we write x_i for the approximate node points and x_i^0 for the exact node points. Now in order to have $e_2 > E$ also, it is also necessary to have $x_2 < x_2^0$; for otherwise (x_1^0, x_2^0) would be contained in (x_1, x_2); and so on—to obtain $e_3 > E$, we must have $x_3 < x_3^0$. This can be done for all subintervals but the last. But $x_{n-1} < x_{n-1}^0$ implies that $e_n < E$. So it is clear that not all of the e's can be greater than E, and a similar argument shows that they cannot all be less than E.

This method may be easily extended to arbitrary Sturm–Liouville problems on any interval. We have applied it to a simple quantum mechanics problem—a particle in a rigid box with a linear perturbation—doing the computations on a desk calculator. We used only one Fourier coefficient on each subinterval; from a very bad start (with all five internal nodes in the left $\frac{1}{4}$ of the box) we had, in about ten steps, bounded the sought eigenvalue between the two neighboring eigenvalues, and had a weighted subinterval average eigenvalue within 1% of the correct eigenvalue.

It has been proposed that this method be used to solved the Hartree equations for the excited states of atoms.

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Note on the Dynamics of Gravitational Sources*

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This paper is concerned with multipole structure for the sources of the gravitational field in the full (axially symmetric) nonlinear gravitational theory. Definitions proposed recently by Janis and Newman for the mass of the source, its linear momentum, dipole moment, and its spin or angular momentum are examined. These definitions are contrasted with those given by other authors. The advantages of the new definitions are discussed and the manner in which they enter into the dynamics of the system is studied. An appendix considers some transformation properties of these multiple moments.

I. INTRODUCTION

IN some of the recent literature[1-4] the sources of a gravitational field have been analyzed by examining its effects at infinity. In the linearized version of the Einstein gravitational theory, solutions of the field equations may be completely characterized by the multipole moments of a bounded source. In the nonlinear theory, it has so far been impossible to determine solutions exactly in terms of source distributions. However, asymptotically exact solutions of the Einstein equations are available,[1,3,5] and these have been used as a basis for defining moments of the source.[1,4,6] Some latitude exists in the possible (reasonable) definitions of these moments, as can be seen by the difference in the "mass" as proposed by Bondi, van der Burg, and Metzner[1] and that proposed by Newman and Unti.[3] Each definition has certain advantages, as as is discussed in Sec. II.

This paper is primarily concerned with the definitions of the multipole moments of the sources and clarification of these definitions. The manner in which these definitions enter into the dynamics of the system is studied. It is evident that the formulations of many dynamic problems depend upon these definitions, as for example scattering problems, absorption of radiation, radiation recoil, etc.

In Sec. II, after a summary of some necessary background material, the definitions of complex quadrupole, dipole, and monopole introduced in Janis and Newman[6] are discussed. It is shown how they are related to the definitions of these multipoles proposed by Bondi *et al.*[1] and Møller.[4] The arguments in favor of the two alternative sets of definitions are presented.

Section III is concerned with the dynamical aspects of the sources. The Bianchi identities, which govern the dependence of the multipole moments on the "time" coordinate, are the basis for this discussion. Some special cases, which are governed by the specialization of the "news" function are examined in detail. We analyze in these cases the time dependence of the monopole moment, mass dipole moment, spin dipole moment (angular momentum), and quadrupole moment.

In the Appendix, some transformation properties of the news, mutipole aspects, and moments are discussed. A representative case is calculated as an example, and it is shown that the transformation properties of the multipole moments are not as simple as might be desired. The transformed expressions, while easy to determine, are unwieldy and do not appear to lend themselves to simple interpretation.

Although all the calculations of the paper can easily be done with greater generality, the presentation is for simplicity confined to the axially symmetric case.

II. MULTIPOLE MOMENTS

The calculations in this paper are based on the results of three previous papers.[7] In NP, spinor and tetrad techniques were used to obtain a set of equations equivalent to the empty-space Einstein field equations. One subset of these, derived from the Bianchi identities, is a set of first-order differential equations for the (complex) physical components

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[7] References 3, 6, and 8, will be referred to as NU, JN, and NP, respectively.
[8] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

of the Weyl tensor, which are defined as follows[9]:

$$\psi_0 = -C_{\alpha\beta\gamma\delta}l^\alpha m^\beta l^\gamma m^\delta, \tag{1a}$$

$$\psi_1 = -C_{\alpha\beta\gamma\delta}l^\alpha n^\beta l^\gamma m^\delta, \tag{1b}$$

$$\psi_2 = -\tfrac{1}{2}C_{\alpha\beta\gamma\delta}(l^\alpha n^\beta l^\gamma n^\delta - l^\alpha n^\beta m^\gamma \bar{m}^\delta), \tag{1c}$$

$$\psi_3 = -C_{\alpha\beta\gamma\delta}n^\alpha l^\beta n^\gamma \bar{m}^\delta, \tag{1d}$$

$$\psi_4 = -C_{\alpha\beta\gamma\delta}n^\alpha \bar{m}^\beta n^\gamma \bar{m}^\delta. \tag{1e}$$

$C_{\alpha\beta\gamma\delta}$ is the Weyl tensor (in empty space, the Riemann tensor), while l^μ, n^μ, m^μ, and $\bar{m}^\mu$ are a complex null tetrad which can be defined in terms of a real orthonormal tetrad. Let a^μ be a timelike unit vector, and b^μ, c^μ, d^μ be three spacelike unit vectors, orthogonal to a^μ and to each other. Then

$$l^\mu = (a^\mu + b^\mu)/\sqrt{2}, \qquad n^\mu = (a^\mu - b^\mu)/\sqrt{2},$$

$$m^\mu = (c^\mu - id^\mu)/\sqrt{2}.$$

A coordinate system is constructed by introducing a family of null hypersurfaces into the normal hyperbolic Riemannian 4-space, which are labeled by a parameter u = const. An affine parameter r can be associated with the null geodesics lying in the hypersurfaces, and each null geodesic of a particular null hypersurface may be labelled by two "angular" coordinates θ, ϕ. The coordinate system is then $x^0 = u$, $x^1 = r$, $x^2 = \theta$, $x^3 = \phi$.[10]

The asymptotic behavior of the Weyl tensor and metric tensor for a large class of asymptotically flat outgoing radiation solutions of the empty-space field equations is derived in NU. For bounded sources ψ_0 should be taken as $O(r^{-5})$. A special case of this (in which the field possesses outgoing quadrupole radiation as well as other properties) is

$$\psi_0 = \psi_0^0 r^{-5} + O(r^{-6}). \tag{2a}$$

In NU it is shown that

$$\psi_1 = \psi_1^0 r^{-4} + O(r^{-5}), \tag{2b}$$

$$\psi_2 = \psi_2^0 r^{-3} + O(r^{-4}), \tag{2c}$$

$$\psi_3 = \psi_3^0 r^{-2} + O(r^{-3}), \tag{2d}$$

$$\psi_4 = \psi_4^0 r^{-1} + O(r^{-2}), \tag{2e}$$

where the superscript zero denotes independence of r.

These results from NP and NU are used in JN to propose the following definition of multipole structure in the full (axially symmetric) nonlinear gravitational theory. When the initial data has the form of Eqs. (2), the source of the field is defined to have a quadrupole structure,[11] with the complex quadrupole moment $Q(u)$ given by

$$Q(u) = -\frac{1}{2}\int_0^\pi \psi_0^0 P_2^2(\cos\theta)\sin\theta\, d\theta, \tag{3}$$

the real part of Q being the mass quadrupole moment, the imaginary part being the spin quadrupole moment. The complex dipole moment is defined as

$$D(u) + iL(u) = -\frac{1}{2}\int_0^\pi \psi_1^0 P_1^1(\cos\theta)\sin\theta\, d\theta. \tag{4}$$

The mass dipole moment $D(u)$ is given by the real part of Eq. (4) while the spin or angular momentum $L(u)$ is given by the imaginary part. The monopole moment (mass) is defined as

$$m(u) = -\frac{1}{4}\int_0^\pi (\psi_2^0 + \bar{\psi}_2^0)P_0(\cos\theta)\sin\theta\, d\theta. \tag{5}$$

(There exists no spin monopole moment.[6]) The $P_n^m(\cos\theta)$ are associated Legendre polynomials. The real parts of these complex moments correspond to "electric" type poles, the imaginary parts to "magnetic"type poles.[12]

We now add to the list of proposed definitions the linear momentum of the system:

$$P(u) = -\frac{1}{4}\int_0^\pi (\psi_2^0 + \bar{\psi}_2^0)P_1(\cos\theta)\sin\theta\, d\theta. \tag{6}$$

The quantities ψ_0^0, ψ_1^0, and $(\psi_2^0 + \bar{\psi}_2^0)$ are named the quadrupole aspect, dipole aspect, and mass aspect, in the order given. Bondi *et al*[1] in their original work, which was then generalized by Sachs,[13] use slightly different definitions of the aspects. Their definitions are related to those of JN by the equations[14]

$$\begin{aligned} M &= -\tfrac{1}{2}[(\psi_2^0 + \bar{\psi}_2^0) + (\sigma^0\sigma_{,0}^{\ 0} + \bar{\sigma}^0\bar{\sigma}_{,0}^{\ 0})], \\ N &= -\tfrac{2}{3}i\psi_1, \\ C &= \tfrac{1}{12}[-2\psi_0^0 + \sigma^0(\sigma^0 + \bar{\sigma}^0)(\sigma^0 - \bar{\sigma}^0)]. \end{aligned} \tag{7}$$

[9] Range and summation convention: Greek lower case 0, 1, 2, 3; Latin lower case 2, 3; Latin upper case 0, 1, 2.

[10] For more detailed discussions of the coordinate system, see Refs. 1 and 3.

[11] It may be desirable to specify more terms of ψ_0, rather than a single term as in Eq. (2a). If the initial datum ψ_0 is given as $\psi_0 = \sum_{n=2}^{N} \psi_0^{n-2} r^{-(n+3)}$, then the source is defined to have the structure of a 2^n-pole, with the 2^n-pole moment proportional to $\int_0^\pi \psi_0^{n-2} P_n^2(\cos\theta)\sin\theta\, d\theta$, for $n \geq 2$.

[12] R. K. Sachs and P. G. Bergmann, Phys. Rev. **112**, 674 (1958).

[13] Reference 5. Note that Bondi *et al.* in Ref. 1 use real quantities. Sachs generalized to complex quantities to include magnetic-type poles as well as electric.

[14] Ordinary differentiation is denoted by a comma: $X_{,0} = \partial X/\partial u$; $X_{,1} = \partial X/\partial r$; $X_{,2} = \partial X/\partial\theta$.

The function $\sigma^0(u, \theta)$ is arbitrary; it describes the flow of information between source and field. $\partial\sigma^0/\partial u \equiv \sigma^0_{,0}$ is called the "news function" by Bondi.

The various multipole moments are defined by Bondi *et al.* as integrals over the aspects M, N, and C. The multipole moments Eqs. (3)–(5) are defined analogously in JN. In addition it is seen that the Goldberg[2] and the Møller[4] definition of the linear momentum of the system

$$P = \frac{1}{2}\int_0^\pi MP_1(\cos\theta)\sin\theta\, d\theta \tag{8}$$

differs from ours by bilinear factors in σ^0 and $\sigma^0_{,0}$.

If we consider a situation in which the news $\sigma^0_{,0}$ is initially zero at "time" $u = u_0$, then is permitted to vary in an arbitrary manner during $u_0 < u < u_1$, and finally returns to zero at $u = u_1$, we find that the mass, as defined by both Bondi and ourselves, diminishes. As shown in Ref. 1, Bondi's mass is given by

$$m_B(u) = \frac{1}{2}\int_0^\pi M(u, \theta)\sin\theta\, d\theta \tag{9}$$

and satisfies

$$\frac{\partial m_B}{\partial u} = -\frac{1}{2}\int_0^\pi |\sigma^0_{,0}|^2 \sin\theta\, d\theta. \tag{10}$$

Since $|\dot\sigma^0|^2$ is positive-definite, Bondi's mass decreases monotonically as long as there is news. There is also another attractive feature which implies that the m_B of Eq. (9) has the properties of "mass"; the time-development equation (10) can be derived from the Einstein psuedo tensor[2] or from the Møller complex.[4]

Alternatively, it is shown in NU that if the mass is defined by Eq. (5) the Bianchi identities lead to the equation

$$\frac{\partial m}{\partial u} = -\frac{1}{2}\int_0^\pi |\dot\sigma^0|^2 \sin\theta\, d\theta + \frac{1}{4}\int_0^\pi \frac{\partial^2}{\partial u^2}(\sigma^0\bar\sigma^0)\sin\theta\, d\theta, \tag{11}$$

which differs from Eq. (10), of course, by the difference in definitions of m and m_B. Eqs. (10) and (11) show us that[15]

$$m_B = m - \frac{1}{4}\int_0^\pi \frac{\partial}{\partial u}(\sigma^0\bar\sigma^0)\sin\theta\, d\theta.^5 \tag{12}$$

[15] It appears that possibly the mass m can be interpreted as arising from just the source or matter, and m_B from the source plus the radiation field. It has been suggested by Møller that m be called the "bare" mass and m_B the "dressed" mass.

Under conditions in which a dynamic period is sandwiched between two static periods, the masses Eqs. (10) and (11) experience exactly the same decrease. This follows at once by integrating Eq. (11) from u_0 to u_1, since $\partial(\sigma^0\bar\sigma^0)/\partial u$ vanishes at u_0 and u_1. Thus m possesses with m_B the most attractive feature of a mass, namely that it should diminish after a burst of radiation.

There is, however, a physical consideration which leads us to prefer the definitions given here over those of Bondi's: our multipole aspects are defined in terms of the Weyl tensor. The tetrad components of the Weyl tensor possess a physical as well as a geometric interpretation. In principle they can be measured by a study of the relative acceleration of two geodesics (i.e., by the methods of geodesic deviation).[16] Therefore our multipole aspects defined in terms of the asymptotic Weyl tensor have not only an invariant significance, but an observational significance. For this reason we will work with our definitions of the aspects and their associated moments in the remainder of the paper.[17]

For completeness, in Appendix A we show and discuss some transformation properties of σ^0, the aspects, and some of the multipole moments.

III. DYNAMICS OF THE SYSTEM

The equations which govern the "time" dependence of the multipole aspects, derived in NP from the Bianchi identities, are given below for the axially symmetric case[14]:

$$\psi^0_{2,0} = (1/\sqrt{2}\sin\theta)\,\partial(V\sin\theta)/\partial\theta - \sigma^0\bar\sigma^0_{,00}, \tag{13a}$$

$$\psi^0_{1,0} = (1/\sqrt{2})\,\partial\psi^0_2/\partial\theta + 2\sigma^0 V, \tag{13b}$$

$$\psi^0_{0,0} = \frac{1}{\sqrt{2}}\sin\theta\,\frac{\partial}{\partial\theta}\left(\frac{\psi^0_1}{\sin\theta}\right) + 3\sigma^0\psi^0_2, \tag{13c}$$

where

$$V \equiv -(1/\sqrt{2}\sin^2\theta)\,\frac{\partial(\bar\sigma^0_{,0}\sin^2\theta)}{\partial\theta}. \tag{14}$$

In Bondi *et al*[1] and in JN it is shown that, in order to avoid angular singularities, σ^0 should be given as a series in associated Legendre polynomials $P^2_m(\cos$

[16] F. A. E. Pirani and A. Schild, Bull. Acad. Pol. Sci. 9, 543 (1961).

[17] It has been suggested that the best definition of the mass would be one which led to its invariance under the Bondi–Metzner supertranslations. It appears to us that a mass defined in this fashion would have to be constant for all time, and hence would be uninteresting for the study of gravitational radiation.

θ), of the form

$$\sigma^0(u, \theta) = \sum_{m=2}^{M} B_m(u) P_m^2(\cos\theta). \tag{15}$$

Equations (13) show us that ψ_2^0 can then be expressed as a finite series in P_m, ψ_1^0 in P_m^1 and ψ_0^0 as a finite series in P_m^2.

The time derivatives of the mass $m(u)$, the linear momentum $P(u)$, the dipole moment $D(u)$, and the spin or angular momentum $L(u)$ will now be considered. Since the mass and dipole aspects may be expressed in Legendre series,

$$\begin{aligned}(\psi_2^0 + \bar{\psi}_2^0) &= -2m(u)P_0 - 6P(u)P_1 + \sum_{m>1} F_m(u)P_m, \\ \psi_1^0 &= -\tfrac{3}{2}[D(u) + iL(u)]P_1^1 + \sum_{m>1} G_m(u)P_m^1,\end{aligned} \tag{16}$$

we have, either by taking the time derivatives of the definitions (4) (5) and (6) or by integrating the above equations (16) and using the orthogonality relationship of Legendre polynomials,[18] the following dynamic equations;

$$\begin{aligned}\frac{\partial m(u)}{\partial u} &= -\frac{1}{4}\int_0^\pi (\psi_{2,0}^0 + \bar{\psi}_{2,0}^0)P_0 \sin\theta\, d\theta, \\ \frac{\partial P(u)}{\partial u} &= -\frac{1}{4}\int_0^\pi (\psi_{2,0}^0 + \bar{\psi}_{2,0}^0)P_1 \sin\theta\, d\theta, \\ \frac{\partial^2 D(u)}{\partial u} &= -\frac{1}{4}\int_0^\pi (\psi_{1,00}^0 + \bar{\psi}_{1,00}^0)P_1^1 \sin\theta\, d\theta, \\ \frac{\partial^2 L(u)}{\partial u^2} &= \frac{1}{4} i \int_0^\pi (\psi_{1,00}^0 - \bar{\psi}_{1,00}^0)P_1^1 \sin\theta\, d\theta.\end{aligned} \tag{17}$$

Upon differentiating Eq. (13b) with respect to u, Eqs. (13) may be used directly in Eqs. (17) to obtain the following:

$$\frac{\partial}{\partial u}\left[m(u) - \frac{1}{4}\int_0^\pi \frac{\partial}{\partial u}(\sigma^0\bar{\sigma}^0)\sin\theta\, d\theta\right] = -\frac{1}{2}\int_0^\pi |\sigma_{,0}^0|^2 \sin\theta\, d\theta, \tag{18}$$

which is the same as Eq. (11); i.e. is the conservation of energy equation. We also have

$$\frac{\partial}{\partial u}\left[P(u) - \frac{1}{4}\int_0^\pi \frac{\partial}{\partial u}(\sigma^0\bar{\sigma}^0)\cos\theta\sin\theta\, d\theta\right] = -\frac{1}{2}\int_0^\pi |\sigma_{,0}^0|^2 \cos\theta\sin\theta\, d\theta, \tag{19}$$

which is the conservation of linear momentum equation. The equation giving the second time derivative of the dipole moment is

$$\begin{aligned}\frac{\partial^2}{\partial u^2} D(u) = &-\frac{1}{2\sqrt{2}}\int_0^\pi [(\bar{\sigma}_{,00}^0 \sin\theta)(\sigma^0 \sin\theta)_{,2} \\ &+ (\bar{\sigma}_{,00}^0 \sin\theta)(\sigma^0 \sin\theta)_{,2}]\, d\theta \\ &+ \frac{1}{\sqrt{2}}\int_0^\pi |\sigma_{,0}^0|^2 \cos\theta \sin\theta\, d\theta,\end{aligned} \tag{20}$$

while the conservation of angular momentum equation can be integrated to give

$$L(u) = \frac{i}{2\sqrt{2}}\int_0^\pi \bar{\sigma}^0 \sin\theta(\sigma^0 \sin\theta)_{,2}\, d\theta + \text{const.} \tag{21}$$

If σ^0 is given in the form of Eq. (15), Eqs. (18)–(21) show that $m_{,0}$, $P_{,0}$, D, and L can be expressed directly in terms of the time dependent coefficients in the Legendre series for σ^0. Defining the constants

$$\kappa_m = (m+2)!/(m-2)!(2m+1),$$
$$\lambda_m = (m+3)\kappa_m/(2m+3),$$

we obtain by substituting Eq. (15) into Eqs. (18)–(21)

$$\frac{\partial}{\partial u}\left[m(u) - \frac{1}{2}\sum_2 \kappa_m \frac{\partial}{\partial u}(B_m\bar{B}_m)\right] = -\sum_2 \kappa_m |B_{m,0}|^2, \tag{22a}$$

$$\frac{\partial}{\partial u}\left[P(u) - \frac{1}{2}\sum_2 \lambda_m \frac{\partial}{\partial u}(\bar{B}_m B_{m+1} + B_m\bar{B}_{m+1})\right] = -\sum_2 \lambda_m(\bar{B}_{m,0}B_{m+1,0} + B_{m,0}\bar{B}_{m+1,0}), \tag{22b}$$

$$\begin{aligned}\frac{\partial^2}{\partial u^2} D(u) = \frac{1}{\sqrt{2}}\sum_2 \lambda_m[&2(B_{m+1,0}\bar{B}_m + B_{m,0}\bar{B}_{m+1,0}) \\ &+ (m+1)(B_{m,00}\bar{B}_{m+1} + \bar{B}_{m,00}B_{m+1} \\ &- B_m\bar{B}_{m+1,00} - \bar{B}_m B_{m+1,00})],\end{aligned} \tag{22c}$$

$$L(u) = \frac{1}{\sqrt{2}} i \sum_2 (m+1)\lambda_m \cdot(B_m\bar{B}_{m+1} - \bar{B}_m B_{m+1}) + \text{const.} \tag{22d}$$

Equation (22b) shows that crossterms between the coefficients of neighboring P_k, P_{k+1} in the expansion of σ^0, Eq. (15), are necessary for momentum recoil. If alternate terms of the series (15) are zero, Eq. (22b) becomes $P_{,0} = 0$; in other words the source does not suffer a recoil. Equations (22c) and (22d) also show dependence upon crossterms of σ^0 for the dipole moment and spin.

As an interesting special case of the above formulation, we let

$$\sigma^0(u, \theta) = B_2(u)P_2^2 + B_3(u)P_3^2. \tag{23}$$

[18] The orthogonality relationship for Legendre polynomials is

$$\int_0^\pi P_m{}^l P_n{}^l \sin\theta\, d\theta = \frac{(m+l)!}{(m-l)!}\frac{2}{2m+1}\delta_{mn}.$$

(This, in linear theory, would be the data for dipole and quadrupole radiation.) Equations (22) then reduce to

$$\begin{aligned}
&\partial m(u)/\partial u - 4(\partial^2/\partial u^2)[\tfrac{3}{5}(B_2\bar{B}_2) + \tfrac{15}{7}(B_3\bar{B}_3)] \\
&\qquad = -8[\tfrac{3}{5}(B_{2,0}\bar{B}_{2,0}) + \tfrac{15}{7}(B_{3,0}\bar{B}_{3,0})], \\
&\partial P(u)/\partial u - \tfrac{12}{7}(\partial^2/\partial u^2)[B_2\bar{B}_3 + \bar{B}_2B_3] \\
&\qquad = -\tfrac{24}{7}(B_{2,0}\bar{B}_{3,0} + \bar{B}_{2,0}B_{3,0}), \\
&\partial^2 D(u)/\partial u^2 = \tfrac{12}{7}\sqrt{2}\,[2(\bar{B}_{2,0}B_{3,0} + B_{2,0}\bar{B}_{3,0}) \\
&+ 3(B_{2,00}\bar{B}_3 + \bar{B}_{2,00}B_3 - B_2\bar{B}_{3,00} - \bar{B}_2B_{3,00})], \\
&\qquad L(u) = \tfrac{36}{7}\sqrt{2}\,i(B_2\bar{B}_3 - \bar{B}_2B_3) + \text{const.}
\end{aligned} \tag{24}$$

Again, the importance of consecutive terms in the expansion of σ^0 is evident. The mass, however, has no dependence on crossterms.

IV. DISCUSSION

In this paper, we have confined ourselves to a discussion of the multipole moments and their dynamics for the important case of retarded solutions. (The case of advanced solutions and mixtures of advanced and retarded solutions is being investigated.)

To the authors, one of the more attractive results of this investigation is the light shed on the effect of the nonlinearity of the field equations. In the linear theory (see JN), there is a complete decoupling of the different modes of the field. (By different modes, we mean different time-dependent multipole moments.) Each of the different terms in the news functions, σ^0, Eq. (15) drives or determines the time dependence of a specific moment. In particular, one obtains the well-known result that the monopole moment or mass and dipole moment are conserved.

In the full theory one sees clearly from Eqs. (18)–(20) how the nonlinearity affects the mass, linear momentum and dipole moment. One can proceed to show how the higher moments are in turn affected. For example, from Eq. (13c), it can be seen that the time dependence of the quadrupole moment is partly determined by the interaction of the quadrupole part of the news function with the mass of the system. It also appears, though the calculation has not yet been carried out in detail, that via the interaction of the monopole, dipole, and quadrupole, an octupole term will automatically be present in general.[19]

One of the more interesting problems to be investigated is the interaction of an incoming and an outgoing mode, i.e., the scattering of the field by another field.

APPENDIX

In Bondi[1] and NU the final coordinate freedom consists of the asymptotic transformation

$$\begin{aligned}
u &= K^{-1}(\theta', \phi')u' + \alpha(\theta', \phi') + O(r'^{-1}), \\
r &= K(\theta', \phi')r' + O(1), \\
x^k &= G^k(\theta', \phi') + O(r^{-1}).
\end{aligned} \tag{25}$$

If axial symmetry is imposed, so that K and α are independent of ϕ, this transformation is referred to as the "Bondi–Metzner group." The transformations with $\alpha = 0$ are equivalent to the Lorentz transformations.[1,5] The "super translations," with $K = 1$, $\alpha \neq 0$, are not as well understood as the Lorentz transformations. These super translations are of greater interest to us here and will be considered in this appendix.

Under the supertranslation $u' = u - \alpha(\theta) + O(r^{-1})$, the function $\sigma^0(u, \theta)$ transforms as[20]

$$\sigma^{0\prime} = \sigma^0 - \tfrac{1}{2}\sin\theta(\alpha_{,2}/\sin\theta)_{,2}, \tag{26}$$

while the mass aspect becomes

$$\begin{aligned}
&(\psi_2^0 + \bar{\psi}_2^0)' = (\psi_2^0 + \bar{\psi}_2^0) - \frac{\alpha_{,2}}{\sin^2\theta} \\
&\cdot[(\sigma^0_{,0} + \bar{\sigma}^0_{,0})\sin^2\theta]_{,2} - \tfrac{1}{2}(\alpha_{,2})^2(\sigma^0_{,00} + \bar{\sigma}^0_{,00}).
\end{aligned} \tag{27}$$

The supertranslations affect the various multipoles defined in Sec. II. To see this, it is only necessary to work with infinitesmal transformations. Let $\alpha(\theta) = -\epsilon(\theta)$ = an infinitesmal. Then under

$$u' = u + \epsilon(\theta), \tag{28}$$

the multipole aspects and σ^0 transform as

$$\begin{aligned}
\sigma^{0\prime} &= \sigma^0 + \tfrac{1}{2}\sin\theta(\epsilon_{,2}/\sin\theta)_{,2}, \\
(\psi_2^0 + \bar{\psi}_2^0)' &= (\psi_2^0 + \bar{\psi}_2^0) + (\epsilon_{,2}/\sin^2\theta) \\
&\qquad \times [(\sigma^0_{,0} + \bar{\sigma}^0_{,0})\sin^2\theta]_{,2}, \\
\psi_1^{0\prime} &= \psi_1^0 - (3/2\sqrt{2})\epsilon_{,2}\{(\psi_2^0 + \bar{\psi}_2^0) + (\sigma^0_{,0}\bar{\sigma}^0 - \bar{\sigma}^0_{,0}\sigma^0) \\
&+ (2\sin\theta)^{-1}[(\sin\theta)^{-1}(\{\sigma^0 - \bar{\sigma}^0\}\sin^2\theta)_{,2}]_{,2}\}, \\
\psi_0^{0\prime} &= \psi_0^0 - 2\sqrt{2}\epsilon_{,2}\psi_1^0.
\end{aligned} \tag{29}$$

As a special case, showing how the multipoles are affected, we take

$$\begin{aligned}
\alpha(\theta) &= -\epsilon(\theta) = -(\epsilon_0 P_0 + \epsilon_1 P_1 + \epsilon_2 P_2, \\
\sigma^0(u, \theta &= B_2(u)\,P_2{}^2 + B_3(u)\,P_3^2,
\end{aligned} \tag{30}$$

[19] A similar result has been obtained by W. Bonner, *Proceedings of the Florence Conference on General Relativity, Problems of Energy and Gravitational Waves* September 1964.

[20] In these transformation equations, the left-hand sides are functions of the new (primed) coordinates, while the right-hand sides are functions of the old coordinates. Hence a Taylor expansion must be made on the unprimed quantities to obtain useful results. This is done in the examples which will be given.

where the ϵ_k are real infinitesmal numbers, P_n and P_n^2 are Legendre polynomials of argument $\cos\theta$, and the $B_k(u)$ are complex functions of u.

In Sec. III it was shown that the multipole aspects can be expressed as finite series in Legendre polynomials:

$$(\psi_2^0 + \bar{\psi}_2^0) = \sum_0 F_m(u)P_n,$$
$$\psi_1^0 = \sum_1 G_m(u)P_m^1, \tag{31}$$
$$\psi_0^0 = \sum_2 H_m(u)P_m^2,$$

where mass, linear momentum, complex dipole, and quadrupole moments are proportional to F_0, F_1, G_1, and H_2, respectively, as illustrated by Eqs. (16) and the discussion following. It is easily shown by Eqs. (29) that a supertranslation does not affect the *form* of the series (31), only the number of terms in each series is changed. Hence after an infinitesmal supertranslation Eq. (28) we have, writing b_k for $\frac{1}{2}(B_k + \bar{B}_k)$,

$$(\psi_2^0 + \bar{\psi}_2^0)' = \sum_0 F_m'(u')P_m, \tag{32}$$

where the new mass and linear momentum are given by

$$-2m'(u') \equiv F_0'(u') = F_0(u') - \epsilon_0 F_{0,0}(u') - \tfrac{1}{3}\epsilon_1 F_{1,0}(u') - \tfrac{1}{5}\epsilon_2[F_{2,0}(u') + 48b_{2,0}(u')], \tag{33}$$

$$-6P'(u') \equiv F_1'(u') = F_1(u') - \epsilon_0 F_{1,0}(u') - \epsilon_1[F_{0,0}(u') + \tfrac{2}{5}F_{2,0}(u') + \tfrac{48}{5}b_{2,0}(u')] - \epsilon_2[\tfrac{2}{5}F_{1,0}(u') + \tfrac{9}{35}F_{3,0}(u') + \tfrac{288}{7}b_{3,0}(u')].$$

It is evident that the supertranslation brings about more of a change than might at first be expected. The new mass is a function of the original mass, its time derivative, the time derivative of the old linear momentum, a component of the news function, and a higher term (F_2) of the series, Eq. (31). Likewise the new linear momentum is a complicated function of the original news, mass, momentum and higher terms.

The complex dipole and quadrupole moments transform in similar fashion. After applying the supertranslation to Eqs. (22) we obtain

$$-\tfrac{3}{2}[D'(u') + iL'(u')] \equiv G_1'(u') = G_1(u') - \epsilon_0 G_{1,0}(u') + \epsilon_1\{(3/2\sqrt{2})F_0(u') - (3/10\sqrt{2})F_2(u') - \tfrac{3}{5}G_{2,0}(u') + \tfrac{90}{7}\sqrt{2}[B_{3,0}(u')\bar{B}_3(u') - \bar{B}_{3,0}(u')B_3(u')] + \tfrac{162}{35}\sqrt{2}[B_{2,0}(u')\bar{B}_2(u') - \bar{B}_{2,0}(u')B_2(u')] + \tfrac{9}{5}\sqrt{2}[\bar{B}_2(u') - B_2(u')]\} + \epsilon_2\{\tfrac{1}{5}G_{1,0}(u') - \tfrac{18}{35}G_{3,0}(u') + (9/10\sqrt{2})F_1(u') - (27/70\sqrt{2})F_3(u') \times \tfrac{54}{7}\sqrt{2}-B_{2,0}(u')\bar{B}_3(u') - \bar{B}_{2,0}(u')B_3(u') + \bar{B}_2(u')B_{3,0}(u') - B_2(u')\bar{B}_{3,0}(u')] + \tfrac{81}{7}\sqrt{2}[\bar{B}_3(u') - B_3(u')]\}, \tag{34}$$

$$-\tfrac{5}{24}Q'(u') \equiv H_2'(u') = H_2(u') - \epsilon_0 H_{2,0}(u') + \epsilon_1[\tfrac{2}{3}\sqrt{2}G_1(u') - \tfrac{2}{7}\sqrt{2}G_3(u') - \tfrac{5}{7}\dot{H}_{3,0}(u')] + \epsilon_2[\tfrac{6}{7}\sqrt{2}G_2(u') - \tfrac{10}{21}\sqrt{2}G_4(u') + \tfrac{2}{7}\dot{H}_{2,0}(u') - \tfrac{5}{7}\dot{H}_{4,0}(u')].$$

Although the components of σ^0 do not enter explicitly in the transformed quadrupole moment, they occur implicitly in the $\dot{H}_2(u')$, through the time-development equations (13). Furthermore the $\dot{F}_k(u')$ and $\dot{G}_k(u')$ are determined by the choice of σ^0, and have been calculated in the example given in Sec. III, Eqs.(22).

From a study of this example it appears as if, by an appropriate choice of the ϵ's in the expansion of $\alpha(\theta)$, one can make at any given "time" u all the mass multipoles except the monopole equal to zero. In this example, it would involve solving the two simultaneous equations for ϵ_1 and ϵ_2 obtained by setting $D'(u')$ and the real part of $Q'(u')$ equal to zero.

Inequality with Applications in Statistical Mechanics*

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We prove for Hermitian matrices (or more generally for completely continuous self-adjoint linear operators in Hilbert space) A and B that $\mathrm{Tr}\,(e^{A+B}) \leq \mathrm{Tr}\,(e^A e^B)$. The inequality is shown to be sharper than the convexity property $(0 \leq \alpha \leq 1)$ $\mathrm{Tr}\,(e^{\alpha A+(1-\alpha)B}) \leq [\mathrm{Tr}\,(e^A)]^\alpha [\mathrm{Tr}\,(e^B)]^{1-\alpha}$, and its possible use for obtaining upper bounds for the partition function is discussed briefly.

1. SUMMARY

OUR results are summarized in the following theorems.[1]

Theorem I. For two $n \times n$ Hermitian matrices A and B

$$\mathrm{Tr}\,(e^{A+B}) \leq \mathrm{Tr}\,(e^A e^B). \tag{1}$$

Theorem II. For two $n \times n$ positive-definite matrices A and B, and $0 \leq \alpha \leq 1$,

$$\mathrm{Tr}\,(A^\alpha B^{1-\alpha}) \leq [\mathrm{Tr}\,(A)]^\alpha [\mathrm{Tr}\,(B)]^{1-\alpha}. \tag{2}$$

Proofs of these theorems (which carry over to completely continuous self adjoint linear operators in Hilbert space) are given in the following two sections.

A consequence of Theorems I and II is[2]:

Corollary: For two $n \times n$ Hermitian matrices A and B, and $0 \leq \alpha \leq 1$,

$$\mathrm{Tr}\,(e^{\alpha A+(1-\alpha)B}) \leq [\mathrm{Tr}\,(e^A)]^\alpha [\mathrm{Tr}\,(e^B)]^{1-\alpha}. \tag{3}$$

The convexity property (3) has been used[3] to obtain an upper bound for the partition function (in the usual notation) $Z = \mathrm{Tr}\,(e^{-\beta H})$ of an antiferromagnetic chain. Equation (1) can also be used to obtain upper bounds for the partition function if we separate the Hamiltonian in a way that enables us to compute the upper bound. In view of (2), the inequality (1) is sharper than (3), so that in general, (1) will probably give us better bounds than (3). Work along these lines is at present in progress.

2. PROOF OF THEOREM I

The proof rests on the following two Lemmas.

Lemma 1. For an $n \times n$ matrix X,

$$|\mathrm{Tr}\,(X)^{2m}| \leq \mathrm{Tr}\,(XX^\dagger)^m, \tag{4}$$

where m is a positive integer and † denotes Hermitian conjugate.

Lemma 2.[1] For two $n \times n$ Hermitian matrices A and B,

$$|\mathrm{Tr}\,(AB)^{2^k}| \leq \mathrm{Tr}\,(A^{2^k}B^{2^k}), \tag{5}$$

where k is a positive integer.

Lemma 1 is a special case of a theorem due to Weyl.[4]

To prove Lemma 2, we first note that with $X = AB$, $X\dagger = BA$ in Lemma 1, we have

$$|\mathrm{Tr}\,(AB)^{2m}| \leq \mathrm{Tr}\,(ABBA)^m = \mathrm{Tr}\,(A^2B^2)^m, \tag{6}$$

where the last equality follows from the cyclic property of the trace. We now proceed by induction.

The case $k = 1$ of (5) is just the case $m = 1$ of (6). And if we assume (5) to be true for $k = l$, we have from (6)

$$|\mathrm{Tr}\,(AB)^{2^{l+1}}| = |\mathrm{Tr}\,(AB)^{2(2^l)}| \leq |\mathrm{Tr}\,(A^2B^2)^{2^l}|.$$

The result follows if we then use our inductive assumption with A^2 and B^2 in place of A and B.

The theorem is proved from Lemma 2 by taking $I + 2^{-k}A$ and $I + 2^{-k}B$ in place of A and B, respectively, and proceeding to the limit $k \to \infty$.

We remark that the obvious generalization of (5), namely,

$$|\mathrm{Tr}\,(ABC)^{2^k}| \leq \mathrm{Tr}\,(A^{2^k}B^{2^k}C^{2^k}) \tag{7}$$

is not true, so that Theorem I has no obvious generalization. A counter example to (7) (for $k = 1$) is

$$A = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 2 & 0 & -2 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 2 \end{bmatrix}, \tag{8}$$

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[1] Theorem I, and Lemma 2 in Sec. 2 (for positive-definite matrices only), have recently been proved independently by S. Golden, Phys. Rev. **137**, B1127 (1965).

[2] D. Ruelle, Helv. Phys. Acta **36**, 789 (1963).

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[4] H. Weyl, Proc. Natl. Acad. Sci. U. S. **35**, 408 (1949); see also G. Polya, *ibid.* **36**, 49 (1950).

for which Tr $(A^2B^2C^2)$ = Tr $(B^2A^2C^2)$ = 0 and Tr $(ABC)^2 = 9$.

3. PROOF OF THEOREM II

We order the eigenvalues a_i of A, and b_i of B in decreasing order, $a_1 \geq a_2 \geq \cdots \geq a_n \geq 0$, $b_1 \geq b_2 \geq \cdots \geq b_n \geq 0$, and use Fan's result[5]

$$\sum_{i=1}^{k} (\varphi_i, B^{1-\alpha}\varphi_i) \leq \sum_{i=1}^{k} b_i^{1-\alpha}, \qquad k = 1, 2, \cdots, n,$$

which holds for an arbitrary orthonormal set of vectors $\{\varphi_i\}$. Choosing the φ_i to be eigenvectors of A and summing by parts gives us

$$\text{Tr } (A^\alpha B^{1-\alpha}) = \sum_{i=1}^{n} a_i^\alpha (\varphi_i, B^{1-\alpha}\varphi_i)$$

$$\leq \sum_{i=1}^{n} a_i^\alpha b_i^{1-\alpha}$$

$$\leq \left(\sum_{i=1}^{n} a_i\right)^\alpha \left(\sum_{i=1}^{n} b_i\right)^{1-\alpha}$$

$$= [\text{Tr } (A)]^\alpha [\text{Tr } (B)]^{1-\alpha},$$

where the last inequality is just Hölder's inequality for positive real numbers.

[5] K. Fan, Proc. Natl. Acad. Sci. U. S. 35, 652 (1949).

ACKNOWLEDGMENTS

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Oblique Incidence on Plane Boundary between Two General Gyrotropic Plasma Media*

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(Received 12 March 1965; final manuscript received 22 April 1965)

The problem of a characteristic electromagnetic wave incident obliquely on a plane boundary between two different gyrotropic plasma media is solved. Two characteristic transmitted waves and two characteristic reflected waves will result. The corresponding reflection and transmission coefficients have been evaluated. The particular degenerate cases of free space–gyrotropic medium, gyrotropic medium–free space, and gyrotropic medium–perfect conductor are solved in the appendices.

I. INTRODUCTION

OVER the past half-century, many attacks have been made on selected portions of the problem of oblique incidence of electromagnetic waves from free space on a sharply bounded ionosphere. The isotropic case has been discussed in detail by Stratton[1] and by Budden,[2] and their results are in agreement with the ones found originally by Snell (1591–1626), Fresnel (1788–1827), and Brewster (1781–1868). Booker[3–5] treated the obliquely incident wave in the anisotropic ionosphere and derived the well-known "Booker quartic equation" for the refractive index, and his results are given in detail by Budden.[2] Bremmer[6] gave an expression for the reflection coefficients, applicable to the lossless case. Yabroff[7] gave curves showing reflection coefficients as a function of the angle of incidence for various directions of the earth's magnetic field. Additional

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† Consultant to the Antenna Laboratory, Department of Electrical Engineering, The Ohio State University, Columbus, Ohio; Electrical Engineering Department, The University of Kansas, Lawrence, Kansas.

[1] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill Book Company, Inc., New York, 1941).

[2] K. G. Budden, *Radio Waves in the Ionosphere* (Cambridge University Press, Cambridge, England, 1961).

[3] H. G. Booker, Proc. Roy. Soc. (London) **A155**, 235 (1936).

[4] H. G. Booker, Phil. Trans. Roy. Soc. London **A237**, 411 (1939).

[5] H. G. Booker, J. Geophys. Res. 54, 243 (1949).

[6] H. Bremmer, *Terrestrial Radio Waves* (Elsevier Publishing Company, New York, 1949).

[7] I. W. Yabroff, Proc. IRE 45, 750 (1957).

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detailed discussion of this problem has been given by Budden.[2]

During the past two years a study of electromagnetic scattering by three-dimensional iostropic plasma bodies has taken place[8,9] in the Antenna Laboratory, The Ohio State University, Columbus, Ohio. A modified geometrical-optics method has been used with excellent results. It has been suggested[9] that this method be extended to anisotropic three-dimensional plasma bodies where no general theoretical solution has been given up to now. The present paper and its appendices could be applied to this problem.

In the present paper the problem of a characteristic electromagnetic wave incident obliquely on a plane boundary between two different gyrotropic plasma media is solved. It is shown that two characteristic transmitted waves and two characteristic reflected waves will result. The corresponding reflection and transmission coefficients are evaluated. The important particular degenerate cases of free space–gyrotropic medium, gyrotropic medium–free space, and gyrotropic medium–perfect conductor are solved in the appendices.

Some related gyrotropic boundary-value problems have been discussed previously by the author[10-12] and an extensive bibliography has been given.[10,12]

II. BOOKER QUARTIC EQUATION

Let a plane electromagnetic wave propagate in a homogeneous, gyrotropic, plasma medium in an arbitrary direction with respect to the coordinate system. Assuming harmonic time variation exp $(+i\omega t)$, each field component of this wave will contain the factor

$$\exp(-in\mathbf{k}\cdot\mathbf{R}) = \exp[-ik(S_1x + S_2y + qz)] \quad (1)$$

where $n = c/v$ is the refractive index and $|\mathbf{k}| = k = \omega/c$. One may obtain from Eq. (1)

$$n^2 = S_1^2 + S_2^2 + q^2. \quad (2)$$

Taking θ as the angle between the direction of the wave normal and the positive z axis, one obtains

$$q = n\cos\theta, \quad (3a)$$

and using Eq. (2) also

$$(S_1^2 + S_2^2)^{\frac{1}{2}} = n\sin\theta. \quad (3b)$$

The direction cosines of the wave normal are

$$\cos\tau' = S_1/n; \quad \cos\tau'' = S_2/n; \quad \cos\theta = q/n, \quad (3c)$$

where τ', τ'', θ are the angles of the wave normal with the corresponding axes x, y, z. The value of the refractive index n may be determined for a given wave with known S_1, S_2, once the variable q has been found, by using Eq. (2). The value of the variable q may be found as a solution of the Booker quartic equation.

Consider a plane electromagnetic wave in a homogeneous, gyrotropic, plasma medium, for which all field components depend on x, y, z only through the factor given in Eq. (1). Then we may write symbolically

$$\partial/\partial x \equiv -ikS_1; \quad \partial/\partial y \equiv -ikS_2; \quad \partial/\partial z \equiv -ikq. \quad (4)$$

The fields in the gyrotropic plasma medium must satisfy the first Maxwell's equation

$$\nabla\times\mathbf{H} = i\omega\mathbf{D} = i\omega(\epsilon_0\mathbf{E} + \mathbf{P}). \quad (5a)$$

Using Eq. (4), this may be rewritten in a matrix form

$$[S]\eta_0\mathbf{H} = -[I]\mathbf{E} - (1/\epsilon_0)\mathbf{P} \quad (5b)$$

where $\eta_0 = (\mu_0/\epsilon_0)^{\frac{1}{2}}$, the matrix $[S]$ is defined by

$$[S] = \begin{bmatrix} 0 & -q & S_2 \\ q & 0 & -S_1 \\ -S_2 & S_1 & 0 \end{bmatrix} \quad (5c)$$

and the identity matrix $[I]$ is defined by

$$[I] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (5d)$$

The second Maxwell's equation for the gyrotropic

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[8] L. Peters, Jr., W. G. Swarner, and D. T. Thomas, "Further Studies of the Radar Cross Section of Plasma-Clad Bodies." Second Symposium on Plasma Sheath, Boston, Massachusetts, 1962 (Pergamon Press, to be published).

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[11] H. Unz, "Electromagnetic Waves in Longitudinally Magnetized Ferrites between Two Conducting Parallel Planes," Report No. 1021-10, pp. 1–40, 1 December 1961, Antenna Laboratory, The Ohio State University, Columbus, Ohio.

[12] H. Unz, "Propagation in Arbitrarily Magnetized Ferrites between Two Conducting Parallel Planes," (includes Biblioggraphy). Report No. 1021-22, pp. 1–38, 1 November 1962, Antenna Laboratory, The Ohio State University, Columbus, Ohio.

plasma medium

$$\nabla \times \mathbf{E} = -i\omega\mathbf{B} = -i\omega\mu_0\mathbf{H} \tag{6a}$$

may be written in a matrix form as follows:

$$[S]\mathbf{E} = \eta_0\mathbf{H}. \tag{6b}$$

In a gyrotropic plasma medium one may find the constitutive relation

$$(1/\epsilon_0)\mathbf{P} = [M]\mathbf{E} \tag{7}$$

where the derivation of the matrix $[M]$ has been given by Budden[2] and may be found in Appendix A. The matrix $[M]$ is usually called the susceptibility matrix.

Substituting Eqs. (6b) and (7) into Eq. (5b) and rearranging, one may find

$$\{[S][S] + [I] + [M]\}\mathbf{E} = 0 \tag{8}$$

which is equivalent to three homogeneous equations with three unknowns E_x, E_y, E_z. For a nontrivial solution, the determinant of the coefficients must be zero:

$$\det |[S][S] + [I] + [M]| = 0. \tag{9}$$

Equation (9) gives a quartic equation for the variable q which is called the Booker quartic:

$$F(q) \equiv \alpha q^4 + \beta q^3 + \gamma q^2 + \delta q + \epsilon = 0. \tag{10}$$

The derivation of the Booker quartic has been given by Budden[2] and it may be found in Appendix B.

For each homogeneous, gyrotropic plasma medium one will have in general four distinct solutions for q, noted as q_1, q_2, q_3, q_4. Two of them belong to upgoing waves and two of them belong to downgoing waves. In the general case when Z is not zero, no root of the Booker quartic can be real: two of the roots must have negative imaginary parts, and the other two must have positive imaginary parts. For oblique incidence, one can define the "upgoing" waves (in the positive z direction) by

$$\text{Im}\,(q_1) < 0; \qquad \text{Im}\,(q_2) < 0 \tag{11a}$$

and the "downgoing" waves (in the negative z direction) by

$$\text{Im}\,(q_3) > 0; \qquad \text{Im}\,(q_4) > 0. \tag{11b}$$

The real part of q may be either positive or negative, i.e., the directions of the wave normal and the "ray" could be different.

When $Z = 0$, the coefficients in the Booker quartic are all real, and the roots are therefore either real or are conjugate complex pairs. To decide whether a real value of q refers to an upgoing or downgoing wave, it is convenient to give Z a very small nonzero value, and to examine the sign of Im (q) as above. A more detailed discussion of the above has been given by Budden.[2]

III. FIELD COMPONENTS

Equation (8) gives three homogeneous linear equations with three unknowns, the details of which are given in Appendix B. For a nontrivial solution the determinantal Eq. (9) should hold, and one obtains the Booker quartic equation for the q variable. According to the theory of homogeneous, linear equations, one may ignore now the last equation implicit in (8); the remaining two equations may be rewritten as follows from Appendix B.

$$(1 - q^2 - S_2^2 + M_{xx})E_x + (S_1S_2 + M_{xy})E_y = -(S_1q + M_{xz})E_z, \tag{12a}$$

$$(S_1S_2 + M_{yx})E_x + (1 - q^2 - S_1^2 + M_{yy})E_y = -(S_2q + M_{yz})E_z, \tag{12b}$$

where the components of the matrix $[M]$ may be found in Appendix A. From Eqs. (12) one may find E_x and E_y in terms of the E_z component

$$\frac{E_x}{E_z} = \pi_x = \frac{-(S_1q + M_{xz})(1 - q^2 - S_1^2 + M_{yy}) + (S_1S_2 + M_{xy})(S_2q + M_{yz})}{(1 - q^2 - S_2^2 + M_{xx})(1 - q^2 - S_1^2 + M_{yy}) - (S_1S_2 + M_{xy})(S_1S_2 + M_{yx})} \tag{13a}$$

$$\frac{E_y}{E_z} = \pi_y = \frac{-(1 - q^2 - S_2^2 + M_{xx})(S_2q + M_{yz}) + (S_1q + M_{xz})(S_1S_2 + M_{yx})}{(1 - q^2 - S_2^2 + M_{xx})(1 - q^2 - S_1^2 + M_{yy}) - (S_1S_2 + M_{xy})(S_1S_2 + M_{yx})}. \tag{13b}$$

From Eq. (6b) and using the definitions above, one may obtain

$$\eta_0H_x/E_z = \eta_x = S_2 - q\pi_y, \tag{13c}$$

$$\eta_0H_y/E_z = \eta_y = -S_1 + q\pi_x, \tag{13d}$$

$$\eta_0H_z/E_z = \eta_z = -S_2\pi_x + S_1\pi_y. \tag{13e}$$

Equations (13) give all the field components in a homogeneous, gyrotropic plasma medium in terms of the E_z component. Once E_z has been found, all the rest of the field components of the hybrid wave may be found.

IV. REFLECTED AND TRANSMITTED WAVES

Consider a horizontal plane boundary $z = 0$ between two homogeneous, gyrotropic plasma media, and let the x, y axes be in the boundary plane and the z axis be measured vertically upward (Fig. 1). The two different media will be denoted by "A" and "B". The value of the field quantity F at $z = 0$ on the boundary in the top medium "B" will be denoted by $F(+0)$, and the corresponding value in the bottom medium "A" will be denoted by $F(-0)$. These are the values immediately adjacent to the boundary, on opposite sides of it. Then the following boundary conditions must hold:

$$E_x(+0) = E_x(-0), \tag{14a}$$

$$E_y(+0) = E_y(-0), \tag{14b}$$

$$H_x(+0) = H_x(-0), \tag{14c}$$

$$H_y(+0) = H_y(-0). \tag{14d}$$

There are two additional boundary conditions:

$$D_z(+0) = D_z(-0), \tag{15a}$$

$$B_z(+0) = B_z(-0). \tag{15b}$$

However, the boundary conditions in Eqs. (15) are equivalent to boundary conditions in Eqs. (14) and may be derived from them, through Maxwell's equations. Therefore, they will not be needed here.

Let a characteristic wave be incident on the boundary $z = 0$ from medium A below, with its wave normal making the angles τ', τ'', θ_I with the corresponding x, y, z axes, in a clockwise direction. In case the above angles are complex, they will represent an inhomogeneous plane wave[2]. In general, there are two possible characteristic waves in medium A, incident on the plane boundary $z = 0$ from below, and the following analysis applies to both of them equally well. Any field component F_i in the incident wave is given by

$$F_i = F^i \exp\,[-ik(S_1x + S_2y + q^A z)], \tag{16}$$

where F^i is a constant. One could take $q^A = q_1^A$ or $q^A = q_2^A$ where both are "upgoing" waves in the positive z direction defined by Eq. (11a). The values of $q_{1,2}^A$ are derived from the corresponding Booker quartic equation given in Appendix B.

In general, there will be two reflected waves in the lower medium A and two transmitted waves in the upper medium B, with their corresponding wave normals at angles θ_r (actually θ_{r3}, θ_{r4}) and θ_t (actually θ_{t1}, θ_{t2}), respectively, as measured from the positive z axis in a clockwise direction (Fig. 1). For the case of normal incidence, each set will correspond to the ordinary and the extraordinary wave.

Any field component F_r for the reflected waves in the lower medium A is given by

$$F_{r3} = F_3^r \exp\,[-ik(S_1x + S_2y + q_3^A z)], \tag{17a}$$

$$F_{r4} = F_4^r \exp\,[-ik(S_1x + S_2y + q_4^A z)], \tag{17b}$$

where F_3^r and F_4^r are constants. q_3^A and q_4^A will be two solutions of the Booker quartic equation in medium A and will be defined by Eq. (11b), giving "downgoing" waves in the negative z direction.

Any field component F_t for the transmitted waves in the upper medium B is given by

$$F_{t1} = F_1^t \exp\,[-ik(S_1x + S_2y + q_1^B z)], \tag{18a}$$

$$F_{t2} = F_2^t \exp\,[-ik(S_1x + S_2y + q_2^B z)], \tag{18b}$$

where F_1^t and F_2^t are constants. q_1^B and q_2^B will be two solutions of the Booker quartic equation in medium B and will be defined by Eq. (11a), giving "upgoing" waves in the positive z direction.

In Eqs. (16), (17), and (18) all the field components depend on the same exponential form in their variation in the x, y directions. This is necessary since they will have to obey the boundary conditions in Eqs. (14) at $z = 0$, where the x, y dependence of all components should be cancelled out. In other words, once S_1 and S_2 have been determined for the given incident wave, their values remain the same for the reflected waves and the transmitted waves. The values of the angles of reflection θ_r and the angles of transmission θ_t may be found from the given

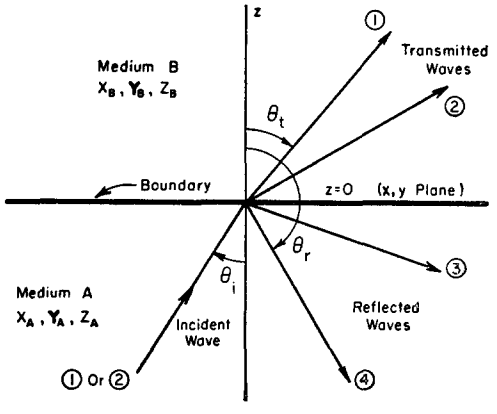

FIG. 1. Oblique incidence on plane boundary.

values S_1, S_2, and the corresponding values $q_{3,4}^{A}$ and $q_{1,2}^{B}$ found from the Booker quartic equation, in accordance with the relationships given in Sec. II.

V. REFLECTION AND TRANSMISSION COEFFICIENTS

The boundary condition in Eq. (14a) states that the x component of the total electric field is continuous across the boundary $z = 0$ as one passes from medium B to medium A. Taking $z = 0$ in Eqs. (16), (17), (18) and substituting into Eq. (14a) one obtains

$$E_{x1}^{t} + E_{x2}^{t} = E_{x}^{i} + E_{x3}^{r} + E_{x4}^{r} \tag{19a}$$

where the term $\exp[-ik(S_1x + S_2y)]$ has been canceled on both sides. Similarly, by substituting as above in the rest of the boundary conditions given in Eqs. (14), one obtains

$$E_{y1}^{t} + E_{y2}^{t} = E_{y}^{i} + E_{y3}^{r} + E_{y4}^{r}, \tag{19b}$$

$$H_{x1}^{t} + H_{x2}^{t} = H_{x}^{i} + H_{x3}^{r} + H_{x4}^{r}, \tag{19c}$$

$$H_{y1}^{t} + H_{y2}^{t} = H_{y}^{i} + H_{y3}^{r} + H_{y4}^{r}. \tag{19d}$$

Using Eqs. (13), one may rewrite Eqs. (19) in terms of the corresponding E_z components, as follows:

$$\pi_{x1}^{B}E_{z1}^{t} + \pi_{x2}^{B}E_{z2}^{t} - \pi_{x3}^{A}E_{z3}^{r} - \pi_{x4}^{A}E_{z4}^{r} = \pi_{x}^{A}E_{z}^{i}, \tag{20a}$$

$$\pi_{y1}^{B}E_{z1}^{t} + \pi_{y2}^{B}E_{z2}^{t} - \pi_{y3}^{A}E_{z3}^{r} - \pi_{y4}^{A}E_{z4}^{r} = \pi_{y}^{A}E_{z}^{i}, \tag{20b}$$

$$\eta_{x1}^{B}E_{z1}^{t} + \eta_{x2}^{B}E_{z2}^{t} - \eta_{x3}^{A}E_{z3}^{r} - \eta_{x4}^{A}E_{z4}^{r} = \eta_{x}^{A}E_{z}^{i}, \tag{20c}$$

$$\eta_{y1}^{B}E_{z1}^{t} + \eta_{y2}^{B}E_{z2}^{t} - \eta_{y3}^{A}E_{z3}^{r} - \eta_{y4}^{A}E_{z4}^{r} = \eta_{y}^{A}E_{z}^{i}, \tag{20d}$$

where the subscripts 1, 2, 3, 4 represent the waves corresponding to q_1, q_2, q_3, q_4; the superscripts A, B represent plasma medium A and medium B, and the superscripts t, r, i represent the transmitted waves, the reflected waves, and the incident waves, respectively (Fig. 1). Terms on the right-hand side in Eqs. (20) for the incident waves could be used for either of the two "upgoing" incident characteristic waves in plasma medium A, i.e., one could take either $q^{A} = q_1^{A}$ or $q^{A} = q_2^{A}$. Both cases are included in the present choice of notation for the incident wave.

Equations (20) are four inhomogeneous linear equations with four unknowns, E_{x1}^{t}, E_{x2}^{t}, E_{x3}^{r}, E_{x4}^{r}, where the value of E_x^{i} is known. Those equations may be solved, by using determinants, to give

$$T_1 = \frac{E_{x1}^{t}}{E_{x}^{i}} = \frac{1}{D}\begin{vmatrix} \pi_{x}^{A} & \pi_{x2}^{B} & \pi_{x3}^{A} & \pi_{x4}^{A} \\ \pi_{y}^{A} & \pi_{y2}^{B} & \pi_{y3}^{A} & \pi_{y4}^{A} \\ \eta_{x}^{A} & \eta_{x2}^{B} & \eta_{x3}^{A} & \eta_{x4}^{A} \\ \eta_{y}^{A} & \eta_{y2}^{B} & \eta_{y3}^{A} & \eta_{y4}^{A} \end{vmatrix}, \tag{21a}$$

$$T_2 = \frac{E_{x2}^{t}}{E_{x}^{i}} = \frac{1}{D}\begin{vmatrix} \pi_{x1}^{B} & \pi_{x}^{A} & \pi_{x3}^{A} & \pi_{x4}^{A} \\ \pi_{y1}^{B} & \pi_{y}^{A} & \pi_{y3}^{A} & \pi_{y4}^{A} \\ \eta_{x1}^{B} & \eta_{x}^{A} & \eta_{x3}^{A} & \eta_{x4}^{A} \\ \eta_{y1}^{B} & \eta_{y}^{A} & \eta_{y3}^{A} & \eta_{y4}^{A} \end{vmatrix}, \tag{21b}$$

$$R_3 = \frac{E_{x3}^{r}}{E_{x}^{i}} = \frac{-1}{D}\begin{vmatrix} \pi_{x1}^{B} & \pi_{x2}^{B} & \pi_{x}^{A} & \pi_{x4}^{A} \\ \pi_{y1}^{B} & \pi_{y2}^{B} & \pi_{y}^{A} & \pi_{y4}^{A} \\ \eta_{x1}^{B} & \eta_{x2}^{B} & \eta_{x}^{A} & \eta_{x4}^{A} \\ \eta_{y1}^{B} & \eta_{y2}^{B} & \eta_{y}^{A} & \eta_{y4}^{A} \end{vmatrix}, \tag{21c}$$

$$R_4 = \frac{E_{x4}^{r}}{E_{x}^{i}} = \frac{-1}{D}\begin{vmatrix} \pi_{x1}^{B} & \pi_{x2}^{B} & \pi_{x3}^{A} & \pi_{x}^{A} \\ \pi_{y1}^{B} & \pi_{y2}^{B} & \pi_{y3}^{A} & \pi_{y}^{A} \\ \eta_{x1}^{B} & \eta_{x2}^{B} & \eta_{x3}^{A} & \eta_{x}^{A} \\ \eta_{y1}^{B} & \eta_{y2}^{B} & \eta_{y3}^{A} & \eta_{y}^{A} \end{vmatrix}, \tag{21d}$$

$$D = \begin{vmatrix} \pi_{x1}^{B} & \pi_{x2}^{B} & \pi_{x3}^{A} & \pi_{x4}^{A} \\ \pi_{y1}^{B} & \pi_{y2}^{B} & \pi_{y3}^{A} & \pi_{y4}^{A} \\ \eta_{x1}^{B} & \eta_{x2}^{B} & \eta_{x3}^{A} & \eta_{x4}^{A} \\ \eta_{y1}^{B} & \eta_{y2}^{B} & \eta_{y3}^{A} & \eta_{y4}^{A} \end{vmatrix}, \tag{21e}$$

Equations (21) represent the solution of the problem in terms of transmission and reflection coefficients.

We will get one set of solutions in Eqs. (21) for the incident characteristic wave of the first kind $q^{A} = q_1^{A}$, and another set of solutions for the incident characteristic wave of the second kind $q^{A} = q_2^{A}$. The two incident characteristic waves are independent of each other and their solutions could be superimposed. The corresponding transmission and reflection coefficients could be rewritten for the two cases as follows:

$${}_1T_1 = E_{z1}^{t}/E_{z1}^{i}, \qquad {}_2T_1 = E_{z1}^{t}/E_{z2}^{i} \tag{22a}$$

$${}_1T_2 = E_{z2}^{t}/E_{z1}^{i}, \qquad {}_2T_2 = E_{z2}^{t}/E_{z2}^{i} \tag{22b}$$

$${}_1R_3 = E_{z3}^{r}/E_{z1}^{i}, \qquad {}_2R_3 = E_{z3}^{r}/E_{z2}^{i} \tag{22c}$$

$${}_1R_4 = E_{z4}^{r}/E_{z1}^{i}, \qquad {}_2R_4 = E_{z4}^{r}/E_{z2}^{i} \tag{22d}$$

and their values may be found from the corresponding Eqs. (21).

VI. SUMMARY

The problem of a characteristic electromagnetic wave incident obliquely on a plane boundary between two different gyrotropic plasma media has been solved. The amplitudes of two characteristic

transmitted waves and two characteristic reflected waves have been found. The corresponding reflection and transmission coefficients have been evaluated in terms of four-by-four determinant ratios.

The above general solution may be used for particular cases, when one medium is free space, or a perfect conductor. However, in those cases the general solution will become degenerate, and one will have to find the results by evaluating indetermined forms. It will be much simpler to solve the particular problems by starting from the beginning, along lines similar to the above general solution.

Solutions of some important particular cases may be found in the Appendices. In Appendix C the problem of a plane electromagnetic wave with arbitrary polarization incident in free space on a general gyrotropic plasma medium with a plane boundary is solved. In Appendix D the problem of a characteristic electromagnetic wave in a general gyrotropic plasma incident on a free space with a plane boundary is solved. In Appendix E the same problem is solved when the characteristic wave is incident on a plane boundary of a perfect conductor. All the above solutions are degenerate cases of the general solution given previously.

The above solutions may be used for the study of electromagnetic scattering by three-dimensional gyrotropic plasma bodies by using the modified geometrical-optics method.[8,9] Some inherent difficulties might be encountered there, especially since the normal of the phase front of the wave does not usually have the same direction as the energy flow.[2] Another related problem of interest will be the problem of an electromagnetic wave of arbitrary polarization in free space incident obliquely on a general gyrotropic plasma slab, which could be solved along lines similar to the above. The solution of this problem will be given elsewhere.[13]

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APPENDIX A: THE SUSCEPTIBILITY MATRIX

The derivation of the susceptibility matrix $[M]$ introduced in Eq. (7) has been given by Budden.[2] However, in the following analysis we will use alternative notation in accordance with Ratcliffe[14] and the present author[15,16] for the derivation of the matrix $[M]$. Taking the charge of the electron as $-e$ (where $e = |e|$ is a positive number) and denoting the static magnetic field by $\mathbf{H}_0$, one may define:

$$X = \omega_N^2/\omega^2 = Ne^2/\epsilon_0 m\omega^2, \tag{A1a}$$

$$\mathbf{Y} = \omega_H/\omega = \mu_0 e\mathbf{H}_0/m\omega = Y_x\mathbf{i}_x + Y_y\mathbf{i}_y + Y_z\mathbf{i}_z, \tag{A1b}$$

$$U = 1 - iZ = 1 - i\nu/\omega. \tag{A1c}$$

It can be shown[14,15] that the constitutive relations are

$$-\epsilon_0 X\mathbf{E} = U\mathbf{P} + i(\mathbf{Y}\times\mathbf{P}). \tag{A2}$$

Equation (A2) is similar to the one given by Budden,[2] except that according to Eq. (A1b) there is a difference in the sign of $\mathbf{Y}$ between the present usage and his definition.

Equation (A2) may be rewritten in a matrix form as follows:[15]

$$\epsilon_0[E] = [Y][P] \tag{A3a}$$

$$[Y] = -\frac{1}{X}\begin{bmatrix} U & -iY_z & iY_y \\ iY_z & U & -iY_x \\ -iY_y & iY_x & U \end{bmatrix}. \tag{A3b}$$

From Eq. (A3a) one may obtain

$$(1/\epsilon_0)[P] = [Y]^{-1}[E] = [M][E], \tag{A4a}$$

where $[M]$ is called the susceptibility matrix. It may be found[15] to be

$$[M] = \frac{-X}{U(U^2 - Y^2)}\begin{bmatrix} U^2 - Y_x^2 & iUY_z - Y_xY_y & -iUY_y - Y_xY_z \\ -iUY_z - Y_xY_y & U^2 - Y_y^2 & iUY_x - Y_yY_z \\ iUY_y - Y_xY_z & -iUY_x - Y_yY_z & U^2 - Y_z^2 \end{bmatrix}. \tag{A4b}$$

[13] H. Unz, "Oblique Incidence on General Magneto-Plasma Slab," Antenna Laboratory, The Ohio State University, Columbus, Ohio, Report 1116-36 (1963), pp 1–18.
[14] J. A. Ratcliffe, *The Magneto-Ionic Theory and Its Applications to the Ionosphere* (Cambridge University Press, Cambridge, England, 1959).
[15] H. Unz, "The Magneto-Ionic Theory for Drifting Plasma," IRE, Trans. Antennas Propagation 10, 459 (1962).
[16] H. Unz, "Drifting Plasma Magneto-Ionic Theory for Oblique Incidence," IEEE, Trans. Antennas Propagation 13, 595 (1965).

Taking into account our definition in Eq. (A1b), the matrix $[M]$ above may be shown to be identical with the one given by Budden.[2]

APPENDIX B: BOOKER QUARTIC EQUATION

The Booker quartic equation may be derived from the determinantal equation given in Eq. (9):

$$\det |[S][S] + [I] + [M]| = 0, \tag{B1a}$$

where the matrix $[S]$ and the identity matrix $[I]$ are defined in Eqs. (5c) and (5d), respectively, and the matrix $[M]$ is given in Appendix A. Equation (B1a) may be rewritten explictly in the following form:

$$\begin{vmatrix} 1 - q^2 - S_2^2 + M_{xx} & S_1S_2 + M_{xy} & S_1q + M_{xz} \\ S_1S_2 + M_{yx} & 1 - q^2 - S_1^2 + M_{yy} & S_2q + M_{yz} \\ S_1q + M_{zx} & S_2q + M_{zy} & 1 - S_1^2 - S^2 + M_{zz} \end{vmatrix} = 0. \tag{B1b}$$

Equation (B1b) is identical with the one given by Budden.[2] Developing the determinantal equation above, one will obtain in accordance with Budden[2]

$$F(q) \equiv \alpha q^4 + \beta q^3 + \gamma q^2 + \delta q + \epsilon = 0, \tag{B2}$$

where by defining

$$Y^2 = Y_x^2 + Y_y^2 + Y_z^2, \tag{B3a}$$

$$C^2 = 1 - S_1^2 - S_2^2, \tag{B3b}$$

the coefficients in Eq. (B2) will be of the form

$$\alpha = U(U^2 - Y^2) + X(Y_z^2 - U^2), \tag{B4a}$$

$$\beta = 2XY_z(S_1Y_x + S_2Y_y), \tag{B4b}$$

$$\gamma = 2(C^2U - X)[Y^2 - U(U - X)] + X[Y^2 - C^2Y_z^2 + (S_1Y_x + S_2Y_y)^2], \tag{B4c}$$

$$\delta = -2C^2XY_z(S_1Y_x + S_2Y_y) = -C^2\beta, \tag{B4d}$$

$$\epsilon = (C^2U - X)[(C^2U - X)(U - X) - C^2Y^2] - C^2X(S_1Y_x + S_2Y_y)^2. \tag{B4e}$$

Several particular cases are discussed in detail by Budden.[2]

APPENDIX C: FREE SPACE–GYROTROPIC MEDIUM

In the following analysis we will consider a plane wave in free space, of arbitrary polarization, obliquely incident on a plane boundary of an arbitrary gyrotropic plasma. We will assume in Fig. 1 that medium A is free space ($X_A = 0$) and medium B is the gyrotropic plasma. Let us represent each component of the field of the incident wave in free space by

$$F_i = F^i \exp [-ik(S_1x + S_2y + Cz)] \tag{C1}$$

where one has[2]

$$\cos \theta_i = C, \tag{C2a}$$

$$\sin \theta_i = (S_1^2 + S_2^2)^{\frac{1}{2}}, \tag{C2b}$$

$$S_1^2 + S_2^2 + C^2 = 1. \tag{C2c}$$

Similarly, let us represent each component of the reflected wave from the plane boundary back into free space by

$$F_r = F^r \exp [-ik(S_1x + S_2y - Cz)], \tag{C3}$$

where similarly one has

$$\cos \theta_r = -C, \tag{C4a}$$

$$\sin \theta_r = (S_1^2 + S_2^2)^{\frac{1}{2}}, \tag{C4b}$$

$$\theta_r = \pi - \theta_i. \tag{C4c}$$

There will be two characteristic transmitted waves into the general gyrotropic plasma medium, and their field components will be of the form

$$F_{t1} = F_1^t \exp [-ik(S_1x + S_2y + q_1^B z)], \tag{C5a}$$

$$F_{t2} = F_2^t \exp [-ik(S_1x + S_2y + q_2^B z)], \tag{C5b}$$

where Eqs. (C5) will represent[2] "upgoing" waves in the positive z direction, as defined by Eq. (11a).

Applying the boundary conditions at $z = 0$ in Eqs. (14) one obtains from Eqs. (C1), (C3), and (C5), after canceling exp $[-i(S_1x + S_2y)]$

$$E_{x1}^t + E_{x2}^t = E_x^i + E_x^r, \tag{C6a}$$

$$E_{y1}^t + E_{y2}^t = E_y^i + E_y^r, \tag{C6b}$$

$$H_{x1}^t + H_{x2}^t = H_x^i + H_x^r, \tag{C6c}$$

$$H_{y1}^t + H_{y2}^t = H_y^i + H_y^r. \tag{C6d}$$

It is well known[1] that for a plane wave in free space, exp $(-i\mathbf{k}\cdot\mathbf{R})$, one has

$$\mathbf{E}\cdot\mathbf{k} = 0, \tag{C7a}$$

$$\mathbf{H} = (1/\omega\mu_0)(\mathbf{k}\times\mathbf{E}), \tag{C7b}$$

where $\mathbf{k}$ is the vector wavenumber in the direction

of propagation. One has for the incident wave according to Eq. (C1):

$$\mathbf{k}_i = k[S_1\mathbf{i}_x + S_2\mathbf{i}_y + C\mathbf{i}_z]. \tag{C8}$$

Using Eqs. (C7) and (C8) one obtains for the incident wave

$$CE_z^i = -S_1E_x^i - S_2E_y^i, \tag{C9a}$$

$$\eta_0H_z^i = -S_2E_x^i + S_1E_y^i, \tag{C9b}$$

$$\eta_0H_x^i = S_2E_z^i - CE_y^i, \tag{C9c}$$

$$\eta_0H_y^i = CE_x^i - S_1E_z^i. \tag{C9d}$$

From Eqs. (C9) one may obtain

$$C\eta_0H_x^i = -S_1S_2E_x^i - (1 - S_1^2)E_y^i, \tag{C10a}$$

$$C\eta_0H_y^i = (1 - S_2^2)E_x^i + S_1S_2E_y^i. \tag{C10b}$$

Using Eqs. (C9a), (C9b), and (C10), one may obtain all the field components of the incident wave in free space if E_x^i and E_y^i are known. They are independent because of the arbitrary polarization of the wave. Similarly, one has for the reflected wave according to Eq. (C3):

$$\mathbf{k}_r = k[S_1\mathbf{i}_x + S_2\mathbf{i}_y - C\mathbf{i}_z]. \tag{C11}$$

Similarly to the above one may obtain the field relations for the reflected wave in the form

$$CE_z^r = S_1E_x^r + S_2E_y^r, \tag{C12a}$$

$$\eta_0H_z^r = -S_2E_x^r + S_1E_y^r, \tag{C12b}$$

$$C\eta_0H_x^r = S_1S_2E_x^r + (1 - S_1^2)E_y^r, \tag{C12c}$$

$$C\eta_0H_y^r = -(1 - S_2^2)E_x^r - S_1S_2E_y^r, \tag{C12d}$$

where all the components of the reflected wave are determined from E_x^r and E_y^r for the arbitrary polarized reflected wave.

Substituting Eqs. (13), (C10), and (C12) in the boundary conditions in Eqs. (C6) and rearranging, one may obtain

$$\pi_{x1}^BE_{z1}^t + \pi_{x2}^BE_{z2}^t - E_x^r = E_x^i, \tag{C13a}$$

$$\pi_{y1}^BE_{z1}^t + \pi_{y2}^BE_{z2}^t - E_y^r = E_y^i, \tag{C13b}$$

$$-C\eta_{x1}^BE_{z1}^t - C\eta_{x2}^BE_{z2}^t + S_1S_2E_x^r + (1 - S_1^2)E_y^r = S_1S_2E_x^i + (1 - S_1^2)E_y^i, \tag{C13c}$$

$$C\eta_{y1}^BE_{z1}^t + C\eta_{y2}^BE_{z2}^t + (1 - S_2^2)E_x^r + S_1S_2E_y^r = (1 - S_2^2)E_x^i + S_1S_2E_y^i. \tag{C13d}$$

From Eqs. (C13) one is able to find the unknowns E_{z1}^t, E_{z2}^t, E_x^r, E_y^r if the incident wave components of the electric field E_x^i, E_y^i are given, by the use of determinants.

After rearranging, one obtains

$$D = \begin{vmatrix} \pi_{x1}^B & \pi_{x2}^B & -1 & 0 \\ \pi_{y1}^B & \pi_{y2}^B & 0 & -1 \\ -C\eta_{x1}^B & -C\eta_{x2}^B & S_1S_2 & 1 - S_1^2 \\ C\eta_{y1}^B & C\eta_{y2}^B & 1 - S_2^2 & S_1S_2 \end{vmatrix}, \tag{C14a}$$

$$\tfrac{1}{2}DE_{z1}^t = E_x^i \begin{vmatrix} \pi_{y2}^B & 0 & -1 \\ -C\eta_{x2}^B & S_1S_2 & 1 - S_1^2 \\ C\eta_{y2}^B & 1 - S_2^2 & S_1S_2 \end{vmatrix} - E_y^i \begin{vmatrix} \pi_{x2}^B & -1 & 0 \\ -C\eta_{x2}^B & S_1S_2 & 1 - S_1^2 \\ C\eta_{y2}^B & 1 - S_2^2 & S_1S_2 \end{vmatrix}, \tag{C14b}$$

$$\tfrac{1}{2}DE_{z2}^t = -E_x^i \begin{vmatrix} \pi_{y1}^B & 0 & -1 \\ -C\eta_{x1}^B & S_1S_2 & 1 - S_1^2 \\ C\eta_{y1}^B & 1 - S_2^2 & S_1S_2 \end{vmatrix} + E_y^i \begin{vmatrix} \pi_{x1}^B & -1 & 0 \\ -C\eta_{x1}^B & S_1S_2 & 1 - S_1^2 \\ C\eta_{y1}^B & 1 - S_2^2 & S_1S_2 \end{vmatrix}. \tag{C14c}$$

The values of E_x^r and E_y^r may be found by substituting Eqs. (C14) into Eqs. (C13a) and (C13b).

By assuming in Fig. 1 that the plane of incidence (plane of paper) is the x–z plane, with the y axis normal to the plane of the paper, one may distinguish between two cases.

Case I: Perpendicular polarization:

$$E_x^i = 0; \qquad E_y^i \neq 0.$$

Case II: Parallel polarization:

$$E_x^i \neq 0; \qquad E_y^i = 0.$$

However, for a general gyrotropic medium in medium B, the reflected wave will have both perpendicular and parallel polarizations for each one of the cases above.

APPENDIX D: GYROTROPIC MEDIUM–FREE SPACE

In the following analysis we will consider a characteristic electromagnetic wave in a gyrotropic plasma medium, obliquely incident on a plane boundary of free space. We will assume in Fig. 1 that medium A is a general gyrotropic plasma medium and that medium B is free space ($X_B = 0$). Let us represent each component of the field of the incident wave in the gyrotropic medium by

$$F_i = F^i \exp [-ik(S_1x + S_2y + q^A z)] \quad \text{(D1)}$$

where F^i is a constant. One could take $q^A = q_1^A$ or $q^A = q_2^A$ where both are "upgoing" waves in the positive z direction as defined by Eq. (11a).

In general there will be two characteristic reflected waves in the lower medium A, and their field components are given by

$$F_{r3} = F_3^r \exp [-ik(S_1x + S_2y + q_3^A z)], \quad \text{(D2a)}$$

$$F_{r4} = F_4^r \exp [-ik(S_1x + S_2y + q_4^A z)], \quad \text{(D2b)}$$

where F_3^r and F_4^r are constants. q_3^A and q_4^A will represent the two "downgoing" waves in the negative z direction in accordance with the definition in Eq. (11b). All four q^A are solutions of the Booker quartic equation in medium A.

The transmitted wave into free space (medium B) will be given by

$$F_t = F^t \exp [-ik(S_1x + S_2y + Cz)]. \quad \text{(D3)}$$

The direction of the transmitted wave θ_t in free space is given in accordance to Snell's law[2] by

$$S_1^2 + S_2^2 = \sin \theta_t = n_A \sin \theta_i, \quad \text{(D4)}$$

where θ_i is the angle of incidence of the characteristic wave in medium A.

Applying the boundary conditions at $z = 0$ in Eqs. (14), one obtains from Eqs. (D1), (D2), and (D3), after canceling the common factor $\exp [-i(S_1x + S_2y)]$:

$$E_{x3}^r + E_{x4}^r + E_x^i = E_x^t, \quad \text{(D5a)}$$

$$E_{y3}^r + E_{y4}^r + E_y^i = E_y^t, \quad \text{(D5b)}$$

$$H_{x3}^r + H_{x4}^r + H_x^i = H_x^t, \quad \text{(D5c)}$$

$$H_{y3}^r + H_{y4}^r + H_y^i = H_y^t, \quad \text{(D5d)}$$

where E^i, H^i could be for either one of the 1, 2 characteristic "upgoing" waves in medium A. E^t, H^t will represent a plane wave in free space (medium B) with relationships similar to Eqs. (C8), (C9), and (C10).

Substituting Eqs. (13) and identities similar to Eqs. (C10) for the transmitted wave, one obtains after rearranging

$$\pi_{x3}^A E_{z3}^r + \pi_{x4}^A E_{z4}^r - E_x^t = -\pi_x^A E_z^i, \quad \text{(D6a)}$$

$$\pi_{y3}^A E_{z3}^r + \pi_{y4}^A E_{z4}^r - E_y^t = -\pi_y^A E_z^i, \quad \text{(D6b)}$$

$$C\eta_{x3}^A E_{z3}^r + C\eta_{x4}^A E_{z4}^r + S_1S_2E_x^t + (1 - S_1^2)E_y^t = -C\eta_x^A E_z^i, \quad \text{(D6c)}$$

$$C\eta_{y3}^A E_{z3}^r + C\eta_{y4}^A E_{z4}^r - (1 - S_2^2)E_x^t - S_1S_2E_y^t = -C\eta_y^A E_z^i, \quad \text{(D6d)}$$

where the terms on the right-hand side could be used with subscripts 1 or 2, depending on the characteristic wave which is incident on the boundary.

Equations (D6) are four inhomogeneous linear equations with four unknowns. Once E_z^i of the incident characteristic wave has been given (i.e., E_{z1}^i or E_{z2}^i), one is able to find the four unknowns, E_{z3}^r, E_{z4}^r, E_x^t, E_y^t, by using determinants. In general, the transmitted wave will not possess the same polarization properties as the incident wave but will still be linearly polarized.

APPENDIX E: GYROTROPIC MEDIUM–PERFECT CONDUCTOR

In the following analysis we will consider a characteristic electromagnetic wave in a gyrotropic plasma medium, incident on a perfectly conducting plane boundary. We will assume in Fig. 1 that medium A is a gyrotropic plasma medium and medium B is a perfect conductor. Let us represent each component of the field of the incident wave and of the reflected waves as in the corresponding equations (D1) and (D2).

The corresponding boundary conditions at $z = 0$ for the perfect conductor plane boundary may be given by

$$E_x^i + E_{x3}^r + E_{x4}^r = 0, \quad \text{(E1a)}$$

$$E_y^i + E_{y3}^r + E_{y4}^r = 0. \quad \text{(E1b)}$$

Substituting Eqs. (13) into Eqs. (E1) and rearranging, one obtains

$$\pi_{x3}^A E_{z3}^r + \pi_{x4}^A E_{z4}^r = -\pi_x^A E_z^i, \quad \text{(E2a)}$$

$$\pi_{y3}^A E_{z3}^r + \pi_{y4}^A E_{z4}^r = -\pi_y^A E_z^i, \quad \text{(E2b)}$$

where E_z^i may denote E_{z1}^i with the corresponding $q^A = q_1^A$ for one "upgoing" characteristic wave, or it may denote E_{z2}^i with the corresponding $q^A = q_2^A$ for the other "upgoing" characteristic wave.

Equations (E2) may be solved by determinants to give the corresponding reflection coefficients as follows:

$${}_1R_3 = \frac{E_{z3}^r}{E_{z1}^i} = \frac{\pi_{y1}^A\pi_{x4}^A - \pi_{x1}^A\pi_{y4}^A}{\pi_{x3}^A\pi_{y4}^A - \pi_{y3}^A\pi_{x4}^A}, \quad \text{(E3a)}$$

$${}_1R_4 = \frac{E_{z4}^r}{E_{z1}^i} = \frac{\pi_{x1}^A\pi_{y3}^A - \pi_{y1}^A\pi_{x3}^A}{\pi_{x3}^A\pi_{y4}^A - \pi_{y3}^A\pi_{x4}^A}, \quad \text{(E3b)}$$

$${}_2R_3 = \frac{E_{z3}^r}{E_{z2}^i} = \frac{\pi_{y2}^A\pi_{x4}^A - \pi_{x2}^A\pi_{y4}^A}{\pi_{x3}^A\pi_{y4}^A - \pi_{y3}^A\pi_{x4}^A}, \quad \text{(E3c)}$$

$${}_2R_4 = \frac{E_{z4}^r}{E_{z2}^i} = \frac{\pi_{x2}^A\pi_{y3}^A - \pi_{y2}^A\pi_{x3}^A}{\pi_{x3}^A\pi_{y4}^A - \pi_{y3}^A\pi_{x4}^A}. \quad \text{(E3d)}$$

Once the reflection coefficients have been found, the total fields may be calculated.

On the Unitary Representations of the Galilei Group. II. Two-Particle Systems*

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Mackey's theory is used to study the kinematics of a nonrelativistic two-particle system. We consider the helicity coupling and the l–S coupling and derive a Jacob–Wick's formula relating these two couplings (Glebsch–Gordan coefficients).

INTRODUCTION

IN a previous article,[1] we have constructed the unitary irreducible representations of those central extensions G_M of the Galilei group G which give the unitary projective irreducible representations of G.[2] We have used the method of Mackey.[3] We have also obtained by the limiting process $M \to 0$ the irreducible representations named class II by Inönü and Wigner.[4,5]

In the present work, we study the nonrelativistic kinematics of a two-particle system. We will be concerned mainly with the case of nonzero total mass. The case $M + M' = 0$ will be only sketched. The method used to reduce the projective representation of the Galilei group corresponding to the system is again a method given by Mackey. This method has been recently applied to the Poincaré group by Moussa and Stora[6] in a very elegant and useful manner.

Systems of two nonrelativistic particles have been previously studied by Levy–Leblond in the framework of group theory.[7] The case considered corresponds to the $l - S$ coupling and the method is the one applied by Wightman to the Poincaré group.[8] Levy–Leblond's procedure is very satisfactory from the physical point of view. It seems to us, however, that the more abstract method of Mackey gives a profound insight into the structure of the problem and that the equivalence of the different physical schemes (helicity, spin, ···) becomes transparent in this frame. From this point of view, our work may be considered as a useful complement to the one of Levy–Leblond. Further, we have studied the helicity coupling and its relation to the l–S coupling (nonrelativistic Jacob–Wick's formula[9]) which have not been considered by Levy–Leblond.

The order of the material is as follows. In Secs. I and II, we define a representation of $G_{M+M'}$ from two given representations $[M \mid U_0, j]$, $[M' \mid U'_0, j']$ corresponding to G_M, $G_{M'}$ respectively. Sections III to VI are devoted to the reduction of this representation of $G_{M+M'}$; the method consists in giving some structure to the arguments of the functions forming the representation space. This structure is obtained successively from the double coset method (Sec. III), the covariance property (Sec. IV), and a Fourier factorization (Sec. V). In Sec. VI, we calculate the Clebsch–Gordan coefficients between the l–S and helicity couplings.

I. REPRESENTATION OF $G_M \otimes G_{M'}$

We consider the two groups G_M and $G_{M'}$. We also consider the closed subgroups $K = T \times \mathcal{O}_0$ of G_M and $K' = T \times \mathcal{O}_0$ of $G_{M'}$ together with the unitary irreductible representations $L(K)$, $L'(K')$ acting in the Hilbert spaces $\mathfrak{K}(L)$ and $\mathfrak{K}(L')$. We restrict ourselves to little groups of first kind corresponding to the characters $(1, E_0, \mathbf{p}_0)$ and $(1, E'_0, \mathbf{p}_0)$.

We construct the following induced representation of $G_M \otimes G_{M'}$.

1. Representation Space

Let f be a function from $G_M \otimes G_{M'}$ into $\mathfrak{K}(L) \otimes \mathfrak{K}(L')$, covariant along left cosets of $G_M \otimes G_{M'}$

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[4] E. Inönü and E. P. Wigner, Nuovo Cimento 9, 705 (1952).

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mod $(K \otimes K')$ according to the law (invariance property)

$$f(gk, g'k') = f(g, g')L^*(k)L'^*(k'), \tag{1}$$

where

$$g = \{\exp i\theta, a, \Gamma\}_M \in G_M,$$
$$g' = \{\exp i\theta', a', \Gamma'\}_{M'} \in G_{M'},$$
$$k \in K, \quad k' \in K', \quad f \in \mathfrak{C}(L) \otimes \mathfrak{C}(L').$$

By definition, two elements (g_1, g_1') and (g_2, g_2') are in the same left coset of $G_M \otimes G_{M'}$ mod $K \otimes K'$ if and only if[10]

$$g_1 \tilde{K} g_2 \quad \text{and} \quad g_1' \tilde{K}' g_2',$$

and thus

$$g_2^{-1} g_1 \in K \quad \text{and} \quad g_2'^{-1} g_1' \in K'.$$

As in Part I, we pick a suitable representative $(\Gamma_p, \Gamma_{p'})$ in each coset and consider the corresponding restriction $\varphi(p, p')$ of f to these points. We take as left invariant measure the product

$$d\Omega_{V_0}(p)\, d\Omega_{V_0'}(p'), \tag{2}$$

where $d\Omega_{V_0}(p)[d\Omega_{V_0'}(p')]$ is given by Part I, Eq. (17) [(2) is independent of the representatives, which is an essential property when the equivalence of representations is considered]. We further suppose that the set of functions $\phi(p, p')$ forms a Hilbert space with respect to the scalar product

$$\langle \varphi_2 \mid \phi_1 \rangle = \int d\Omega_{V_0}(p)\, d\Omega_{V_0'}(p') \varphi_2^\dagger(p, p') \varphi_1(p, p'). \tag{3}$$

The Hilbert space so constructed will be our representation space $\mathfrak{C}(G_M \otimes G_{M'})$.

2. Definition of the Representation

Now, in the Hilbert space $\mathfrak{C}(G_M \otimes G_{M'})$ we define a representation of $G_M \otimes G_{M'}$ by requiring that

$$[U(g, g')f](\Gamma_p, \Gamma_{p'}) = f(g^{-1}\Gamma_p, g'^{-1}\Gamma_{p'}). \tag{4}$$

The second member of (4) is to be transformed by means of (1) and expressed in terms of the restricted function φ.

II. REPRESENTATION OF $G_{M+M'}$

What we are interested in is not a representation of $G_M \otimes G_{M'}$ but a representation of groups of the kind $G_{M''}$ with some M''. However, the representation (4) will give us such a representation if we can find a subgroup of $G_M \otimes G_{M'}$ which is isomorphic to some $G_{M''}$.

Let us then consider the following subgroup of $G_M \otimes G_M$,

$$[(\exp i\theta, a, \Gamma)_M, (\exp i\theta', a, \Gamma)_{M'}]. \tag{5}$$

As it can be shown, this subgroup is isomorphic to $G_{M+M'}$ in the following one-to-one correspondence (the freedom left in θ, θ' is meaningless)[11]

$$[(\exp i\theta, a, \Gamma)_M, (\exp i\theta', a, \Gamma)_{M'}]$$
$$\Leftrightarrow [\exp i(\theta + \theta'), a, \Gamma]_{M+M'}, \tag{6}$$

As a result, if we reduce the representation (4) to the subgroup (5) we will obtain a representation of G_{M+M}, given by

$$\{U[(\exp i\theta, a, \Gamma)_M, (\exp i\theta', a, \Gamma)_{M'}]f\}(\Gamma_p, \Gamma_{p'})$$
$$= f[(\exp i\theta, a, \Gamma)_M^{-1}\Gamma_p; (\exp i\theta', a, \Gamma)_{M'}^{-1}\Gamma_{p'}] \tag{7}$$

together with the scalar product (3) and the invariance property (1). Now from this invariance and with the notations of Part I.

$$\{U[(\exp i\theta, a, \Gamma)_M, (\exp i\theta', a, \Gamma)_{M'}]f\}(\Gamma_p, \Gamma_{p'})$$
$$= \langle \exp i\theta, a \mid 1p\rangle\langle \exp i\theta', a \mid 1p'\rangle$$
$$\times D^j(\Gamma_p^{-1}\Gamma\Gamma_t)D^{j'}(\Gamma_{p'}^{-1}\Gamma\Gamma_{t'})f(\Gamma_t, \Gamma_{t'})$$
$$= \langle \exp i(\theta + \theta'), a \mid 1, p + p'\rangle$$
$$\times D^j(\Gamma_p^{-1}\Gamma\Gamma_t)D^{j'}(\Gamma_{p'}^{-1}\Gamma\Gamma_{t'})f(\Gamma_t, \Gamma_{t'}), \tag{8}$$

where j, j' refer to the respective representations of the little group R corresponding to L and L' and $t = \Gamma^{-1}p$, $t' = \Gamma^{-1}p'$.

We are going to reduce the representation (8) of $G_{M+M'}$. The idea of the method is the following. The main feature of the representations (4) and (8) is to deal with functions which are restrictions of the f's to the chosen representatives $(\Gamma_p, \Gamma_{p'})$ of the cosets. However, in (4) and (8), these representatives are "direct data" i.e., they are given without any structure. Accordingly, the representations (4) and (8) are given as a whole and do not give immediately their composition. What we are going to do is to build up representatives of the left cosets from simpler elements. The functions $f(\Gamma_p, \Gamma_{p'})$ will then be constructed from certain functions defined on the "simplest" factor of $(\Gamma_p, \Gamma_{p'})$ and giving an irreducible representation space of $G_{M+M'}$.

The starting point is to consider the representation (8) as the representation

[10] The notation $g_1 \sim g\tilde{K}_2$ means that g_1 and g_2 are in the same left coset of G_M mod K.

[11] We thus see that the mass is conserved in nonrelativistic two-particle systems. This is to be related to Bargmann's selection rule.

$$\{U[(\exp i\theta, a, \Gamma)_M; (\exp i\theta', a, \Gamma)_{M'}]f\}(g, g')$$
$$= f[(\exp i\theta, a, \Gamma)_M^{-1}g, (\exp i\theta', a, \Gamma)_{M'}^{-1}g'] \quad (7')$$
$$[(g, g') \text{ is any element of } G_M \otimes G_{M'}],$$

where full use has been made of the invariance property (I). This corresponds to the way in which any induced representation is built.

The reduction will proceed in three steps (Secs. III, IV, V).

III. REDUCTION: FIRST STEP—THE DOUBLE COSETS

Let us consider in $G_M \otimes G_{M'}$ the so-called double cosets of $G_M \otimes G_{M'}$ mod $K \otimes K'$ on the left, $G_{M+M'}$ on the right.[12]

1. Labeling of the Double Cosets

Let us first look at double cosets of $G_M \otimes G_{M'}$ where translations have been eliminated. The reason why we proceed in this way lies in the total freedom left in the translation part of the elements belonging to K or K' and hence in the fact that belonging to a double coset restricts nothing but the homogeneous part of the arguments. Accordingly, we will write Γ instead of $(1, 0, \Gamma)$. We will also use the general notation Λ_p for any $\Gamma \in G_M$ transforming the character p_0 into p and $\Lambda_{p'}$ for any $\Gamma \in G_{M'}$ transforming p_0' into p'.

Now, two homogeneous elements $(\Lambda_{p_1}, \Lambda_{p_1'})$ and $(\Lambda_{p_2}, \Lambda_{p_2'})$ belong to the same coset $G_M \otimes G_{M'}$ mod $G_{M+M'}$, $K \otimes K'$ if and only if there exist an homogeneous $\gamma \in G_{M+M'}$, an element $r_M \in \mathcal{P}_0$ and an element $r'_{M'} \in \mathcal{P}_0$ such that

$$\gamma^{-1}(\Lambda_{p_1}, \Lambda_{p_1'})(r, r') = (\Lambda_{p_2}, \Lambda_{p_2'})$$

and thus

$$(\Lambda_{p_1}, \Lambda_{p_1'})(r, r')(\Lambda_{p_2}, \Lambda_{p_2'})^{-1} = (\Lambda, \Lambda) = \gamma$$

or

$$(\Lambda_{p_1} r \Lambda_{p_2}^{-1}, \Lambda_{p_1'} r' \Lambda_{p_2'}^{-1}) = (\Lambda, \Lambda). \quad (9)$$

This implies that we may go from p_2 to p_1 and from p_2' to p_1' by the same homogeneous transformation Λ. We thus have ($q_0 = 1$)

$$\begin{bmatrix} E_1 \\ \mathbf{p}_1 \end{bmatrix} = \begin{bmatrix} E_2 - \mathbf{p}_2\cdot\mathbf{v} + \frac{1}{2}M\mathbf{v}^2 \\ R^{-1}(\mathbf{p}_2 - M\mathbf{v}) \end{bmatrix};$$
$$\begin{bmatrix} E_1' \\ \mathbf{p}_1' \end{bmatrix} = \begin{bmatrix} E_2' - \mathbf{p}_2'\cdot\mathbf{v} + \frac{1}{2}M'\mathbf{v}^2 \\ R^{-1}(\mathbf{p}_2' - M'\mathbf{v}) \end{bmatrix}, \quad (10)$$

and thus

$$\begin{bmatrix} E_1 + E_1' \\ \mathbf{p}_1 + \mathbf{p}_1' \end{bmatrix} = \begin{bmatrix} E_2 + E_2' - (\mathbf{p}_2 + \mathbf{p}_2')\cdot\mathbf{v} + \frac{1}{2}(M + M')\mathbf{v}^2 \\ R^{-1}[(\mathbf{p}_2 + \mathbf{p}_2') - (M + M')\mathbf{v}] \end{bmatrix}. \quad (10')$$

Hence, if $(\Lambda p_1, \Lambda p_1')$ and $(\Lambda p_2, \Lambda p_2')$ are in the same double coset,

$$U = E_1 + E_1' - \frac{(\mathbf{p}_1 + \mathbf{p}_1')^2}{2(M + M')} = E_2 + E_2' - \frac{(\mathbf{p}_2 + \mathbf{p}_2')^2}{2(M + M')}. \quad (11)$$

We have also from the definition of our functions f

$$E_1 - \mathbf{p}_1/2M = E_2 - \mathbf{p}_2/2M \quad (12a)$$
$$E_1' - \mathbf{p}_1'/2M' = E_2 - \mathbf{p}_2'/2M'. \quad (12b)$$

If these conditions are also sufficient, this will allow us to label the double cosets by the values of the invariant

$$E_1 + E_1' - (\mathbf{p}_1 + \mathbf{p}_1')^2/2(M + M'), \quad (13)$$

which varies from E_0 to E_0' to ∞.

As a matter of fact, (11) [together with (12a, b) which hold by definition] implies the existence of a transformation Λ transforming both p_2 into p_1 and p_2' into p_1' (Λ is not unique). The general form of Λ is

$$\Lambda_{p_1} r \Lambda_{p_2}^{-1} = \Lambda_{p_1'} r' \Lambda_{p_2'}, \quad (14)$$

for such transformations are the most general ones leading from p_2 to p_1 and p_2' to p_1'.

2. Invariance of the Double Cosets

Let us consider arguments g, g' of the form

$$g = \Lambda\Lambda_{p^0} r, \qquad g' = \Lambda\Lambda_{p'^0} r',$$

where

$$\Lambda = (\Lambda, \Lambda) \in G_{M+M'}, \qquad r \in \mathcal{P}_0, \qquad r' \in \mathcal{P}_0$$

and where Λ_{p^0}, $\Lambda_{p'^0}$ are fixed in G_M, $G_{M'}$, respectively. (g, g') is the most general element of the double coset to which $(\Lambda_{p^0}, \Lambda_{p'^0})$ belongs. Now, such an element (g, g') retains its form under the action of $G_{M+M'}$ on the left. For, if $\gamma = (\gamma, \gamma) \in G_{M+M'}$,

$$\gamma(g, g') = [\gamma\Lambda\Lambda_{p^0} r, \gamma\Lambda\Lambda_{p'^0} r'] = [\lambda\Lambda_{p^0} r, \lambda\Lambda_{p'^0} r'], \quad (15)$$

where $\lambda = \gamma\Lambda \in G_{M+M'}$ (group property). Hence $\gamma(g, g')$ still belongs to the same double coset.

[12] A double coset of G mod T of the left, V on the right is defined as follows: g_1 and g_2 belonging to G are in the same double coset if there exists an element t in T and an element v in V such that $v^{-1}g_1 t = g_2$.

3. First Reduction of the Functions f

From our actual point of view, the first feature of (8) lies in the identity (7′) which relates the value of $U(\gamma)f$ at the point (g, g') to the value of f at the point $(\gamma^{-1}g, \gamma^{-1}g')$. Now, because of the invariance of the double cosets under $G_{M+M'}$, (g, g') and $(\gamma^{-1}g, \gamma^{-1}g')$ are in the same double coset. Hence $[U(\gamma)f](g, g')$ will be completely determined if we know the restriction of f to the double coset of (g, g').

This result leads us to consider the functions f as direct integrals over U of their respective restrictions f_V to the double cosets and on the other hand, to consider (7′) as identical to the set of restricted representations we get in that way. Let us point out that as the labeling parameter is nothing but the total internal energy, it will appear that the reduced representations are equivalent.

IV. REDUCTION: SECOND STEP—THE COVARIANCE PROPERTY

Let us now take into account the second feature of (7′) namely its "maximal" simplicity with respect to the covariance property.

1. The (r, r') Covariance

We consider a particular double coset. Let $(\Lambda_{p^x}, \Lambda_{p'^x})$ be its representative. The corresponding reduced space is built up with functions which are equal to zero everywhere except at the points $(\gamma\Lambda_{p^x}r, \gamma\Lambda_{p'^x}r')$. Let us point out that the value of $U_\epsilon f(\epsilon \in G_{M+M'})$ at the point above can be expressed in terms of f at the point

$$(\epsilon^{-1}\gamma\Lambda_{p^x}r, \epsilon^{-1}\gamma\Lambda_{p'^x}r')$$

having the same (r, r') component. It then results that the points of a double coset which have the same (r, r') component provide a new invariant subspace. But because of the invariance property (1) these finer representations corresponding to different (r, r') are all equivalent. We thus limit ourselves to considering the standard type which evidently corresponds to the choice $r = r' = 1$. This step leaves us with the following restriction of the functions f:

$$f^x(\gamma) = f(\gamma\Lambda_{p^x}1, \gamma\Lambda_{p'^x}1) \tag{16}$$

and hence with functions defined in $G_{M+M'}$ (but depending in their form on $V^x \Leftrightarrow (p^x, p'^x)$]. With these notations, we have reduced the identity (7′) to the set of following identities

$$(U_\epsilon f^x)(\gamma) = f^x(\epsilon^{-1}\gamma), \tag{17}$$

where $\epsilon, \gamma \in G_{M+M'}$ and (p^x, p'^x) labels the double cosets.

2. The $(\mathcal{P}_{p^x}, \mathcal{P}_{p'^x})$ Covariance

A. A Further Reduction

The representation (17) is not yet the representation (8) because some covariance is still left. For consider

$$f^x(\gamma\cdot\epsilon) = f(\gamma\Lambda_{p^x}\Lambda_{p^x}^{-1}\epsilon\Lambda_{p^x}, \gamma\Lambda_{p'^x}\Lambda_{p'^x}^{-1}\epsilon\Lambda_{p'^x})$$

where $\gamma, \epsilon \in G_{M+M'}$.

If

$$\Lambda_{p^x}^{-1}\epsilon\Lambda_{p^x} \in \mathcal{P}_0 \quad \text{and} \quad \Lambda_{p'^x}^{-1}\epsilon\Lambda_{p'^x} \in \mathcal{P}_0 \tag{18}$$

then the following covariance property still holds

$$\begin{aligned} f^x(\gamma\epsilon) &= f(\gamma\Lambda_{p^x}, \gamma'\Lambda_{p'^x})L^*(\Lambda_{p^x}^{-1}\epsilon\Lambda_{p^x})L'^*(\Lambda_{p'^x}^{-1}\epsilon\Lambda_{p'^x}) \\ &= f^x(\gamma)L^*(\Lambda_{p^x}^{-1}\epsilon^{-1}\Lambda_{p^x})L'^*(\Lambda_{p'^x}^{-1}\epsilon\Lambda_{p'^x}). \end{aligned} \tag{19}$$

Now, what is the translation of (18) in terms of the elements of $G_{M+M'}$? Using the relation [Part I, Eq. (10)] we can prove the following *theorem*: The element (ϵ, ϵ) belongs to $(\mathcal{P}_{p^x}, \mathcal{P}_{p'^x})$ if and only if ϵ, as an element of $G_{M+M'}$, belongs to $\mathcal{P}_{p^x}$ and is such that its rotation part belongs to $\mathcal{P}_{q^x}$, where

$$P^x = p^x + p'^x, \tag{20}$$

$$q^x = (M'p^x - Mp'^x)/(M + M'). \tag{21}$$

Such elements ϵ form a subgroup of $\mathcal{P}_{p^x}$.

For later use let us point out that in the case where either $\mathbf{P}^x = 0$ or $\mathbf{P}^x$ is parallel to $\mathbf{p}^x$ (and hence to $\mathbf{p}'^x$), this latter subgroup is

$$\mathcal{P}_{p^x} \cap \mathcal{P}_{q^x}.$$

As a result of (19), we may proceed to a further restriction of (7′). For consider the left cosets of the subgroup of $G_{M+M'}$ which is isomorphic to $(\mathcal{P}_{p^x}, \mathcal{P}_{p'^x})$ and pick a representative in each such coset. Because of the invariance property (19) the values of the functions f^x at these points transform among themselves under $G_{M+M'}$. Hence we get an invariant subspace and correspondingly a subrepresentation of (17). All such representations are obviously equivalent and according to our program, we limit ourselves to one of them.

B. The Variables P and q

Let us characterize the domain of the functions forming the corresponding representation space. We have the following theorem if $\mathbf{p}^x + \mathbf{p}'^x = 0$.

Theorem: The left cosets of $G_{M+M'}$ mod $\mathbf{P}_{p^x} \cap \mathbf{P}_{q^x}$ are labeled by two quantities P and q which are

to be interpreted as the total momentum and the relative momentum respectively.

Proof: First of all we remark that these left cosets may be labeled by the two variables P and P_-, where P is any character in the orbit of P^x in $G_{M+M'}$, and P_- is any character in the orbit of q^x in the same group. Unlike the case of Poincaré theory, the quantity P_- may not be interpreted generally as the relative momentum of the system. To make this point clear, we first note that since $\mathcal{O}_{P^x} \cap \mathcal{O}_{q^x}$ is isomorphic to $(\mathcal{O}_{p^x}, \mathcal{O}_{p'^x})$, the left cosets may as well be labeled by the quantities (p, p') where $p(p')$ is any character of the orbit of $p^x(p'^x)$ in $G_M(G_{M'})$. As a result, they may also be characterized by the variables

$$P = p + p',$$
$$q = (M'p - Mp')/(M + M').$$

It is q which is the relative momentum. Now, it happens that the values of q and P_- corresponding to the same left coset are generally different unlike the case of Poincaré group. The reason why lies in the fact that we have to work here with three groups G_M, $G_{M'}$, $G_{M+M'}$ instead of one as in relativistic theory. As we are going to see, the relations between P_- and q is given by

$$P_- = q + (P - P^x). \tag{22}$$

However, in the physically important case where $\mathbf{P} = \mathbf{P}^x = 0$, $P_- = q$ and can be interpreted as a relative momentum. We are going to prove these statements, while determining the respective domains of the variables P, P_-, and q.

The *domain* of P consists of all the values P compatible with the condition $[P = (1, E_+, \mathbf{p})]$

$$E_+ - (\mathbf{P})^2/2(M + M') = E^x + E'^x. \tag{23}$$

This domain is generated by the values p, p' such that (if $\mathbf{P}^x = 0$)

$$E - \mathbf{p}^2/2M = E^x - \mathbf{p}^{x2}/2M = U_0$$
$$E' - \frac{\mathbf{p}^2}{2M} = E'^x - \frac{\mathbf{p}'^{x2}}{2M'} = U_0'$$
$$E + E' - \frac{(\mathbf{p} + \mathbf{p}')^2}{2(M + M')} = E^x + E'^x = U^x$$

according to the formula $P = p + p'$.

As for the domain of P_- when P is fixed, we note that it is generated by applying to q^x the transformations of the type $\Gamma_P\Omega$, where Γ_P is a particular transformation leading from P^x to P; for example

$$\Gamma_P = (\mathbf{P}/(M + M)', 1). \tag{24}$$

Ω is any transformation $\epsilon\mathcal{O}_{P^x} = SU_2$. Hence there is a one-to-one correspondence between the values of P_- for P fixed and the points on a sphere. The value of P_- corresponding to the choice (24) of Γ_P and to $\Omega = R$ is from Part I, Eq. (8′),

$$P_- = \Gamma_P R q^x$$
$$= \left(E_-^x + \frac{R\mathbf{q}\cdot\mathbf{P}}{M + M'} + \frac{1}{2}\frac{\mathbf{P}^2}{M + M'}\,; Rq^x + \mathbf{P}\right). \tag{25}$$

Now, applying $\Gamma_P R$ to p^x and p'^x successively, we see that

$$q = \left(\frac{M'E^x - ME'^x}{M + M'} + \frac{R\mathbf{q}^x\cdot\mathbf{P}}{M + M'}\,, Rq^x\right). \tag{26}$$

Since $P^x = (E_+^x, 0)$, (25) and (26) give immediately the relation (22) and the stated result concerning the case $\mathbf{P}^x = \mathbf{P} = 0$.

We now prove that $\mathbf{q}^2$ is a constant. We have indeed

$$\mathbf{q}^2 = (R\mathbf{q}^x)^2 = \mathbf{q}^{x2}$$

and as

$$\mathbf{q}^x = (M'\mathbf{p}^x - M\mathbf{p}'^x)/(M + M')$$

we have more precisely

$$(\mathbf{q}^x)^2 = [2MM'/(M + M')]\{U^x - U_0 - U_0'\}.$$

We also have from (26)

$$E_- = \frac{M'E - ME'}{M + M'} = \frac{M'E^x - ME'^x}{M + M'} + \frac{R\mathbf{q}'^x\cdot\mathbf{P}}{M + M'}.$$

Hence, taking into account the fact that $\mathbf{P}^x = 0$, we obtain after some calculation

$$E_- = \frac{M'U_0 - MU_0'}{M + M'} + \frac{M' - M}{2MM'}\mathbf{q}^2 + \frac{\mathbf{q}\cdot\mathbf{P}}{M + M'}. \tag{27}$$

E_- depends on nothing but $\mathbf{q}$ when P is fixed.

C. *New covariance Property*

The covariance law (19) takes now the form

$$f^x(\Gamma_{Pq}\varphi) = f(\Gamma_{Pq}\Lambda_{p^x}\Lambda_{p^x}^{-1}\varphi\Lambda_{p^x},\ \Gamma_{Pq}\Lambda_{p'^x}\Lambda_{p'^x}^{-1}\varphi\Lambda_{p'^x})$$
$$= D(\Lambda_{p^x}^{-1}\varphi^{-1}\Lambda_{p^x})D'(\Lambda_{p'^x}^{-1}\varphi^{-1}\Lambda_{p'^x})f^x(\Gamma_{Pq}), \tag{28}$$

where $\varphi \in \mathcal{O}_{P^x} \cap \mathcal{O}_{q^x}$ if $p^x = 0$. We replace the notation L by D since in the present homogeneous

case, L is reduced to the representation of the little group.

When we compute the representations of $G_{M+M'}$ we will have however to take the translations into account. We must then replace (28) by the following law:

$$f^{\varkappa}[(\exp i\theta, a, 1)\Gamma_{P_\varrho}\varphi] = \langle(\exp i\theta, a)^{-1} \mid 1P\rangle \times D(\Lambda_{p^\varkappa}^{-1}\varphi^{-1}\Lambda_{p^\varkappa})D'(\Lambda_{p'^\varkappa}^{-1}\varphi^{-1}\Lambda_{p'^\varkappa})f^{\varkappa}(\Gamma_{P_\varrho}). \quad (29)$$

3. Linear Representation of $G_{M+M'}$

Suppose we have made a suitable choice for the representatives Γ_{P_ϱ} in each left coset. Let us then consider the corresponding Hilbert space $\mathfrak{H}$. According to the definition (7'), we obtain in $\mathfrak{H}$ the following representation of $G_{M+M'}$

$$[U(\exp i\theta, a, \Gamma)f^{\varkappa}](\Gamma_{P_\varrho}) = f^{\varkappa}[(\exp i\theta, a, \Gamma)^{-1}\Gamma_{P_\varrho}]. \quad (30)$$

We now write

$$(\exp i\theta, a, \Gamma)^{-1}\Gamma_{P_\varrho} = (\exp i\theta', -\Gamma^{-1}a, 1)\Gamma_{P'_{\varrho'}}\Gamma_{P'_{\varrho'}}^{-1}\Gamma^{-1}\Gamma_{P_\varrho} \quad (31)$$

with

$$P' = \Gamma^{-1}P, \qquad q' = \Gamma^{-1}q = (M'\Gamma^{-1}p - M\Gamma^{-1}p')/(M + M').$$

The second member of (31) has the form of the argument of $f^{\varkappa}$ in (29) with

$$\varphi = \Gamma_{P'}^{-1}q'\Gamma^{-1}\Gamma_{P_\varrho}.$$

We also point out that

$$\langle(\exp i\theta', -\Gamma^{-1}a, 1)^{-1} \mid 1, \Gamma^{-1}P\rangle = \langle\exp i\theta, a \mid 1, P\rangle \quad (32)$$

Using (29), (30), (31) and (32) we then obtain for our present reduction of (7') the form

$$[U(\exp i\theta, a, \Gamma)f^{\varkappa}](\Gamma_{P_\varrho}) = \langle\exp i\theta, a \mid 1, P\rangle \times D(\Lambda_{p^\varkappa}^{-1}\Gamma_{P_\varrho}^{-1}\Gamma\Gamma_{P'_{\varrho'}}\Lambda_{p^\varkappa}) \times D'(\Lambda_{p'^\varkappa}^{-1}\Gamma_{P_\varrho}^{-1}\Gamma\Gamma_{P'_{\varrho'}}\Lambda_{p'^\varkappa})f^{\varkappa}(\Gamma_{P',\varrho'}) \quad (33)$$

where $(p^\varkappa, p'^\varkappa)$ labels the double cosets and

$$\Gamma_{P_\varrho}^{-1}\Gamma\Gamma_{P'_{\varrho'}} \in (\mathcal{P}_{p^\varkappa}, \mathcal{P}_{p'^\varkappa})$$

We recall that $(\mathcal{P}_{p^\varkappa}, \mathcal{P}_{p'^\varkappa}) \Leftrightarrow \mathcal{P}_{P^\varkappa} \cap \mathcal{P}_{q^\varkappa}$ if $P^\varkappa = 0$.

With the set (33) of the representations $(p^\varkappa, p'^\varkappa)$ the covariance property (1) has been completely taken into account. This set must then be equivalent to the representation (8).

V. REDUCTION: THIRD STEP—THE HELICITY COUPLING; THE l–S COUPLING

The reduction (33) leaves us with functions $f^{\varkappa}(\Gamma_{P_\varrho})$ which are equal to $f(\Gamma_{P_\varrho}\Lambda_{p^\varkappa}, \Gamma_{P_\varrho}\Lambda_{p'^\varkappa})$ and are of the form $f(\Lambda_p, \Lambda_{p'})$, where $\Lambda_p(\Lambda_{p'})$ is some representative of the left coset $p(p')$ of $G_M(G_{M'})$ mod $K(K')$.

Obtaining the representatives $\Lambda_p(\Lambda_{p'})$ from

$$\Gamma_{P_\varrho}\Lambda_{p^\varkappa}[\Gamma_{P_\varrho}\Lambda_{p'^\varkappa}]$$

we have now some structure for our former arguments in (8) and accordingly some reduction of (8). However the structure can be made finer as it appears from what follows. So far the representatives Γ_{P_ϱ}, the characters $p^\varkappa$, $p'^\varkappa$, the representatives $(\Lambda_{p^\varkappa}, \Lambda_{p'^\varkappa})$ of the double cosets are formal arguments. We are going to show that a suitable choice of these elements leads on the one hand to a further decomposition of (33) and on the other hand to the "helicity coupling" and the "l–S coupling," respectively. We proceed in four steps.

1. Little Group $\mathcal{P}_0$ and Condition on $p^\varkappa$, $p'^\varkappa$

First of all we take

$$(1, p_0) = (1, E_0, \mathbf{0}), \quad (1, p'_0) = (1, E'_0, \mathbf{0}) \quad (34)$$

and because of the equivalence of the representation labeled by U (double cosets) we limit ourselves to a particular double coset.

Now, we take $p^\varkappa$, $p'^\varkappa$ such that

$$\mathbf{P}^\varkappa = 0, \qquad \mathbf{q}^\varkappa = \mathbf{e}_3,$$

then

$$P^\varkappa = (1, E_+^\varkappa, 0), \qquad q^\varkappa = (1, E_-^\varkappa, \mathbf{e}_3), \quad (35)$$

and the double cosets are labeled by $E_+^\varkappa$ which will run from $E_0 + E'_0$ to ∞. Such a choice of $p^\varkappa$, $p'^\varkappa$ is made possible in any double coset by a suitable choice of the energies $E^\varkappa$, $E'^\varkappa$ of $p^\varkappa$, $p'^\varkappa$ respectively. Hence we are loosing no generality provided $M + M' \neq 0$.

An immediate result of (35) is that any transformation belonging to $R_{P^\varkappa} \cap R_{q^\varkappa}$ is a rotation around the third axis $\mathbf{e}_3$, and conversely.

2. Factorization of Γ_{P_ϱ}

It is possible to make for Γ_{P_ϱ} a very interesting choice. Indeed we may take an element of the form $\Gamma_P\Omega_q$, where Γ_P is independent of P. More precisely, let P, q be two quantities such that there exists an element $\Gamma \in G_{M+M'}$ having the following property

$$\Gamma P^\varkappa = P \quad (36)$$

$$\Gamma q^\varkappa = (M'\Gamma p - M\Gamma p')/(M + M') = q.$$

We associate with P a fixed element Γ_P {suitably chosen; we will take usually $\Gamma_P = [\mathbf{P}/(M + M'), 1]$} such that $\Gamma_P P^x = P$. Now let Ω_q be the element of the little group $\mathcal{P}_{Px}$ leading from q^x to $\Gamma_P^{-1} q$. We then take $\Gamma_{Pq} = \Gamma_P \Omega_q$. As a matter of fact, the kernel of the latter discussion lies in the isomorphism of our present little group to the rotation group.

The interest of this factorization is seen if we note that Ω_q being a rotation (it belongs to $\mathcal{P}_{Px}$), we may Fourier-analyze the functions $f^x(\Gamma_P \Omega_q)$ in terms of the relevant representations of $\mathcal{P}_{Px} = SU_2$, namely D^l. We write symbolically

$$f^x_{uu'}(\Gamma_P \Omega_q) = \tilde{f}^{l\mu'\mu}_{uu'}(\Gamma_P) D^{l*}_{\mu\mu'}(\Omega_q) N(U^x, j), \qquad (37)$$

where the normalization factor will be defined later (Sec. VI). $D^{l*}_{\mu\mu'}(\Omega_q) = D^l_{\mu'\mu}(\Omega_q^{-1})$. The functions $f^x_{uu'}$ depend intrinsically on our choice of Λ_{px}, $\Lambda_{p'x}$. The same is thus true for the functions $f^{l\mu'\mu}_{uu'}$. In particular according to the choice we make for the representatives, the null coefficients $f^{l\mu'\mu}_{uu'}$ will be found different. This will be illustrated in our application.

We expect that this development of $f^x_{uu'}$ leads to a new reduction of (7') where the reduced functions will be the functions $\tilde{f}^{l\mu'\mu}_{uu'}$ defined on the Λ_P. Let us show this property in the helicity scheme and in the l–S scheme successively.

3. The Helicity Coupling

In the present section and in the next one we are going to study two possibilities of reducing the last freedom left in (33), namely that one concerning the choice of Λ_{px}, $\Lambda_{p'x}$.

A. Helicity Amplitudes

The characteristic of the helicity formalism is to take Λ_{px}, $\Lambda_{p'x}$ in such a way that they commute with $\mathcal{P}_{px}$, $\mathcal{P}_{p'x}$, respectively. Then the arguments of the matrices D, D' appearing in (27), (36) belong to $\mathcal{P}_{Px} \cap \mathcal{P}_{qx}$ and are rotations around $\mathbf{e}_3 = \mathbf{q}^x$. Hence if we take the generator of the rotations around $\mathbf{e}_3$ among the basis variables we may write

$$D_{\sigma\lambda}(\varphi) = \exp i\varphi (M^j_3)_{\sigma\lambda}$$

and

$$D'_{\mu\nu}(\varphi) = \exp i\varphi (M^{j'}_3)_{\mu\nu},$$

where

$$\varphi \in \mathcal{P}_{Px} \cap \mathcal{P}_{qx}.$$

In the exponential, φ is used for the rotation angle corresponding to φ; j and j' designate the irreducible representations of SU_2 to which D and D' correspond, respectively; M^j_3 and $M^{j'}_3$ are the corresponding representatives of the generator $(M_3)_{0p}$. We have

$$M^j_3 = \begin{bmatrix} j & & \\ & \ddots & \\ & & -j \end{bmatrix} \qquad M^{j'}_3 = \begin{bmatrix} j' & & \\ & \ddots & \\ & & -j' \end{bmatrix}$$

and

$$D(\varphi) = D^j(\varphi) = \begin{bmatrix} \exp i\varphi j & & \\ & \ddots & \\ & & \exp(-i\varphi j) \end{bmatrix}$$

$$D'(\varphi) = D^{j'}(\varphi) = \begin{bmatrix} \exp i\varphi j' & & \\ & \ddots & \\ & & \exp(-i\varphi j') \end{bmatrix}$$

Hence if we take $\sigma, \lambda = (j, \cdots, -j)$ and $\mu, \nu = (j', \cdots, -j')$, we have

$$D^j_{\sigma\lambda}(\varphi) = (\exp i\varphi\sigma)\delta_{\sigma\lambda} \quad D^{j'}_{\mu\nu}(\varphi) = (\exp i\varphi\mu)\delta_{\mu\nu}. \qquad (38)$$

σ and μ are then projections of M_3 on the polarization axis $\mathbf{q}^x = \mathbf{e}_3$. Now, representatives Λ_{px}, $\Lambda_{p'x}$ satisfying the above condition are given for example by the pure Galilei transformations

$$\Gamma_{px} = (\mathbf{p}^x/M, 1) \qquad \Gamma_{p'x} = (\mathbf{p}'^x/M, 1) \qquad (39)$$

For as in the present case, $\mathbf{P}^x = 0$ and $\mathbf{q}^x = e_3$, $\mathbf{p}^x$ and $\mathbf{p}'^x$ must be parallel to $\mathbf{e}_3$. Hence they are kept invariant by the transformations of $\mathcal{P}_{Px} \cap \mathcal{P}_{qx}$. Now

$$p = (\Gamma_P \Omega_q \Gamma_{px})_M p_0, \qquad p' = (\Gamma_P \Omega_q \Gamma_{p'x})_{M'} p'_0$$

are such that

$$p + p' = P \quad \text{and} \quad (M'p - Mp')/(M + M') = q,$$

so that we may write

$$\theta_p = (\Gamma_P \Omega_q \Gamma_{px})_M, \qquad \theta_{p'} = (\Gamma_P \Omega_q \Gamma_{p'x})_{M'},$$

θ_p, $\theta_{p'}$ being two homogeneous transformations.

B. The Helicity Representation and its Reductions

Let us denote by ψ^x the wavefunctions f^x corresponding to the values (39) of Λ_{px}, $\Lambda_{p'x}$. For these wavefunctions, we have from (28) the following covariance property

$$\psi^x_{\sigma\sigma'}[(\exp i\theta, a, 1)\Gamma_{Pq}\varphi] = \langle (\exp i\theta, a, 1)^{-1} \mid 1P \rangle \times \exp[-i(\sigma + \sigma')\varphi] \psi^x_{\sigma\sigma'}(\Gamma_{Pq}). \qquad (40)$$

On the other hand, they constitute a Hilbert space where the group $G_{M+M'}$ is represented by ($P' = \Gamma^{-1}P$, $q' = \Gamma^{-1}q$):

$$[U(\exp i\theta, a, \Gamma)\psi^x]_{\sigma\sigma'}(\Gamma_{Pq}) = \langle \exp i\theta, a \mid 1, P\rangle \times \exp[i(\sigma+\sigma')\varphi]\psi^x_{\sigma\sigma'}(\Gamma_{P'q'}), \quad (41)$$

where φ is the angle corresponding to the rotations $\Gamma^{-1}_{Pq}\Gamma\Gamma_{P',q'}$ around $\mathbf{e}_3$.

We are going to reduce this representation by using the factorization $\Gamma_P\Omega_q$ of Γ_{Pq} according to (37).

First we have from (40) $\tilde{\psi}^{l\mu'\mu} = \tilde{\psi}^{l\mu'\mu}\delta_{\mu',\sigma+\sigma'}$. For if $\varphi \in \mathcal{P}_{P^x} \cap \mathcal{P}_{q^x}$, φ and $\Omega_q\varphi$ belong to $\mathcal{P}_{P^x}$ so that according to (37) and (38)

$$\psi^x_{\sigma\sigma'}(\Gamma_P\Omega_q\varphi) = \tilde{\psi}^{l\mu'\mu}_{\sigma\sigma'}(\Gamma_P)\exp(i\mu'\varphi)D^l_{\mu'\mu}(\Omega_q^{-1})N(U^x l).$$

On the other hand, from (40)

$$\psi^x_{\sigma\sigma'}(\Gamma_P\Omega_q\varphi) = \exp[-i(\sigma+\sigma')\varphi]\psi_{\sigma\sigma'}(\Gamma_P\Omega_q) = \tilde{\psi}^{l\mu'\mu}_{\sigma\sigma'}(\Gamma_P)\exp[-i(\sigma+\sigma')\varphi]D^l_{\mu'\mu}(\Omega_q^{-1})N(U^x, l). \quad (43)$$

Comparing (42) and (43), we obtain the stated result: μ' may be restricted to the value

$$\mu' = \sigma + \sigma'. \quad (44)$$

Since φ is an arbitrary rotation around $\mathbf{e}_3$. As a result, the invariance property (40) can be written

$$\psi^x_{\sigma\sigma'}[(\exp i\theta, a, 1)\Gamma_{Pq}\varphi] = \langle(\exp i\theta, a, 1)^{-1} \mid 1P\rangle \times \exp[-i(\sigma+\sigma')\varphi]\tilde{\psi}^{l\mu}_{\sigma\sigma'}(\Gamma_P)D^l_{\sigma+\sigma',\mu}(\Omega_q^{-1})N(U^x, l). \quad (45)$$

We now compute the representation (41). We show that

$$\{U[\exp i\theta, a, \Gamma]\psi^x\}_{\sigma\sigma'}(\Gamma_P\Omega_q) = [\tilde{U}(\exp i\theta, a, \Gamma)\tilde{\psi}]^{l\mu}_{\sigma\sigma'} \times (\Gamma_P)D^l_{\sigma+\sigma',\mu}(\Omega_q^{-1})N(U^x, l), \quad (46)$$

with $(P' = \Gamma^{-1}P)$,

$$\{\tilde{U}(\exp i\theta, a, \Gamma)\tilde{\psi}\}^{l\mu}_{\sigma\sigma'}(\Gamma_P) = \langle \exp i\theta, a \mid 1P\rangle D^l_{\mu\mu'}(\Gamma_P^{-1}\Gamma\Gamma_{P'})\tilde{\psi}^{l\mu'}_{\sigma\sigma'}(\Gamma_{P'}), \quad (47)$$

which is the standard form of irreducible representation for mass $(M + M')$ and spin l so that the reduction of (8) is completely performed with (46).

Let us prove (46) and (47).

According to (41) we have to analyze the quantities $\psi^x_{\sigma\sigma'}(\Gamma_{P'q'})$, where $P' = \Gamma^{-1}P$, $q' = \Gamma^{-1}q$. First of all we write

$$\Gamma_{P'q'} = \Gamma_{P'}\Omega_{q'} \quad (48)$$

and

$$\Gamma^{-1}_{Pq}\Gamma\Gamma_{P'q'} = \Omega_q^{-1}R\Omega_{q'} \quad (49)$$

with

$$A = \Gamma_P^{-1}\Gamma\Gamma_{P'} \in \mathcal{P}_{P^x}. \quad (50)$$

We will use also

$$\Omega_{q'}^{-1} = \Omega_{q'}^{-1}A^{-1}\Omega_q\Omega_q^{-1}A, \quad = \Gamma^{-1}_{P'q'}\Gamma^{-1}\Gamma_{Pq}\Omega_q^{-1}A. \quad (51)$$

Now, from (37), (38), (44), and φ being the angle introduced in (41), we obtain

$$\psi^x_{\sigma\sigma'}(\Gamma_{P'q'}) = \tilde{\psi}^{l\mu}_{\sigma\sigma'}(\Gamma_{P'})\exp[-i(\sigma+\sigma')\varphi] \times D^l_{\sigma+\sigma',\lambda}(\Omega_q^{-1})D^l_{\lambda\mu}(A)N(U^x, l).$$

Taking this latter formula into account in (41) leads to the stated result.

4. The *l*–S Coupling

A. Definition of the Amplitudes

The present representation is defined by the amplitudes

$$\Lambda_{p^x} = \Gamma_{p^x}\Omega_q^{-1}, \qquad \Lambda_{p'^x} = \Gamma_{p'^x}\Omega_q^{-1}, \quad (52)$$

where Ω_q belongs to $\mathcal{P}_{P^x}$ and hence to $\mathcal{P}_0$ since $\mathbf{p}_0 = \mathbf{P}^x = 0$.

B. Covariance Property and representation

The covariance property is here particularly simple since if we denote by $\phi^x(\Gamma_P\Omega_q)$ the corresponding wavefunctions, we have

$$\phi^x_{\tau\tau'}(\Gamma_P\Omega_q\varphi) = \phi^x_{\tau\tau'}(\Gamma_P\Omega_q). \quad (53)$$

Let us first note that

$$\phi^x_{\tau\tau'}(\Gamma_P\Omega_q) = D^j_{\tau\sigma}(\Omega_q)D^{j'}_{\tau'\sigma'}(\Omega_q)\psi^x_{\sigma\sigma'}(\Gamma_P\Omega_q), \quad (54)$$

which is the relation between the present representation and the former one;

$$\phi^x_{\tau\tau'}(\Gamma_P\Omega_q) = f_{\tau\tau'}(\Gamma_P\Omega_q\Gamma_{p^x}\Omega_q^{-1}, \Gamma_P\Omega_q\Gamma_{p'^x}\Omega_q^{-1}).$$

Now as $\mathbf{p}_0 = 0$, $\Omega_q \in \mathcal{P}_0$. Hence,

$$\phi^x_{\tau\tau'}(\Gamma_P\Omega_q) = f_{\sigma\sigma'}(\Gamma_P\Omega_q\Gamma_{p^x}, \Gamma_P\Omega_q\Gamma_{p'^x})\tilde{D}^j_{\sigma\tau}(\Omega_q)\tilde{D}^{j'}_{\sigma'\tau'}(\Omega_q) = D^j_{\tau\sigma}(\Omega_q)D^{j'}_{\tau'\sigma'}(\Omega_q)\psi^x_{\sigma\sigma'}(\Gamma_P\Omega_q).$$

Now, the property (53) is directly obtained from (54) and (40). The converse of (55) is

$$\psi^x_{\sigma\sigma'}(\Gamma_P\Omega_q) = D^j_{\sigma\tau}(\Omega_q^{-1})D^{j'}_{\sigma'\tau'}(\Omega_q^{-1})\phi^x_{\tau\tau'}(\Gamma_P\Omega_q). \quad (55)$$

As to the corresponding representation of $G_{M+M'}$, it is easily deduced from (33) by taking (52) into account.

C. First Reduction—Fourier Decomposition

We now apply the considerations of (V.2). According to (44) where we put $\sigma + \sigma' = 0$, we see

that the functions ϕ can be expanded as follows:

$$\phi^{x}_{\tau\tau'}(\Gamma_P\Omega_q) = \tilde{\phi}^{lm}_{\tau\tau'}(\Gamma_P)D^{l}_{0m}(\Omega_q^{-1})N(U^x, l). \quad (56)$$

We are going to determine the representation corresponding to the functions $\tilde{\phi}^{lm}$ from the one obtained with functions $\tilde{\psi}^{lm}$. From (55), (56), we have

$$[U(\exp i\theta, a, \Gamma)\psi^x]_{\sigma\sigma'}(\Gamma_P\Omega_q) = N(U^x, l)D^{j}_{\sigma\tau}(\Omega_q^{-1})D^{j'}_{\sigma'\tau'}(\Omega_q^{-1})D^{l}_{0m}(\Omega_q^{-1}) \times [\tilde{U}(\exp i\theta, a, \Gamma)\tilde{\phi}]^{lm}_{\tau\tau'}(\Gamma_P). \quad (57)$$

On the other hand,

$$[U(\exp i\theta, a, \Gamma)\psi^x]_{\sigma\sigma'}(\Gamma_P\Omega_q) = \langle \exp i\theta, a \mid 1, P\rangle \times D^{j}_{\sigma\tau}(\Omega_q^{-1}A\Omega_{q'})D^{j'}_{\sigma'\tau'}(\Omega_q^{-1}A\Omega_{q'})\psi^{x}_{\tau\tau'}(\Gamma_{P'}\Omega_{q'}).$$

Hence from (55)

$$[U(\exp i\theta, a, \Gamma)\psi^x]_{\sigma\sigma'}(\Gamma_P\Omega_q) = \langle \exp i\theta, a \mid 1, P\rangle D^{j}_{\sigma\tau}(\Omega_q^{-1})D^{j'}_{\sigma'\tau'}(\Omega_q^{-1})D^{j}_{\tau u}(A) \times D^{j'}_{\tau' u'}(A)D^{l}_{0m'}(\Omega_{q'}^{-1})\tilde{\phi}^{lm'}_{tt'}(\Gamma_{P'})N(U^x, l). \quad (58)$$

We thus obtain from (57) and (58)

$$D^{l}_{0m}(\Omega_q^{-1})[\tilde{U}(\exp i\theta, a, \Gamma)\tilde{\phi}]^{lm}_{\tau\tau'}(\Gamma_P) = \langle \exp i\theta, a \mid 1, P\rangle \times D^{j}_{\tau t}(A)D^{j'}_{\tau' t'}(A)D^{l'}_{0m'}(\Omega_{q'}^{-1})\tilde{\phi}^{l'm'}_{tt'}(\Gamma_{P'}).$$

Taking then into account that

$$D^{l'}_{0m'}(\Omega_{q'}^{-1}) = D^{l'}_{0m''}(\Omega_q^{-1})D^{l'}_{m''m'}(A) \quad (59)$$

and varying Ω_q over the little group $\mathcal{P}_{P^z}$, we obtain from (58) and (59)

$$[U(\exp i\theta, a, \Gamma)\tilde{\phi}]^{lm}_{\tau\tau'}(\Gamma_P) = \langle \exp i\theta, a \mid 1P\rangle D^{j}_{\tau t}(A)D^{j'}_{\tau' t'}(A)D^{l}_{mm'}(A)\tilde{\phi}^{lm'}_{tt'}. \quad (60)$$

Comparing (60) with Part I, Eq. (23), we can interpret the present realization of (33) as the representation of $G_{M+M'}$ induced by the representation

$$D^{j} \otimes D^{j'} \otimes \left(\bigoplus_{l=0}^{\infty} D^{l}\right) \quad (61)$$

of the little group $\mathcal{P}_{P^z} \equiv SU_2$.

D. Second Reduction

The induced representation (60) is still reducible. However, the reduction of the tensor product (67) can be obtained immediately by considering the J, l, S amplitudes

$$\varphi^{J\mu}_{lS}(\Gamma_P) = c(t, t', \tau; j, j', S) \times c(\tau, m, \mu; S, l, J)\tilde{\phi}^{lm}_{tt'}(\Gamma_P) \quad (62)$$

which transform irreducibly.

One obtains finally for (8) the following reduction

$$[M \mid U_0 j] \otimes [M' \mid U_0' j'] \Leftrightarrow \int_{\oplus U_0+U_0'}^{\infty} dU^x \times \bigoplus_{l=0}^{\infty} \bigoplus_{S=|j-j'|}^{j+j'} \bigoplus_{J=|l-S|}^{l+S} [M + M' \mid U^x, J] \quad (63)$$

with the scalar product

$$(\Phi_2, \Phi_1) = \int_{U_0+U_0}^{\infty} dV^x \int dP\ \delta\left(E - \frac{P^2}{2(M+M^2)} - U^x\right) \times \int dq\ \delta\left(U^x - \frac{\mathbf{q}^2}{2MM'}(M+M') - U_0 - U_0'\right) \times \delta\left(E_- - \frac{M'U_0 - MU_0'}{M+M'} - \frac{\mathbf{P}\cdot\mathbf{q}}{M+M'} - \frac{\mathbf{q}^2}{2M} + \frac{\mathbf{q}^2}{2M'}\right)\phi^*{}_2(P, q,)\phi_1(P, q,), \quad (64)$$

where U labels the double cosets and (P, Z) the left cosets of $G_{M+M'}$ mod $(\mathcal{P}_{p^z}, \mathcal{P}_{p'^z})$. This result agrees completely with the one of Levy–Leblond, except for the value of E_-.[7]

VI. CLEBSCH–GORDAN COEFFICIENTS

To obtain a physical interpretation, we only need to relate the functions ψ or ϕ to state vectors in the Hilbert space associated with the system and to interpret these corresponding state vectors (see Part I, Sec. IV).

For that purpose let us first of all write the functions $f_{ss'}(\Gamma_p, \Gamma_{p'})$ as

$$f_{ss'}(\Gamma_p, \Gamma_{p'}) = \langle \Gamma_p, s; \Gamma_{p'}, s' \mid f\rangle \quad (65)$$

considering f as the wavefunction representing the state $|f\rangle$ in the basis $|\Gamma_p, s; \Gamma_{p'}, s'\rangle$. We have

$$|f\rangle = \int d\Omega_{E_0}(p)\, d\Omega_{E_0'}(p')f_{ss'}(\Gamma_p, \Gamma_{p'}) \times |\Gamma_p, s; \Gamma_{p'}, s'\rangle. \quad (66)$$

Now, if we consider the helicity coupling, the wavefunctions take the more structured form

$$f_{\sigma\sigma'}(\Gamma_P\Omega_q\Gamma_{p^z}, \Gamma_P\Omega_q\Gamma_{p'^z}) = \psi^{z}_{\sigma\sigma'}(\Gamma_P\Omega_q) = \tilde{\psi}^{l\mu}_{\sigma\sigma'}(\Gamma_P)D^{l}_{\sigma+\sigma',\mu}(\Omega_q^{-1})N(U^z, l) \quad (67)$$

and accordingly the states of the corresponding basis will be labeled as follows

$$|\Gamma_P\Omega_q\Gamma_{p^z}, \sigma; \Gamma_P\Omega_q\Gamma_{p'^z}, \sigma'\rangle, \quad (68)$$

with the following domain of variation: σ, $\sigma' = (j, \cdots, -j)$, for P fixed, $\mathbf{q}$ can take any value

compatible with

$$\mathbf{q}^2 = \frac{2MM'}{M+M'}[U - U_0 - U_0']$$

where

$$U = E_+ - \frac{\mathbf{P}^2}{2(M+M')}$$

and E_- is given by (27); P is then varied in such a way that U remains equal to a constant U which is in a one-to-one correspondence with the couple (p, p'^x) with $\mathbf{p}^x + \mathbf{p}'^x = 0$; finally, U runs over the domain $(U_0 + U_0', \infty)$.

In that scheme, we have for $|f\rangle$ the representation

$$|f\rangle = \int_{U_0+U_0'}^{\infty} dU^x \int d\Omega_{U^x}(P) \bar{\psi}^{l\mu}_{\sigma\sigma'}(\Gamma_P) \times |\Gamma_P, \mu, l, U^x, \sigma, \sigma'\rangle, \quad (69)$$

with

$$|\Gamma_P, \mu, l, U^x, \sigma, \sigma'\rangle = \int dq\, \delta\Big(E_- - \frac{M'U_0 - MU_0'}{M+M'} - \mathbf{P}\cdot\mathbf{q} - \frac{\mathbf{q}^2}{2M} + \frac{\mathbf{q}^2}{2M'}\Big) \times D^l_{\sigma+\sigma',\mu}(\Omega_q^{-1}) N(V^x, l) \times |\Gamma_P \Omega_q \Gamma_{p^x}, \sigma; \Gamma_P \Omega_q \Gamma_{p^x}, \sigma'\rangle . \quad (70)$$

We are now in position of determing the value of $N(U, l)$.

This normalization factor will be so chosen that

$$\int d\Omega_{U_0}(p)\, d\Omega_{U_0'}(p') \langle f_2 \mid f_1\rangle(p, p') = \int dU^x \int d\Omega_{U^x}(P) \langle \bar{\psi}_2 \mid \bar{\psi}_1\rangle(P). \quad (71)$$

Hence from (70), and putting for the sake of simplicity

$$g(\mathbf{q}) = (M'U_0 - MU_0')/(M+M') + \mathbf{P}\cdot\mathbf{q} + \mathbf{q}^2(M' - M)/2MM',$$

we have

$$[N(U, l)]^{-2} = \int d\hat{q}\, \delta[E_- - g(\mathbf{q})] D^{+l}_{\sigma_2+\sigma_2',\mu_2}(\Omega_q^{-1}) D^l_{\sigma_1+\sigma_1',\mu_1}(\Omega_q^{-1}).$$

As $\mathbf{q}^2$ is a constant, we have

$$[N(U^x, l)]^{-2} = \frac{2MM'}{M+M'}(U^x - U_0 - U_0') \times \int d\hat{q}_{\blacktriangle} D^{+l}_{\sigma_2+\sigma_2^x,\mu_2}(\Omega_q^{-1}) D^l_{\sigma_1+\sigma_1^x,\mu_1}(\Omega_q^{-1}) \quad (72)$$

where $\hat{q}$ is the unit vector in the direction of $\mathbf{q}$. But from the orthonormality relations for the irreducible representations of the rotation group, the integral in (72) is equal to

Hence $[4\pi/(2l+1)]\delta_{\sigma_2+\sigma_2',\sigma_1+\sigma_1'}\delta_{\mu_2\mu_1}$.

$$N(U^x, l) = \left[\frac{M+M'}{2MM'(U^x - U_0 - U_0')} \frac{2l+1}{4\pi}\right]^{\frac{1}{2}}. \quad (73)$$

Let us now determine the Clebsch–Gordan coefficients between the helicity and the l–S schemes.

We have seen that the relation between the wavefunction $\psi^x(\Gamma_P\Omega_q)$ in the helicity representation and the wavefunction $\phi^x(\Gamma_P\Omega_q)$ in the l–S representation is given by (55). Hence the following relation holds between the corresponding basis vectors

$$D^i_{\sigma\tau}(\Omega_q) D^{i'}_{\sigma'\tau'}(\Omega_q) \times |\Gamma_P \Omega_q \Gamma_{p^x} \Omega_q^{-1}, \tau; \Gamma_P \Omega_q \Gamma_{p'^x} \Omega_q^{-1}, \tau'\rangle = |\Gamma_P \Omega_q \Gamma_{p^x}, \sigma; \Gamma_P \Omega_q \Gamma_{p'^x}, \sigma'\rangle \quad (74)$$

or conversely

$$|\Gamma_P \Omega_q \Gamma_{p^x} \Omega_q^{-1}\tau; \Gamma_{P_x} \Omega_q \Gamma_{p'^x} \Omega_q^{-1}\tau'\rangle = D^i_{\tau\sigma}(\Omega_q^{-1}) D^{i'}_{\tau'\sigma'}(\Omega_q^{-1}) \times |\Gamma_P \Omega_q \Gamma_{p^x}, \sigma; \Gamma_P \Omega_q \Gamma_{p'^x}, \sigma'\rangle. \quad (75)$$

Using (70) and (75), we eventually see that the Clebsch–Gordan coefficients between the helicity and the l–S schemes are

$$\langle \Lambda_p, \tau; \Lambda_{p'}, \tau' \mid \Gamma_P, \mu, l, U^x, \sigma, \sigma'\rangle = N(U^x, l) D^l_{\sigma+\sigma',\mu}(\Omega_q^{-1}) D^i_{\tau\sigma}(\Omega_q) D^{i'}_{\tau'\sigma'}(\Omega_q) \quad (76)$$

with

$$p + p' = P, \qquad \Lambda_p = \Gamma_P \Omega_q \Gamma_{p^x} \Omega_q^{-1},$$

and

$$\Lambda_{p'} = \Gamma_P \Omega_q \Gamma_{p'^x} \Omega_q^{-1}.$$

The formula (76) is the *Jacob–Wick formula for the Galilei group.*[9]

As for the physical interpretation, we make the following comment. If, given a total energy U^x, we limit ourselves to the states of total linear momentum $\mathbf{P}$ equal to zero, on the one hand there is no need to distinguish between q and P_- and on the other hand the amplitudes $\Gamma_P\Omega_q\Gamma_{p^x}$ and $\Gamma_P\Omega_q\Gamma_{p'^x}$ become exactly the helicity amplitudes Γ_P', $\Gamma_{P'}$ introduced in Part I. Indeed, $\mathbf{p}^x$ and $\mathbf{p}'^x$ are parallel to $\mathbf{e}_3$; $\mathbf{p}$, $\mathbf{p}'$ and $\mathbf{q}$ are colinear; $\mathbf{q} = \mathbf{p}$ and hence is a rotation leading from the direction $\mathbf{e}_3$ to the direction $\mathbf{p}$. We thus have, since $\Gamma_P = 1$,

$$\Gamma_P \Omega_q \Gamma_{p^x} = (0, R)(\mathbf{p}^x/M, 1) = (\mathbf{p}/M, R)$$

and

$$\Gamma_P \Omega_Q \Gamma_{P'^*} = (-\mathbf{p}/M, R),$$

where R is the "helicity" rotation.

This result still holds if $\mathbf{P}$ is parallel to $\mathbf{p}$ but not in the other cases, which is related to the nonconservation of a helicity eigenstate $|p, \sigma\rangle$ when a velocity nonparallel to $\mathbf{p}$ is imparted to the system.

We knew already from the work of Jacob and Wick that the helicity coupling method has to be used only in a frame where the momenta of the particles are opposite to each other. Our considerations show how to proceed if $\mathbf{P}$ is not parallel to $\mathbf{p}$.

In the present work, we have considered only the case where the total mass is different from zero. If $M + M' = 0$, the coset method is still valid for reducing the product representation. However, in this case, the double cosets will be labeled by the modulus of the total linear momentum.

Note added in proof. It is worth mentioning explicitly that to apply directly the general formalism to the amplitudes (52) would require some (secondary) modification. It is this difficulty that we have avoided by using the results obtained for the helicity coupling.

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[13] R. Stora informs us that a work analogous to ours has been performed by J. C. Guillot (unpublished).

Observations on the Spherical Model of a Ferromagnet*

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A discrepancy between the methods of the grand and the canonical ensemble which arose in the study of the spherical model of a ferromagnet even for properties of individual spins is traced to an incorrect order of taking limits. The spin system must be considered for a small but not vanishing field first, and the limit of zero field must only be taken after the limit of an infinite number of particles has been taken. For this case no discrepancy between the two ensembles arises. A calculation proceeding entirely at zero field cannot be considered as logically admissible; discrepancies arising in this case are thus of no physical consequence.

I. INTRODUCTION

IN 1952, Berlin and Kac introduced the so-called "spherical model" of a ferromagnet into the literature.[1] The model is a modification of the Ising model. Like the Ising model it has scalar "spins" ϵ_i on fixed sites, interacting through nearest neighbor interaction of the form $-J\epsilon_i\epsilon_j$. It differs from the Ising model in that the spins are not restricted to the values $+1$ and -1 but may assume any real value. The magnitude of the spins is held in the mean to something like ± 1 by the side condition

$$\sum_{i=1}^{N} \epsilon_i^2 = N. \tag{1}$$

Berlin and Kac interpreted this condition rigorously. In other words, they accepted (1) as a microcanonical constraint, and derived the properties of their model with considerable labor. In particular they had to carry out a very difficult contour integration. Such integrations are known to be associated with microcanonical constraints generally.

Following this paper, Lewis and Wannier[2] wrote a short article pointing out that the spherical model lends itself very well to the grand canonical approach. In that approach the spins are left free entirely, but a variable S conjugate to $\sum_i \epsilon_i^2$ is introduced. The statistics of this relaxed problem are carried through, and in the end the parameter S is adjusted in such a way that the condition (1) is valid in the mean. It seemed to us that the equivalence of the two procedures is a cornerstone of all thermal physics. Indeed, this point of view seemed to be justified by the early results. After a calculation which is almost trivial in its simplicity, Lewis and Wannier reproduced all thermodynamic results of Berlin and Kac. However, some time later, discrepancies began to be noted. The first one was in $\sum_i \epsilon_i^4$. This did not seem very serious. For this quantity is intimately associated with the fluctuation in the spherical constraint (1) and a discrepancy is thus not very surprising. However, it was then noted that there is a discrepancy in the probability distribution of an individual spin. The distribution comes out to be Gaussian about 0 for all temperatures by the grand method. The micro method, on the other hand, yields a double peak about $+1$ and -1 below the Curie point. Lewis and Wannier admitted these discrepancies.[3] A general paper by Lax followed which pointed out that discrepancies of this sort are to be expected whenever the contour integration of the micro method does not proceed over a normal saddle point.[4]

We wish to take up the preceding question again after a lapse of some years because we feel that important physical principles are at stake in this discussion. If the preceding results are taken at face value they are equivalent to the assertion that the Maxwellian distribution might be right for a gas whose total energy is kept fixed, but that an entirely different distribution might arise if the gas is placed into a constant-temperature bath. In other words, the stability of the atomic scale parameters with respect to macroscopic constraints is called into question. The entire edifice of statistical thermodynamics rests on that stability. It is therefore proper to re-examine the results discussed earlier to see if the discrepancy described previously is genuine. It is the purpose of the following paper to argue that the discrepancy arose from a freak situation. The properties were calculated at points of discontinuity in the phase behavior of the system.

* This work has been supported by the U. S. Office of Naval Research.

[1] T. H. Berlin and M. Kac, Phys. Rev. 86, 821 (1952).

[2] H. W. Lewis and G. H. Wannier, Phys. Rev. 88, 682 (1952).

[3] H. W. Lewis and G. H. Wannier, Phys. Rev. 90, 1131 (1953).

[4] M. Lax, Phys. Rev. 97, 1419 (1955).

Two limiting processes are associated with these points: passage to the limit of zero magnetic field and passage to the limit of infinite N. In Ref. 2 these limits were taken in the order given. If the order of the two limiting processes is reversed the discrepancy between the two modes of computation disappears. The discrepancy is therefore not between the two forms of statistics, but within one form of statistics. This result does of course not explain away entirely the discrepancy previously found. But it salvages the principles of statistical mechanics by showing that *if proper care is taken* the result of a statistical calculation is independent of the ensemble enployed in computing it.

II. SPIN PROBABILITIES WITHOUT FIELD

In this section we shall work out the previously discussed discrepancy. In other words we shall compute the probability distribution for an individual spin ϵ_1 using either ensemble and assuming no field. The energy of the model then equals

$$E = -\tfrac{1}{2}J \sum_{(i,j)} \epsilon_i\epsilon_j. \tag{2}$$

Here the summation is over nearest-neighbor pairs i, j, and each pair is counted twice. J is the interaction energy. Introducing the abbreviation

$$K = J/2kT, \tag{3}$$

we can now write two kinds of partition functions. The microcanonical partition function Q_m reads

$$Q_m = \int_{-\infty}^{\infty} \cdots \int d\epsilon_1 \cdots d\epsilon_N \cdot \exp\left[K \sum_{(i,j)} \epsilon_i\epsilon_j\right] \delta\left(N - \sum_{i=1}^{N} \epsilon_i^2\right)$$

$$= \int_{-\infty}^{\infty} \cdots \int d\epsilon_1 \cdots d\epsilon_N \cdot \exp\left[K \sum_{(i,j)} \epsilon_i\epsilon_j\right] \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dS \exp\left[S\left(N - \sum_{i=1}^{N} \epsilon_i^2\right)\right]$$

or

$$Q_m = \frac{1}{2\pi i} \int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS \exp[NS] \int_{-\infty}^{\infty} \cdots \int d\epsilon_1 \cdots d\epsilon_N \cdot \exp\left[-S \sum_{i=1}^{N} \epsilon_i^2 + K \sum_{(i,j)} \epsilon_i\epsilon_j\right]. \tag{4}$$

On the other hand, if the grand canonical method is employed we construct a grand partition function $Q_g(S)$ as follows

$$Q_g(S) = \int_{-\infty}^{\infty} \cdots \int d\epsilon_1 \cdots d\epsilon_N \cdot \exp\left[K \sum_{(i,j)} \epsilon_i\epsilon_j - S \sum_{i=1} \epsilon_i^2\right] \tag{5}$$

and impose the side condition

$$\partial[\ln Q_g(S)]/\partial S = -N. \tag{6}$$

Now we observe that in either ensemble

$$Q = \int_{-\infty}^{\infty} P(\epsilon_1)\, d\epsilon_1 = \int_{-\infty}^{\infty} P(x)\, dx = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} P(\epsilon_1)\, \delta(\epsilon_1 - x)\, d\epsilon_1\right] dx \tag{7}$$

$$P(x) = \int_{-\infty}^{\infty} P(\epsilon_1)\, \delta(\epsilon_1 - x)\, d\epsilon_1,$$

which is equivalent to inserting $\delta(\epsilon_1 - x)$ into the integrand of Q. We may thus define

$$p(x) = P(x)/Q. \tag{8}$$

$p(x)dx$ then represents the probability that a single spin have a value between x and $x + dx$.

Our problem has now been transformed into the evaluation of Q and $P(x)$ micro and grand canonically. To achieve this we may apply the following orthogonal transformations:

$$\epsilon = (V)y, \tag{9a}$$

where (V) is a matrix whose elements are

$$V_{ks} = N^{-\frac{1}{2}}[\cos 2\pi N^{-1}(k-1)(s-1) + \sin 2\pi N^{-1}(k-1)(s-1)], \tag{9b}$$

then we have

$$\epsilon_1 = \sum_{k=1}^{N} V_{1k}y_k = N^{-\frac{1}{2}} \sum_{i=1}^{N} y_i \tag{10}$$

and

$$y_1 = N^{-\frac{1}{2}} \sum_{i=1}^{N} \epsilon_i, \tag{11}$$

$$\sum_{i,j} \epsilon_i\epsilon_j = \sum_{p} \lambda_p y_p^2, \tag{12}$$

$$\sum_{p=1}^{N} \epsilon_p^2 = \sum_{p=1}^{N} y_p^2. \tag{13}$$

It is found for the case of a simple cubic three-dimensional net of spins that the quantities λ_p equal

$$\lambda_p = 2\cos\frac{2\pi}{N}(p-1) + 2\cos\frac{2\pi n_1}{N}(p-1) + 2\cos\frac{2\pi n_1 n_2}{N}(p-1). \tag{14}$$

After these transformations we find the following results in the microcanonical case:

$$Q_m = \frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS \exp[NS] \int_{\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N \cdot\exp\left[-S\sum_{i=1}^{N}\epsilon_i^2 + K\sum_{(i,j)}\epsilon_i\epsilon_j\right]$$

$$= \frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS \exp[NS] \int_{-\infty}^{\infty}\cdots\int dy_1\cdots dy_N \cdot\exp\left[-S\sum_{i=1}^{N}y_i^2 + K\sum_{i=1}^{N}\lambda_i y_i^2\right]$$

$$= \frac{1}{2\pi i}\pi^{N/2}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS \cdot\exp\left[NS - \frac{1}{2}\sum_{i=1}^{N}\ln(S-K\lambda_i)\right]$$

or

$$Q_m = \pi^{N/2}2Ke^{-\frac{1}{4}N\ln 2K}\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)}, \tag{15}$$

where

$$g(z) = 2Kz - \tfrac{1}{2}f(z), \tag{16}$$

$$f(z) = \lim_{N=\infty} N^{-1}\sum_{i=2}^{N}\ln(z-\tfrac{1}{2}\lambda_i) = \frac{1}{(2\pi)^3}\iiint_0^{2\pi}\frac{d\omega_1\,d\omega_2\,d\omega_3}{z-(\cos\omega_1+\cos\omega_2+\cos\omega_3)}dz, \tag{17}$$

$$z = S/2K; \qquad z_0 > \tfrac{1}{2}|\lambda_{\max}| = \tfrac{1}{2}\lambda_1. \tag{18}$$

Now, for $T > T_c(K < K_c)$ with $T_c = (3.9568)J/k$ or

$$4K_c = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} d\omega_1\,d\omega_2\,d\omega_3 \cdot[3-(\cos\omega_1+\cos\omega_2+\cos\omega_3)]^{-1} = 0.50546,$$

the saddle point exists; thus

$$Q_m(S) = 2K\pi^{\frac{1}{4}N}\exp(-\tfrac{1}{2}N\ln 2K)\cdot\frac{\exp[Ng(z_s)]}{(z_s-\frac{1}{2}\lambda_1)^{\frac{1}{2}}[2\pi N(\partial^2 g/\partial z^2)_{z_s}]^{\frac{1}{2}}} \tag{19}$$

with z_s determined from

$$4K = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} d\omega_1\,d\omega_2\,d\omega_3 \cdot[z_s-(\cos\omega_1+\cos\omega_2+\cos\omega_3)]^{-1}. \tag{20}$$

However for $T < T_c$ the saddle point sticks to the point at $z = 3$, and in the neighborhood of $z = 3$ it is found by analytic continuation that

$$f(z) = f(3) + 4K_c(z-3) - (2^{\frac{1}{2}}/3\pi)(z-3)^{\frac{3}{2}} + o[(z-3)^2],$$

$$g(z) = g(3) + 2(K-K_c)(z-3) + (2^{-\frac{1}{2}}/3\pi)(z-3)^{\frac{3}{2}} + o[(z-3)^2].$$

Hence

$$Q_m = 2K\pi^{\frac{1}{4}N}e^{-\frac{1}{4}N\ln 2K}[N2\pi(K-K_c)]^{-\frac{1}{2}}e^{Ng(3)}. \tag{21}$$

Furthermore,

$$P_m(x) = \frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS\exp[NS]\int_{-\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N \cdot\exp\left[-S\sum_{i=1}^{N}\epsilon_i^2 + K\sum_{(i,j)}\epsilon_i\epsilon_j\right]\delta(\epsilon_1-x)$$

$$= \frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS\exp[NS]\int_{-\infty}^{\infty}\cdots\int dy_1\cdots dy_N \cdot\exp\left[-S\sum_{i=1}^{N}y_i^2 + \sum_{i=1}^{N}\lambda_i y_i^2\right]\delta\left(N^{-\frac{1}{2}}\sum_{i=1}^{N}y_i - x\right)$$

$$= \frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS\exp[NS]\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} dq \cdot\exp[qx]\int_{-\infty}^{\infty}\cdots\int dy_1\cdots dy_N \cdot\exp\left[-S\sum_{i}^{N}y_i^2 + \sum_{i=1}^{N}\lambda_i y_i^2 - N^{-\frac{1}{2}}q\sum_{i=1}^{N}y_i\right]$$

$$= \frac{1}{2\pi i}\pi^{\frac{1}{4}N}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dS \cdot\exp\left[NS - \frac{1}{2}\sum_{i=1}^{N}\ln(S-K\lambda_i)\right] \cdot\frac{1}{\pi^{\frac{1}{2}}}\left[\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S-K\lambda_i}\right]^{-\frac{1}{2}} \cdot\exp\left[-x^2\Big/\left(\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S-K\lambda_i}\right)\right]$$

$$= 2K\pi^{\frac{1}{4}N}e^{-\frac{1}{2}\ln 2K}\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}}e^{Ng(z)} \cdot\frac{1}{\pi^{\frac{1}{2}}}\left[\frac{1}{2KN}\sum_{i=1}^{N}\frac{1}{z-\frac{1}{2}\lambda_i}\right]^{-\frac{1}{2}} \cdot\exp\left[-x^2\Big/\left(\frac{1}{2KN}\sum_{i=1}^{N}\frac{1}{z-\frac{1}{2}\lambda_i}\right)\right].$$

For $T > T_c(K < K_c)$ the saddle point exists and we have

$$P_m(x) = 2K\pi^{\frac{1}{4}N}e^{-\frac{1}{4}N\ln 2K} \cdot\frac{\exp[Ng(z_s)]}{(z_s-\frac{1}{2}\lambda_1)^{\frac{1}{2}}[2\pi N(\partial^2 g/\partial z^2)_{z_s}]^{\frac{1}{2}}}\frac{1}{(2\pi)^{\frac{1}{2}}}\exp(-\tfrac{1}{2}x^2) \tag{22}$$

where the relation

$$\lim_{N\to\infty}\frac{1}{2K}\frac{1}{N}\sum_{i=1}^{N}\frac{1}{z-\frac{1}{2}\lambda_i} = \frac{1}{2K}\left(\frac{d}{dz}f(z)\right)_{z_s} = \frac{1}{2K}4K = 2$$

has been used. Thus we have, combining (19) and (22),

$$p(x) = (2\pi)^{-\frac{1}{2}} \exp(-\tfrac{1}{2}x^2), \tag{23}$$

which is a Gaussian as expected. The width of this Gaussian is such that the expectation value of x^2 equals 1, in agreement with the spherical constraint (1).

For $T < T_c(K > K_c)$, we have instead

$$\begin{aligned}
&\frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz(z-\tfrac{1}{2}\lambda_1)^{-\frac{1}{2}} e^{Ng(z)}\pi^{-\frac{1}{2}} \\
&\cdot\left[\frac{1}{2KN}\sum_{i=1}^{N}\frac{1}{z-\frac{1}{2}\lambda_i}\right]^{-\frac{1}{2}} \\
&\cdot\exp\left\{-x^2\Big/\left[\frac{1}{2KN}\sum_{i=1}^{N}\frac{1}{z-\frac{1}{2}\lambda_i}\right]\right\} \\
&= \frac{1}{2\pi i}\int_{z_0-i\infty}^{z_0+i\infty} dz\, e^{N[g(3)+2(K-K_c)(z-3)]}\pi^{-\frac{1}{2}} \\
&\cdot\left[\frac{1}{2KN}+\frac{2K_c}{K}(z-3)\right]^{-\frac{1}{2}} \\
&\cdot\exp\left\{-x^2(z-3)\Big/\left[\frac{1}{2KN}+\frac{2K_c}{K}(z-3)\right]\right\} \\
&= e^{Ng(3)}\left[\frac{K}{4\pi NK_c(K-K_c)}\right]^{\frac{1}{2}} \\
&\cdot\exp\left\{-\frac{K}{2K_c}\left[\left(1-\frac{K_c}{K}\right)+x^2\right]\right\}\frac{1}{2\pi i}\int_{\alpha_0-i\infty}^{\alpha_0+i\infty} dt\, t^{-\frac{1}{2}} \\
&\cdot\exp\left[t-\frac{1}{4t}\left(\frac{ix}{K_c}[K(K-K_c)]^{\frac{1}{2}}\right)^2\right],
\end{aligned}$$

where the transformation

$$\frac{1}{2KN}+\frac{2K_c}{K}(z-3) = \frac{t}{N(K/K_c)(K-K_c)}$$

has been employed. We now use the expression[5]

$$J_\nu(Z) = \frac{1}{2\pi i}\left(\frac{1}{2}Z\right)^\nu \int_{c-i\infty}^{c+i\infty}\exp\left(t-\frac{Z^2}{4t}\right)t^{-\nu-1}\,dt$$

and obtain finally

$$\begin{aligned}
P_m(x) &= \pi^{\frac{1}{2}N}2Ke^{-\frac{1}{2}N\ln 2K+Ng(3)}\left[\frac{K}{2K_c2\pi N(K-K_c)}\right]^{\frac{1}{2}} \\
&\cdot\exp\left\{-\frac{K}{2K_c}\left[\left(1-\frac{K_c}{K}\right)+x^2\right]\right\}\left(\frac{1}{2}Z\right)^{\frac{1}{2}}J_{-\frac{1}{2}}(Z).
\end{aligned} \tag{24}$$

Combination of (21) and (24) yields then (define $K/K_c \equiv A$ for typographical simplicity)

$$\begin{aligned}
p(x) &= (\tfrac{1}{2}A)^{\frac{1}{2}}\exp\{-\tfrac{1}{2}A[(1-A^{-1})+x^2]\}(\tfrac{1}{2}Z)^{\frac{1}{2}}J_{-\frac{1}{2}}(Z) \\
&= (\tfrac{1}{2}A)^{\frac{1}{2}}\exp\{-\tfrac{1}{2}A[(1-A^{-1})+x^2]\}\pi^{-\frac{1}{2}}\cos Z \\
&= \pi^{-\frac{1}{2}}(\tfrac{1}{2}A)^{\frac{1}{2}}\exp\{-\tfrac{1}{2}A[(1-A^{-1})+x^2]\} \\
&\cdot\{\tfrac{1}{2}\exp[Ax(1-A^{-1})^{\frac{1}{2}}]+\tfrac{1}{2}\exp[-Ax(1-A^{-1})^{\frac{1}{2}}]\}
\end{aligned}$$

or

$$\begin{aligned}
p(x) &= \tfrac{1}{2}\pi^{-\frac{1}{2}}(2A^{-1})^{-\frac{1}{2}} \\
&\cdot(\exp\{-[(1-A^{-1})^{\frac{1}{2}}-x]^2[(2A^{-1})^{\frac{1}{2}}]^{-2}\} \\
&+\exp\{[(1-A^{-1})^{\frac{1}{2}}+x]^2[(2A^{-1})^{\frac{1}{2}}]^{-2}\}),
\end{aligned} \tag{25}$$

which represents a superposition of two displaced Gaussians of width of $(K_c/K)^{\frac{1}{2}} = (T/T_c)^{\frac{1}{2}}$ and a displacement of $\pm(1-K_c/K)^{\frac{1}{2}} = \pm(1-T/T_c)^{\frac{1}{2}}$

In the grand canonical case the same calculation proceeds as follows:

$$\begin{aligned}
Q_g(S) &= \int_{-\infty}^{\infty}\cdots\int d\epsilon_1\cdots d\epsilon_N \\
&\cdot\exp\left[K\sum_{(i,j)}\epsilon_i\epsilon_j - S\sum_{i=1}^{N}\epsilon_i^2\right] \\
&= \int_{-\infty}^{\infty}\cdots\int dy_1\cdots dy_N \\
&\cdot\exp\left[\sum_{i=1}^{N}\lambda_i y_i^2 - S\sum_{i=1}^{N}y_i^2\right]
\end{aligned}$$

or

$$Q_g(S) = \pi^{\frac{1}{2}N}\exp\left[-\frac{1}{2}\sum_{i=1}^{N}\ln(S-K\lambda_i)\right]. \tag{26}$$

The canonical variable S should be fixed by the side condition (6) which leads to

$$\begin{aligned}
1 &= \frac{1}{2N(S_0-6K)}+\frac{1}{2(2\pi)^3} \\
&\cdot\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{d\omega_1\,d\omega_2\,d\omega_3}{S_0-2K(\cos\omega_1+\cos\omega_2+\cos\omega_3)},
\end{aligned} \tag{27}$$

from which we can solve for S_0 for all ranges of temperature even if $T < T_c$, since then the first term of the right-hand side of the above equation can take care of it.

Now, using the fact that

$$\begin{aligned}
\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S_0-K\lambda_i} &= \frac{1}{N}\left(\frac{\partial}{\partial S}\sum_{i=1}^{N}\ln(S-K\lambda_i)\right)_{S_0} \\
&= -2\frac{1}{N}\frac{\partial}{\partial S}(\ln Q_g(S)) = 2,
\end{aligned}$$

we have

[5] W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1949), p. 28.

$$P(x, S_0) = \int_{-\infty}^{\infty} \cdots \int d\epsilon_1 \cdots d\epsilon_N \cdot \exp\left[K \sum_{(i,j)} \epsilon_i\epsilon_j - S_0 \sum_{i=1}^{N} \epsilon_i^2\right] \delta(\epsilon_1 - x)$$
$$= \pi^{\frac{1}{2}N} \exp\left[-\frac{1}{2}\sum_{i=1}^{N} \ln (S_0 - K\lambda_i)\right]\pi^{-\frac{1}{2}} \cdot\left[\frac{1}{N}\sum_{i}^{N}\frac{1}{S_0 - K\lambda_i}\right]^{-\frac{1}{2}} \cdot\exp\left\{-x^2\Big/\left[\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S_0 - K\lambda_i}\right]\right\}$$

or

$$P(x, S_0) = \pi^{\frac{1}{2}N} \cdot\exp\left[-\frac{1}{2}\sum_{i=1}^{N}\ln (S_0 - K\lambda_i)\right](2\pi)^{-\frac{1}{2}}e^{-\frac{1}{2}x^2}. \quad (28)$$

Combination of (26) and (28) thus yields

$$p(x) = (2\pi)^{-\frac{1}{2}}e^{-\frac{1}{2}x^2}, \quad (29)$$

which is a Gaussian for all temperatures, and thus a discrepancy occurs when $T < T_c$.

III. SPIN PROBABILITIES IN THE LIMIT OF A VANISHINGLY SMALL FIELD

To overcome this apparent discrepancy, we may now start with a finite field. Then the microcanonical partition function can be written as

$$Q_m = \int_{\sum_{i=1}^{N}\epsilon_i^2 = N} \cdots \int d\epsilon_1 \cdots d\epsilon_N \cdot\exp\left[K\sum_{(i,j)}\epsilon_i\epsilon_j + 2M\sum_{i}^{N}\epsilon_i\right], \quad (30)$$

where

$$M = \mu_0 H/2kT,$$

with μ_0 = magnetic moment of a single spin; H = external magnetic field.

Following the same manner of calculation as before we end up with the following expressions.

A. Microcanonical Case

$$Q_m(S) = \frac{1}{2\pi i}\pi^{\frac{1}{2}N}\int_{\alpha_0 - i\infty}^{\alpha_0 + i\infty} dS \cdot\exp\left[NS - \frac{1}{2}\sum_{i=1}^{N}\ln (S - K\lambda_i)\right]\exp\left[\frac{NM^2}{S - 6K}\right], \quad (31)$$

$$P_m(x) = \frac{1}{2\pi i}\pi^{\frac{1}{2}N}\int_{\alpha_0 - i\infty}^{\alpha_0 + i\infty} dS \cdot\exp\left[NS - \frac{1}{2}\sum_{i=1}^{N}\ln (S - K\lambda_i)\right]\exp\left[\frac{NM^2}{S - 6K}\right] \cdot\pi^{-\frac{1}{2}}\left[\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S - K\lambda_i}\right]^{-\frac{1}{2}} \cdot\exp\left\{-\left[\frac{M}{S - 6K} - x\right]^2\left[\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S - K\lambda_i}\right]^{-1}\right\}. \quad (32)$$

The saddle-point condition is given by

$$1 = \frac{1}{2N(S - 6K)} + \frac{M^2}{(S - 6K)^2} + \frac{1}{2(2\pi)^3} \cdot\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{d\omega_1\, d\omega_2\, d\omega_3}{S - 2K(\cos\omega_1 + \cos\omega_2 + \cos\omega_3)}. \quad (33)$$

For the case $M \neq 0$ we can always solve the above equation for S. Even for the limiting case $M \to 0$, if we hold the condition $NM \gg 1$ as $N \to \infty$, $M \to 0$, the first term can be neglected. In this case we have

For $T > T_c (K < K_c)$

$$1 \approx \frac{1}{2(2\pi)^3} \cdot\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{d\omega_1\, d\omega_2\, d\omega_3}{S_0 - 2K(\cos\omega_1 + \cos\omega_2 + \cos\omega_3)}. \quad (34)$$

For $T < T_c (K > K_c)$,

$$1 \approx M^2/(S - 6K)^2 + K_c/K \quad (35a)$$

or

$$M/(S - 6K) = \pm(1 - K_c/K)^{\frac{1}{2}}. \quad (35b)$$

Hence

$$Q_m = Q_m(S_0)[2\pi N(\partial^2 G/\partial S^2)_{S_0}]^{-\frac{1}{2}} \quad (36)$$

with

$$G(S) = S - \frac{1}{2}\sum_{i=1}^{N}\ln (S - K\lambda_i) + \frac{M^2}{S - 6K} \quad (37)$$

and

$$P_m(x) = \frac{Q_m(S_0)}{\left[2\pi N\left(\frac{\partial^2 G}{\partial S^2}\right)_{S_0}\right]^{\frac{1}{2}}} \times \frac{1}{\sqrt{\pi}} \times \frac{1}{\left[\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S_0 - K\lambda_i}\right]^{\frac{1}{2}}} \cdot\exp\frac{-\left[\frac{M}{S_0 - 6K} - x\right]^2}{\left[\frac{1}{N}\sum_{i=1}^{N}\frac{1}{S_0 - K\lambda_i}\right]}, \quad (38)$$

which lead to the following:

For $T > T_c(K < K_c)$,

$$p(x) = (2\pi)^{-\frac{1}{2}} e^{-\frac{1}{2}x^2}, \tag{39}$$

again a Gaussian.

For $T < T_c(K > K_c)$ (here, define $B \equiv K_c/K$)

$$p_+(x) = \pi^{-\frac{1}{2}}(2B)^{-\frac{1}{2}} \exp\{-[(1-B)^{\frac{1}{2}} - x]^2[(2B)^{\frac{1}{2}}]^{-2}\} \tag{40a}$$

if $M/(S_0 - 6K) = +(1-B)^{\frac{1}{2}}$ is substituted

or

$$p_-(x) = \pi^{-\frac{1}{2}}(2B)^{-\frac{1}{2}} \exp\{-[(1-B)^{\frac{1}{2}} + x]^2[(2B)^{\frac{1}{2}}]^{-2}\} \tag{40b}$$

if $M/(S_0 - 6K) = -(1-B)^{\frac{1}{2}}$ is substituted.

Here we have a discontinuity which arises from the ambiguity of the sign of square root. We may note that if we take an arithmetical mean of $p_+(x)$ and $p_-(x)$ we do go back to the result (25).

B. Grand Canonical Case

$$Q_s(S) = \pi^{\frac{1}{2}N} \cdot \exp\left[-\frac{1}{2}\sum_{i=1}^{N} \ln(S - K\lambda_i)\right] \exp\left[\frac{NM^2}{S - 6K}\right], \tag{41}$$

$$P(x, S) = \pi^{\frac{1}{2}N} \exp\left[-\frac{1}{2}\sum_{i=1}^{N} \ln(S - K\lambda_i)\right] \cdot \exp\left[\frac{NM^2}{S - 6K}\right] \times \pi^{-\frac{1}{2}}\left[\frac{1}{N}\sum_{i}^{N} \frac{1}{S - K\lambda_i}\right]^{-\frac{1}{2}} \cdot \exp\left\{-\left[\frac{M}{S - 6K} - x\right]^2\left[\frac{1}{N}\sum_{i=1}^{N} \frac{1}{S - K\lambda_i}\right]^{-1}\right\} \tag{42}$$

with the side condition (6)

or

$$1 = \frac{1}{2N(S - 6K)} + \frac{M^2}{(S - 6K)^2} + \frac{1}{2(2\pi)^3} \cdot \int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} \frac{d\omega_1\, d\omega_2\, d\omega_3}{S - 2K(\cos\omega_1 + \cos\omega_2 + \cos\omega_3)} \tag{43}$$

which is the same as the saddle-point condition (33). Thus, the same results follow as under Sec. IIIA. After a comparison with the results obtained in the Sec. II the equivalence of these micro and grand canonical methods can thus be ascertained.

IV. CONCLUSIONS

Since the result (29) cannot be reached by a limiting process from a finite field when $T < T_c$, we are inclined to consider it simply an erroneous answer, arising from an incorrect order of taking limits. The results for vanishingly small field do agree in the two statistics. The equivalence of the two procedures is thereby established, in agreement with the principles of statistical mechanics. One simply has to be cautious when trying to compute the value of a function $f(x)$ at a point of discontinuity x_0. Only $\lim_{\epsilon\to 0} f(x_0 + \epsilon)$ and $\lim_{\epsilon\to 0} f(x_0 - \epsilon)$ are properly defined. This observation has no deep implication for the validity of various ensembles in statistical mechanics.

Wave Scattering and the Geometry of a Strip

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A new method is introduced to find properties of wave and other fields. The relationship between the geometry of the strip and the symmetry of the Helmholtz equation is shown and leads to previously undiscovered properties of the field. The field pattern of the strip is shown to have a particularly simple form and, moreover, to be completely determined by symmetry-like principles.

I. INTRODUCTION

THE problem of wave scattering by a strip has been extensively studied,[1-4] but a class of valuable relations has remained unexplored. These are related to the behavior of the field near the strip ends and stem from the form of the change that the wave field exhibits when an infinitesimal extension of the strip is made. Some of the relations can also be shown for a variety of other scattering obstacles, and the derivations for the strip will be cast in terms that facilitate the generalizations.

II. FORMULATION

We suppose a monochromatic wave process governed by the two-dimensional Helmholtz equation, with a wave field ϕ defined on the (x, y)-plane. If the field were not constrained on the strip then it would be the incident field ϕ^{inc}, which is assumed known. When a boundary condition is imposed on the strip $L_2 < x < L_1$, $y = 0$, a scattered field ϕ^{sc} is induced so that the field ϕ is given by

$$\phi = \phi^{\text{inc}} + \phi^{\text{sc}}. \tag{1}$$

ϕ and ϕ^{sc} are determined by the conditions (a) through (e):

(a) $$(\partial_x^2 + \partial_y^2 + k^2)\phi^{\text{sc}} = 0 \tag{2}$$

at all points not on the closed strip, where "closed" refers to the strip plus its end points.

(b) ϕ^{sc} satisfies Sommerfeld's radiation condition at infinity.[4]

(c) On the strip, either

$$\phi^{\text{sc}} = -\phi^{\text{inc}} \qquad \text{(Dirichlet condition)}$$

or

$$\partial_y\phi^{\text{sc}} = -\partial_y\phi^{\text{inc}} \qquad \text{(Neumann condition)}.$$

When it is necessary to distinguish which boundary condition is assumed, D will be subscripted to functions associated with the Dirichlet condition and N will be subscripted for the Neumann condition.

(d) With Bouwkamp[4] we may also require that $\phi_{\text{D}}^{\text{sc}}$ be symmetric about the line $y = 0$ and that $\phi_{\text{N}}^{\text{sc}}$ be antisymmetric.

(e) ϕ^{sc} is finite everywhere (including the endpoints of the strip). These conditions are known to determine ϕ and ϕ^{sc} uniquely.

We shall be primarily concerned with the field ψ of a unit point source, and view this field as a special case of the general field ϕ. Let $\mathbf{x}$ be the position vector to the point (x, y), and let $\mathbf{x}'$ denote the source point (x', y'), which may be any point not on the closed strip. The field due to a point source at $\mathbf{x}'$ is denoted $\psi(\mathbf{x}, \mathbf{x}', L_1, L_2)$, or often abbreviated as $\psi(\mathbf{x}, \mathbf{x}')$. Conditions (a) through (e) determine ψ when we stipulate that the incident field is the free-space Green's function G:

$$\psi^{\text{inc}} = G(\mathbf{x}, \mathbf{x}') \equiv \tfrac{1}{4}iH_0^{(1)}(k\,|\mathbf{x} - \mathbf{x}'|). \tag{3}$$

III. THE BASIC RELATION

In the Appendix, it is demonstrated from integral equations that the change in ψ associated with an infinitesimal shift in the location of the endpoint L_1 is the same function of $\mathbf{x}$, up to a multiplier, independent of the location of the source. Let $\mathbf{x}_1$ be any fixed point on the plane and not on the closed strip, such that for some $\mathbf{x}_2$ the derivative $\partial_{L_1}\psi(\mathbf{x}_2, \mathbf{x}_1)$ is not zero. For any two points $\mathbf{x}$ and $\mathbf{x}'$ there is a function $\alpha(\mathbf{x}', \mathbf{x}_1, L_1, L_2)$, or briefly written $\alpha(\mathbf{x}', \mathbf{x}_1)$, which is independent of $\mathbf{x}$ and such that

$$\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}') = \alpha(\mathbf{x}', \mathbf{x}_1)\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}_1). \tag{4}$$

Equation (4) can also be derived in ways other than that of the Appendix, and these are instructive. It is easy to show that

$$\partial_{L_1}\psi = \partial_{L_1}\psi^{\text{sc}}, \tag{5}$$

[1] P. M. Morse and P. J. Rubenstein, Phys. Rev. 54, 895 (1938).
[2] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953).
[3] R. A. Schmeltzer and M. Lewin, Quart. Appl. Math. 21, 269 (1964).
[4] C. J. Bouwkamp, Diffraction Theory, Proc. Phys. Soc. (London) 27, 35 (1954).

and that $\partial_{L_1}\psi$ satisfies the Helmholtz equation at all points not on the closed strip even though ψ itself has a singularity at $\mathbf{x} = \mathbf{x}'$. Further, ∂_{L_1} satisfies the symmetry and radiation conditions. It satisfies the same boundary condition on the open strip as does the scattered field associated with zero incident field, since

$$\partial_{L_1}G = \partial_y\partial_{L_1}G = 0 \tag{6}$$

everywhere. It is bounded at $(L_2, 0)$ but we must examine it at the end point of $(L_1, 0)$. For $\mathbf{x}$ near $(L_1, 0)$ the Dirichlet field ψ_D behaves as Re $[(x + iy - L_1)^{\frac{1}{2}}]$ plus terms which have bounded derivatives with respect to L_1. This behavior is discussed by Bouwkamp[4] and may also be shown by the same relation between the Helmholtz and Laplace equations as is used in the Appendix. Similarly ψ_N behaves as Im $[(x + iy - L_1)^{\frac{1}{2}}]$ plus differentiable terms. Hence $\partial_{L_1}\psi$ has a square-root singularity at $(L_1, 0)$. But, since the singularity is a simple square root, some linear combination of $\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}')$ and $\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}_1)$ will be bounded at $(L_1, 0)$. The combination then satisfies all the conditions of Sec. II for a scattered field corresponding to no incident field. These conditions are satisfied by the null function. Since the conditions uniquely determine the scattered field, the null function is the only solution for the combination. This statement is equivalent to Eq. (4). In passing, one notes that $\partial_{L_1}\psi$ is an example of the necessity of condition e), since without that condition ∂_{L_1} could be added to any ψ to form a second distinct field for the same source.

A second way of deriving Eq. (4) is based on considering the extension of the strip from L_1 to $L_1 + \delta L_1$. On the extended strip $L_2 < x < L_1 + \delta L_1$, we know that $\psi(\mathbf{x}, \mathbf{x}', L_1, L_2)$ departs from the boundary condition, though only on the extended increment. The effect of this departure is that of an incident field which has the same departure. The field change $\delta\psi$ is the scattered field associated with illumination of the extended strip by this "incident field." On the extended strip $\psi_D(\mathbf{x}, \mathbf{x}', L_1, L_2)$ is zero up to L_1; and on $L_1 < x < L_1 + \delta L_1$ it is $(x - L_1)^{\frac{1}{2}}$ times a multiplier which depends on $\mathbf{x}'$, plus terms of higher order in $(x - L_1)$. The multiplier will be denoted $-i(2/\pi)^{\frac{1}{2}}S_D(\mathbf{x}', L_1, L_2)$. It may be shown from an integral-equation analysis that the higher-order terms make no contribution as strong as first order in δL_1, and so may be neglected. Thus the "incident field" with which $\delta\psi$ has been associated is the same function of $\mathbf{x}$, whatever the value of $\mathbf{x}'$, up to the multiplier S_D. Essentially the same is true for the Neumann case, where $\partial_y\psi_N(\mathbf{x}, \mathbf{x}', L_1, L_2)$ departs from zero on the extended increment as a strength $(2\pi)^{-\frac{1}{2}}S_N$ times $(x - L_1)^{-\frac{1}{2}}$, plus negligible terms. For either case we may consider two source points simultaneously and regulate the strength of one of the sources so that the "incident field" is zero. Consequently, $\delta\psi$ must also be zero. This statement is again equivalent to Eq. (4), where now $(-a)$ becomes the strength of the regulated source.

A third and last derivation follows from modifying the above argument. One merely observes that since the effective "incident field" which produces $\delta\psi$ is a product of $S(\mathbf{x}', L_1, L_2)$ times a function of $\mathbf{x}$ which is independent of $\mathbf{x}'$, and since the problem is linear in $\mathbf{x}$, it follows that $\delta\psi$, which is just $[\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}'L_1, L_2]\delta L_1$, must also be a product of S times (another) function of $\mathbf{x}$.

This view suggests more relations. It is obvious from the definition of S that

$$\frac{1}{i}\left(\frac{\pi}{2}\right)^{-\frac{1}{2}}S_D(\mathbf{x}', L_1, L_2) = \lim_{\substack{x\to L_1^+ \\ y=0}} (x - L_1)^{-\frac{1}{2}}\psi_D(\mathbf{x}, \mathbf{x}'), \tag{7}$$

and similarly that

$$(2\pi)^{-\frac{1}{2}}S_N(\mathbf{x}', L_1, L_2) = \lim_{\substack{x\to L_1^+ \\ y=0}} (x - L_1)^{\frac{1}{2}}\partial_y\psi_N(\mathbf{x}, \mathbf{x}'). \tag{8}$$

It was shown in the last paragraph that $\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}')$ is equal to $S(\mathbf{x}', L_1, L_2)$ times a function of $\mathbf{x}$ (and L_1 and L_2). It is well known[2] that

$$\psi(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x}', \mathbf{x}). \tag{9}$$

Differentiating Eq. (9) with respect to L_1, one sees that this reciprocity applies also to $\partial_{L_1}\psi$. Thus the function of $\mathbf{x}$ must be proportional to $S(\mathbf{x}, L_1, L_2)$. By comparison with Eq. (4) it must also be proportional to $\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}_1)$, where $\mathbf{x}_1$ is arbitrary. These two requirements are compatible. Since, up to a multiplier, $\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}_1)$ is the same function of $\mathbf{x}$, independent of $\mathbf{x}_1$, that same function results when a limiting process is carried out on $\mathbf{x}_1$. From reciprocity and the behavior at the end points one shows that

$$\lim_{\substack{x_1\to L_1^+ \\ y_1=0}} (x_1 - L_1)^{\frac{1}{2}}\partial_{L1}\psi_D(\mathbf{x}, \mathbf{x}_1) = i(2\pi)^{-\frac{1}{2}}S_D(\mathbf{x}, L_1, L_2). \tag{10}$$

and

$$\lim_{\substack{x_1\to L_1^- \\ y_1=0^+}} (L_1 - x_1)^{\frac{1}{2}}\partial_{L_1}\psi_N(\mathbf{x}, \mathbf{x}_1) = (2\pi)^{-\frac{1}{2}}S_N(\mathbf{x}, L_1, L_2). \tag{11}$$

Thus we have shown that for some c_D and c_N, which

may depend on L_1 and L_2, but are independent of $\mathbf{x}$ and $\mathbf{x}'$,

$$\partial_{L_1}\psi(\mathbf{x}, \mathbf{x}') = cS(\mathbf{x})S(\mathbf{x}'), \tag{12}$$

where the abbreviated notation is used for S. On substituting Eq. (12) into Eqs. (10) and (11) one finds

$$\frac{i}{c_D} = (2\pi)^{\frac{1}{2}} \lim_{\substack{x_1 \to L_1^+ \\ y_1 = 0}} (x_1 - L_1)^{\frac{1}{2}} S_D(\mathbf{x}_1) \tag{13}$$

and

$$\frac{1}{c_N} = (2\pi)^{\frac{1}{2}} \lim_{\substack{x_1 \to L_1^- \\ y_1 = 0^+}} (L_1 - x_1)^{\frac{1}{2}} S_N(\mathbf{x}_1). \tag{14}$$

IV. CHANGE WITH RESPECT TO L_2

It is straightforward to define S_2 and c_2 which describe the derivative with respect to L_2. Because of symmetry, these may be related to S and c. For an arbitrary vector $\mathbf{x}$ corresponding to the point (x, y), we define $R\mathbf{x}$ as the vector to the point $(L_1 + L_2 - x, y)$, so that R corresponds to reflection about the symmetry line $x = \frac{1}{2}(L_1 + L_2)$. From symmetry it follows that

$$\psi(\mathbf{x}, \mathbf{x}') = \psi(R\mathbf{x}, R\mathbf{x}') \tag{15}$$

and

$$\partial_{L_2}\psi(\mathbf{x}, \mathbf{x}') = -\partial_{L_1}\psi(R\mathbf{x}, R\mathbf{x}'). \tag{16}$$

It then follows from Eq. (12) that

$$\partial L_2\psi(\mathbf{x}, \mathbf{x}') = -cS_2(\mathbf{x})S_2(\mathbf{x}'), \tag{17}$$

where we define

$$S_2(\mathbf{x}, L_1, L_2) = S(R\mathbf{x}, L_1, L_2). \tag{18}$$

$S(\mathbf{x}')$ provides a description of the behavior of $\psi(\mathbf{x}, \mathbf{x}')$ for $\mathbf{x}$ near L_1. The behavior near L_1 depends on L_2, and we now consider $\partial_{L_2}S(\mathbf{x}, L_1, L_2)$. One differentiates Eqs. (7) and (8). The derivative can be carried through the limit, and with Eq. (7) and a little symmetry manipulation one obtains

$$\partial_{L_2}S(\mathbf{x}) = \gamma S_2(\mathbf{x}) = \gamma S(R\mathbf{x}), \tag{19}$$

where

$$\gamma_D(L) = -i\left(\frac{\pi}{2}\right)^{\frac{1}{2}} c_D \lim_{\substack{x' \to L_2^- \\ y' = 0}} (L_2 - x')^{-\frac{1}{2}} S_D(\mathbf{x}') \tag{20}$$

and

$$\gamma_N(L) = -(2\pi)^{\frac{1}{2}} c_N \lim_{\substack{x' \to L_2^- \\ y' = 0}} (L_2 - x')^{\frac{1}{2}} \partial_{y'} S_N(\mathbf{x}'), \tag{21}$$

with

$$L = L_1 - L_2. \tag{22}$$

These limits exist because by reciprocity Eqs. (7) and (8) give the field at $\mathbf{x}'$ due to a source at $\mathbf{x}$ vanishingly near $(L_1, 0)$, and the character of the field near $(L_2, 0)$ will be the same as for any ordinary field. By symmetry, γ can depend on L_1 and L_2 only as their difference. From symmetry one shows that

$$\partial_{L_1}S_2(\mathbf{x}) = -\gamma S(\mathbf{x}). \tag{23}$$

From the simple fact that at regular points $\partial_{L_2}\partial_{L_1}\psi = \partial_{L_1}\partial_{L_2}\psi$, one may show with Eqs. (12), (17), (19), and (22) that

$$(\partial_{L_2}c)S(\mathbf{x})S(\mathbf{x}') = (\partial_{L_1}c)S_2(\mathbf{x})S_2(\mathbf{x}'). \tag{24}$$

Since S and S_2 are linearly independent functions of $\mathbf{x}$ this can only be so if

$$\partial_{L_1}c = \partial_{L_2}c = 0. \tag{25}$$

Physically, c represents the limit of the field near L_1 due to a source near L_1, and it is not surprising that the length of the strip is irrelevant to this limit. Since c is independent of L_1 and L_2, it may be determined from the limit as L_1 tends to L_2 and this limit may be determined for the Dirichlet case from Carleman's[5] solution for the logarithmic-kernel integral equation. One finds

$$c_D = 1; \tag{26}$$

the choice of normalization of S_D was of course made with Eq. (26) in mind. Through Babinet's principle[2,4] and the use of the semi-infinite strip instead of a short strip one finds

$$c_N = c_D = c = 1. \tag{27}$$

V. PROPERTIES ASSOCIATED WITH THE SYMMETRY OF THE STRIP

What has been shown so far, except for Eq. (18), is presumably valid for segments of arbitrary smooth curves. We turn now to special properties of the strip. The first is that moving both end points by the same amount is equivalent to translating the strip. From this and the translational symmetry of the Helmholtz equation it follows that on the whole plane

$$(\partial_{L_1} + \partial_{L_2} + \partial_x + \partial_{x'})\psi(\mathbf{x}, \mathbf{x}') = 0 \tag{28}$$

and

$$(\partial_{L_1} + \partial_{L_2} + \partial_x)S(\mathbf{x}) = 0. \tag{29}$$

[5] T. Carleman, Math. Z. 15, 111 (1922).

From Eqs. (12), (17), (18), and (28) it follows that

$$(\partial_x + \partial_{x'})\psi(\mathbf{x}, \mathbf{x}') = S(R\mathbf{x})S(R\mathbf{x}') - S(\mathbf{x})S(\mathbf{x}'). \quad (30)$$

Equation (30) can also be derived from the observation that $(\partial_x+\partial_{x'})$ commutes with the Helmholtz operator, and on the whole plane,

$$(\partial_x + \partial_{x'})G(\mathbf{x}, \mathbf{x}') = 0. \quad (31)$$

It follows that $(\partial_x + \partial_{x'})\psi(\mathbf{x}, \mathbf{x}')$ is free of any singularity at $\mathbf{x} = \mathbf{x}'$, and except for end-point singularities satisfies all of the requirements of the scattered field associated with zero incident field. From Eqs. (7), (8), (13), and (14) one can show that the endpoint singularities can be cancelled without spoiling the boundary condition by addition of the term $[S(\mathbf{x})S(\mathbf{x}') - S(R\mathbf{x})S(R\mathbf{x}')]$. The combination then satisfies all of the requirements without exception and must be the null field. This is equivalent to Eq. (30).

The Dirichlet and Neumann fields for the strip are related. Both ∂_y and $\partial_{y'}$ commute with the Helmholtz operator, and $(\partial_y + \partial_{y'})$ can replace $(\partial_x + \partial_{x'})$ in Eq. (31), so that $(\partial_y\psi_N + \partial_{y'}\psi_D)$ has no singularity at $\mathbf{x} = \mathbf{x}'$, and except for being unbounded at the end points satisfies all conditions for the Dirichelt scattered field corresponding to zero incident field. Examination of the end-point singularities shows that

$$\{\partial_y\psi_N + \partial_{y'}\psi_D - i^{-1}[S_N(\mathbf{x}')S_D(\mathbf{x}) + S_N(R\mathbf{x}')S_D(R\mathbf{x})]\}$$

is free of end-point singularities and is thus necessarily zero. One so obtains

$$\partial_y\psi_N(\mathbf{x}, \mathbf{x}') + \partial_{y'}\psi_D(\mathbf{x}, \mathbf{x}') = i^{-1}[S_N(\mathbf{x}')S_D(\mathbf{x}) + S_N(R\mathbf{x}')S_D(R\mathbf{x})]. \quad (32)$$

It follows from differentiation of Eq. (32) with respect to L_1 that S_N and S_D are related. One may use Eq. (12) and rearrange the resulting terms to equate a function of $\mathbf{x}$ to a function of $\mathbf{x}'$. It follows that both must be independent of $\mathbf{x}$ and $\mathbf{x}'$, and must equal some function ζ which depends only on L. With the use of Eqs. (19), (23), and (29), this result can be put in the form

$$\partial_y S_N(\mathbf{x}) - i(\gamma_D + \gamma_N)S_D(R\mathbf{x}) - i(\partial_x - \zeta)S_D(\mathbf{x}) = 0, \quad (33)$$

and

$$\partial_y S_D(\mathbf{x}) - i(\gamma_D + \gamma_N)S_N(R\mathbf{x}) - i(\partial_x + \zeta)S_N(\mathbf{x}) = 0. \quad (34)$$

One obtains a complementary pair of equations on replacing $\mathbf{x}$ by $R\mathbf{x}$, in which case ∂x is of course to be replaced by $-\partial x$. It follows from differentiation of Eq. (33) with respect to y, a little manipulation, and use of the fact that S satisfies Eq. (2), that

$$\zeta^2 = (\gamma_D + \gamma_N)^2 - k^2. \quad (35)$$

It follows that ζ like γ_D and γ_N depends on L_1 and L_2 only as L.

Another kind of relation follows from the fact that the polar-coordinate rotation operator, $\partial_\theta(=x\partial_y - y\partial_x)$ commutes with the Helmholtz equation. It is easy to show that $\partial_\theta\psi_N$ and $\partial_\theta\psi_D$ both satisfy the Dirichlet condition on the strip. Equivalently, the relation between them may be expressed through the angular relations between S_D and S_N. The relations are simplified if the point of rotation is taken to be the singularity so that the operator is $(\partial_\theta - L_1\partial_y)$. One obtains from the usual considerations

$$(\partial_\theta - L_1\partial_y)S_D(\mathbf{x}) = -i[L\gamma_D S_N(R\mathbf{x}) + \tfrac{1}{2}S_N(\mathbf{x})] \quad (36)$$

and

$$(\partial_\theta - L_1\partial_y)S_N(\mathbf{x}) = -i[L\gamma_N S_D(R\mathbf{x}) + \tfrac{1}{2}S_D(\mathbf{x})]. \quad (37)$$

A complementary pair is obtained when one replaces $\mathbf{x}$ by $R\mathbf{x}$ and $\partial_\theta - L_1\partial_y$ by $-(\partial_\theta - L_2\partial_y)$.

These equations may be used to determine γ_D and γ_N. On differentiating the complement of Eq. (36) with respect to L_1, using Eqs. (19) and (23), dividing by γ_D and then subtracting L times Eq. (33) one obtains an equation of the same form as Eq. (36). Comparison shows that

$$\zeta = \frac{1}{2L}\left(\frac{\gamma_N}{\gamma_D} - 1\right) - \frac{1}{\gamma_D}\frac{d}{dL}\gamma_D. \quad (38)$$

A similar manipulation starting with the complement of Eq. (37) yields

$$\zeta = \frac{1}{2L}\left(1 - \frac{\gamma_D}{\gamma_N}\right) + \frac{1}{\gamma_N}\frac{d}{dL}\gamma_N. \quad (39)$$

Equations (35), (38), and (39) form a pair of second-order ordinary differential equations for γ_N and γ_D. One may verify that Eqs. (35), (38), and (39) are equivalent to the introduction of a function $\eta(t)$ with

$$\frac{\gamma_D}{k} = \frac{1}{4}\left[\frac{1}{\eta(t)}\frac{d}{dt}\eta(t) - \eta(t) - \frac{1}{\eta(t)}\right], \quad (40)$$

$$\frac{\gamma_N}{k} = -\frac{1}{4}\left[\frac{1}{\eta(t)}\frac{d}{dt}\eta(t) + \eta(t) + \frac{1}{\eta(t)}\right], \quad (41)$$

where

$$\frac{d^2\eta(t)}{dt^2} = \frac{1}{\eta(t)}\left[\left(\frac{d\eta(t)}{dt}\right)^2 - 1\right] - \frac{1}{t}\frac{d\eta(t)}{dt} + [\eta(t)]^3, \quad (42)$$

and

$$t = \tfrac{1}{2}kL = \tfrac{1}{2}k(L_1 - L_2). \tag{43}$$

The behavior for small t is determined from Carleman's solution.[5] This with substitution into Eq. (42) yields for small t

$$\eta(t) = -t\Omega - (t^5/128)[8\Omega^3 - 8\Omega^2 + 4\Omega - 1] + O[t^9\Omega^5], \tag{44}$$

where

$$\Omega = \ln \tfrac{1}{4}t - \tfrac{1}{2}i\pi + 0.5772157 \cdots, \tag{45}$$

where the decimal number is Euler's constant. Equation (42) is discussed by Ince[6] on p. 335 and has been solved numerically and tabulated by Myers.[7] Thus γ_D and γ_N are determined.

VI. THE FIELD PATTERN

The behavior far from the strip when the source is also far away is described by the field pattern $\mathfrak{F}$,

$$\mathfrak{F}(\theta, \theta') = \lim_{\substack{|\mathbf{x}'|\to\infty \\ |\mathbf{x}|\to\infty}} \frac{\psi(\mathbf{x}, -\mathbf{x}')}{\tfrac{1}{4}i[H_0(k|\mathbf{x}|)H_0(k|\mathbf{x}'|)]}, \tag{46}$$

where

$$\cos\theta = x/|\mathbf{x}| \tag{47}$$

and

$$\sin\theta = y/|\mathbf{x}|, \tag{48}$$

and the limits are to be taken with θ and θ' held constant. The minus sign occurs in Eq. (46) because θ' is defined as the propagation direction of the incident field, rather than the source direction. We define corresponding limits for S by

$$g(\theta) = \lim_{|x|\to\infty} \frac{S(\mathbf{x})}{\tfrac{1}{4}iH_0(k|\mathbf{x}|)}. \tag{49}$$

Far from the strip the scattered field behaves locally as a plane wave and for this reason one obtains the corresponding limits

$$\begin{aligned} S(R\mathbf{x}) &\to e^{-ik(L_1+L_2)\cos\theta} g(\pi - \theta), \\ S(-\mathbf{x}) &\to g(\theta - \pi), \\ S(-R\mathbf{x}) &+ e^{ik(L_1+L_2)\cos\theta} g(-\theta). \end{aligned} \tag{50}$$

One readily shows that the effect of translation of the strip on the field pattern is described by a phase factor, and correspondingly that

$$g(\theta) = f(\theta)e^{-\frac{1}{2}ik(L_1+L_2)\cos\theta}, \tag{51}$$

where $f(\theta) = g(\theta)|_{L_1+L_2=0}$. From this point on we shall take the strip as centered so that $L_1 + L_2 = 0$. It then follows from Eqs. (12), (17), (22), and (27) that

$$\begin{aligned} \partial_L \mathfrak{F}(\theta, \theta') &= f(\theta)f(\theta' - \pi) + f(\pi - \theta)f(-\theta') \\ &= f(\theta)f(\theta' - \pi) + f(\theta - \pi)f(\theta') \end{aligned} \tag{52}$$

where the second part of the equality is possible because f_D is symmetric in θ and f_N is antisymmetric. Again using the "local plane wave" behavior, one can carry out the limit on Eq. (30) to obtain

$$\begin{aligned} ik(\cos\theta - \cos\theta')\mathfrak{F}(\theta, \theta') \\ = f(\theta - \pi)f(\theta') - f(\theta)f(\theta' - \pi). \end{aligned} \tag{53}$$

From Eqs. (19) and (29) one obtains

$$(k^{-1}\partial_L + \tfrac{1}{2}i\cos\theta)f(\theta) + [\gamma(L)/k]f(\pi - \theta) = 0. \tag{54}$$

Equation (54) and the complement obtained by replacing θ by $\pi - \theta$ form a second-order system of ordinary differential equations for $f(\theta)$. From examination of the behavior for small L, one can show that for small L

$$f_D(\theta) = (2\pi/L)^{\frac{1}{2}}(-\tfrac{1}{2}kL\cos\theta + \{i/\Omega(\tfrac{1}{2}kL)\} + O[L^2]), \tag{55}$$

Equation (55) provides the initial condition for Eq. (54) for the Dirichlet condition.

The Neumann function f_N is expressed in terms of f_D when one takes the limit of Eq. (33) with $L_1 + L_2 = 0$. One finds

$$\begin{aligned} \sin\theta f_N(\theta) = [(\gamma_D + \gamma_N)/k]f_D(\pi - \theta) \\ + (i\cos\theta - \zeta/k)f_D(\theta). \end{aligned} \tag{56}$$

One may take the limit of Eq. (36) and use Eq. (56) to show

$$\begin{aligned} \left(\frac{d}{d(\cos\theta)} + \tfrac{1}{2}ikL\right)f_D(\theta) = \frac{i}{1 - \cos^2\theta} \\ \times \left\{\left[kL\frac{\gamma_D}{k}\left(\frac{\gamma_D + \gamma_N}{k}\right) + \frac{1}{2}\left(i\cos\theta - \frac{\zeta}{k}\right)\right]f_D(\theta) \right. \\ \left. + \left[\frac{\gamma_D + \gamma_N}{k} - kL\frac{\gamma_D}{k}\frac{\zeta}{k} - ikL\frac{\gamma_D}{k}\cos\theta\right]f_D(\pi - \theta)\right\}. \end{aligned} \tag{57}$$

Equation (57) and the complement obtained by interchanging θ and $\pi - \theta$ form a second-order system for $f_D(\theta)$; this time, however, the system is differential in θ. For computation, one may derive starting values from Eq. (54) at one special value of θ. One notes that f_D is even in θ and hence a function only of $\cos\theta$, so that changing the dependent variable to $\cos\theta$ is computationally advanta-

[6] E. L. Ince, *Ordinary Differential Equations* (Dover Publications, Inc., New York, 1956).

[7] J. M. Myers, "Symmetry in Scattering by a Strip," Harvard University thesis, Department of Engineering and Applied Physics (1962).

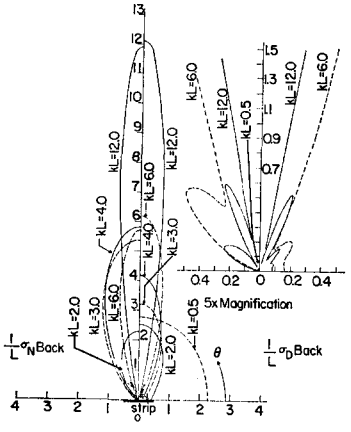

FIG. 1. Back-scattering cross sections vs angle of observation.

geous. Equation (57) may be obtained also as the Fourier transform of the differential equation for $\partial_y \psi_D$ evaluated on the strip. This equation can be obtained from Latta's method.[7,8]

VII. NUMERICAL RESULTS

Equations equivalent to Eqs. (42), (54), and (57) have been numerically integrated and are tabulated in Ref. 7. Some of these results are presented graphically in Figs. 1 and 2, where we have defined the differential cross section

$$\partial\, \sigma(\theta, \theta')/\partial\theta = (1/8\pi k)\mathfrak{F}(\theta, \theta')\mathfrak{F}^*(\theta, \theta'), \quad (58)$$

and the back-scattering cross section

$$\sigma_{\text{back}} = 2\pi\, \partial\, \sigma(\theta, \theta - \pi)/\partial\theta. \quad (59)$$

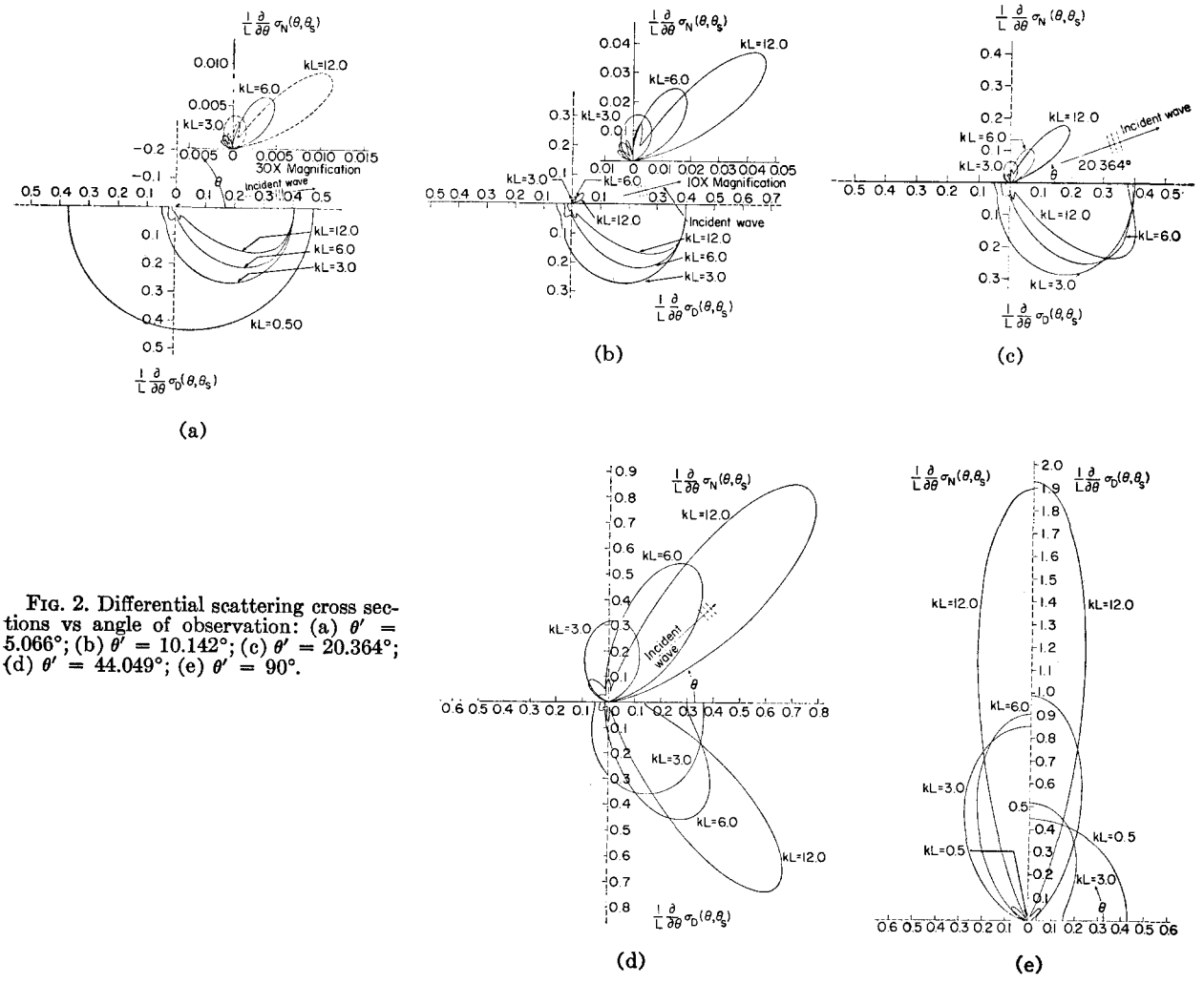

FIG. 2. Differential scattering cross sections vs angle of observation: (a) $\theta' = 5.066°$; (b) $\theta' = 10.142°$; (c) $\theta' = 20.364°$; (d) $\theta' = 44.049°$; (e) $\theta' = 90°$.

[8] G. E. Latta, J. Ratl. Mech. Anal. 5, 821 (1956).

VIII. OTHER OBSTACLES

The results through Sec. IV appear to be valid for any class of sufficiently smooth open curves, except that $S_2(\mathbf{x})$ cannot be replaced by $S(R\mathbf{x})$. Many shapes have additional symmetry properties analogous to those of the strip, though usually not so extensive, so that some of the results of the later sections hold. The field pattern of the rectangle separates variables. The field patterns for the arc, wedge, and arc-backed wedge share a similar property with respect to scattering of cylindrical waves. The disk and hemispherical shell are examples of three-dimensional obstacles for which analogous properties can be shown. A report on electromagnetic scattering by a circular disk is in preparation.

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APPENDIX: DERIVATIONS FROM INTEGRAL EQUATIONS

A. Formulation

As is well known,[2] the formulation of Sec. II is equivalent to

$$-\psi^{sc}(\mathbf{x}, \mathbf{x}') = \oint d\mathbf{x}_0 \Big[G(\mathbf{x}, \mathbf{x}_0) \frac{\partial}{\partial n_0} \psi(\mathbf{x}_0, \mathbf{x}') - \psi(\mathbf{x}_0, \mathbf{x}') \frac{\partial}{\partial n_0} G(\mathbf{x}, \mathbf{x}_0) \Big], \quad \text{(A1)}$$

where the contour is around and infinitesimally close to the strip. It follows that

$$\psi^{sc}(\mathbf{x}, \mathbf{x}') = \int_{L_2}^{L_1} dx_0 \Big[G(\mathbf{x}, \mathbf{x}_0) p(x_0, \mathbf{x}') + q(x_0, \mathbf{x}') \frac{\partial}{\partial y} G(\mathbf{x}, \mathbf{x}_0) \Big], \quad \text{(A2)}$$

where

$$p(x_0, \mathbf{x}') = -\lim_{\epsilon \to 0^+} [\partial_{y_0} \psi(\mathbf{x}_0, \mathbf{x}')|_{y_0 = \epsilon} - \partial_{y_0} \psi(\mathbf{x}_0, \mathbf{x}')|_{y_0 = -\epsilon}] \quad \text{(A3)}$$

and

$$q(x_0, \mathbf{x}') = -\lim_{\epsilon \to 0^+} [\psi(\mathbf{x}_0, \mathbf{x}')|_{y_0 = \epsilon} - \psi(\mathbf{x}_0, \mathbf{x}')|_{y_0 = -\epsilon}]. \quad \text{(A4)}$$

B. Dirichlet Condition

The Dirichlet condition implies that q is identically zero. Condition (c) of Sec. II then yields an integral equation for p,

$$-G(\mathbf{x}, \mathbf{x}')|_{y=0} = \int_{L_2}^{L_1} dx_0 \frac{i}{4} H_0^{(1)}(k\,|x - x_0|) p(x_0, \mathbf{x}') \quad \text{on} \quad L_2 < x < L_1. \quad \text{(A5)}$$

We wish to differentiate Eq. (A5) with respect to L_1. One may not differentiate under the integral because $p(x_0, \mathbf{x}')$ is singular at L_1 and $\partial_{L1} p$ is not integrable. If p were continuous as $x_0 \to L_1$, one could construct a linear combination of $p(x_0, \mathbf{x}')$ and $p(x_0, \mathbf{x}_1)$ which would be zero at $x_0 = L_1$. Then the derivative could be taken under the integral and moreover there would be zero contribution from the evaluation of the integrand at the end point. In fact, this procedure works in spite of the lack of continuity. The Helmholtz equation is related to the Laplace equation in a way which permits us to show that the singularities can be cancelled. The Laplace equation is equivalent to the logarithmic-kernel integral equation, $G(\mathbf{x}, \mathbf{x}')$ is analytic on the closed strip, and it is well known that

$$\tfrac{1}{4} i H_0^{(1)}(k\,|x - x_0|) = \text{const} \ln |x - x_0| + K(x, x_0), \quad \text{(A6)}$$

where K is continuous in x and x' and has continuous first derivatives. From Eq. (A6) and Carleman's solution to the logarithmic-kernel integral equation,[5] it may be shown that p is a function which has a finite slope at L_1 times $(L_1 - x_0)^{-\frac{1}{2}}$. Because the multiplying function has a finite slope at the end point, it follows that for any other source point $\mathbf{x}_1$, there exists an $\alpha_D(\mathbf{x}', \mathbf{x}_1, L_1, L_2)$ such that $p(x_0, \mathbf{x}') - \alpha_D p(x_0, \mathbf{x}_1)$ behaves as $(L_1 - x_0)^{+\frac{1}{2}}$ as x_0 approaches L_1, provided merely that

$$\lim_{x_0 \to L_1} p(x_0, \mathbf{x}_1) \neq 0.$$

(If by any chance this condition were not satisfied one would only have to interchange the labels of $\mathbf{x}'$ and $\mathbf{x}_1$ to obtain a combination of the desired form.) One thus shows that from Eq. (A5) that $\partial_{L_1}[p(x_0, \mathbf{x}') - \alpha_D p(x_0, \mathbf{x}_1)]$ satisfies the integral equation

$$(\partial_{L_1} \alpha_D) G(\mathbf{x}, \mathbf{x}_1)|_{y=0} = \int_{L_2}^{L_1} dx_0 \frac{i}{4} H_0^{(1)}(k\,|x - x_0|) \times \partial_{L_1}[p(x_0, \mathbf{x}') - \alpha_D p(x_0, \mathbf{x}_1)], \quad \text{(A7)}$$

whence, with Eq. (A5), we see

$$0 = \int_{L_2}^{L_1} dx_0 \frac{i}{4} H_0^{(1)}(k\,|x - x_0|)$$

$$\times [\partial_{L_1} p(x_0, \mathbf{x}') - \alpha_D \partial_{L_1} p(x_0, \mathbf{x}_1)]$$
$$\text{on} \quad L_2 < x < L_1. \tag{A8}$$

The Helmholtz equation, with the Dirichlet boundary condition and the Sommerfeld radiation condition, is known to have a unique solution (see Bouwkamp[4]). It follows that the integral Eq. (A5) has a unique solution. Because there is only one solution, the corresponding homogeneous integral equation, (A8) can have only the null solution. Therefore one obtains

$$0 = \partial_{L_1} p(x_0, \mathbf{x}') - \alpha_D \partial_{L_1} p(x_0, \mathbf{x}_1). \tag{A9}$$

With Eq. (A2) and the fact that $q_D = 0$, it is easy to show from Eq. (A9) that

$$\partial_{L_1} \psi(\mathbf{x}, \mathbf{x}') - \alpha_D(\mathbf{x}', \mathbf{x}_1) \partial_{L_1} \psi_D(\mathbf{x}, \mathbf{x}_1) = 0. \tag{A10}$$

C. Neumann Condition

For the Neumann condition, $\partial\psi/\partial y$ and p are zero on the strip and Eq. (A2) yields

$$\psi^{sc}(\mathbf{x}, \mathbf{x}') = \int_{L_2}^{L_1} dx_0 \, q(x_0, \mathbf{x}') \frac{\partial}{\partial y} G(\mathbf{x}, \mathbf{x}_0) \tag{A11}$$

and one obtains the equation which determines q by differentiating Eq. (A22) with respect to y and taking the limit as $y \to 0^+$. Doing this and taking the derivative in Eq. (A11) outside the integral, one obtains

$$-[\partial_y G(\mathbf{x}, \mathbf{x}')]|_{y=0} = \lim_{y \to 0^+} \frac{\partial^2}{\partial y^2} \int_{L_2}^{L_1} dx_0$$
$$\times q(x_0, \mathbf{x}') G(\mathbf{x}, \mathbf{x}_0) \quad \text{on} \quad L_2 < x < L_1. \tag{A12}$$

Because

$$\int_{L_2}^{L_1} dx_0 \, q(x_0, \mathbf{x}') G(\mathbf{x}, \mathbf{x}_0)$$

automatically satisfies the Helmholtz equation, $\partial^2/\partial y^2$ may be replaced by $-(\partial^2/\partial x^2 + k^2)$. When this is done the limit presents no difficulty and one obtains

$$-\left[\frac{\partial}{\partial y} G(\mathbf{x}, \mathbf{x}')\right]\Big|_{y=0} = -\left(\frac{\partial^2}{\partial x^2} + k^2\right)$$
$$\times \int_{L_2}^{L_1} dx_0 \frac{i}{4} H_0^{(1)}(k\,|x_0 - x|) q(x_0, \mathbf{x}')$$
$$\text{on} \quad L_2 < x < L_1. \tag{A13}$$

This is identical, except for the use of a point source, to Eq. (2.26) of Bouwkamp (Ref. 4, p. 43). Equation (A13) may be converted into a pure integral equation by inversion of the differential operator, but of course two undetermined constants emerge, since the operator is of the second order.

These constants are determined by the condition that q, the discontinuity in the field, tend to zero as the end points are approached. Thus Eq. (A13) is well set only when accompanied by boundary conditions. On differentiating Eq. (A13) with respect to L_1, one readily obtains, since q is zero at L_1,

$$0 = -\left(\frac{\partial^2}{\partial x^2} + k^2\right) \int_{L_2}^{L_1} dx_0 \frac{i}{4} H_0^{(1)}(k\,|x_0 - x|)$$
$$\times \frac{\partial}{\partial L_1} q(x_0, \mathbf{x}') \quad \text{on} \quad L_2 < x < L_1. \tag{A14}$$

However, this equation does not imply that $\partial q/\partial L_1$ is zero, since nothing has been said about

$$\lim_{x_0 \to L_1} \frac{\partial}{\partial L_1} q(x_0, \mathbf{x}').$$

(Note that since

$$\lim_{x_0 \to L2} q(x_0, \mathbf{x}') = 0 \tag{A15}$$

for all $L_1 > L_2$, $\partial q/\partial L_1$ does tend to zero as x_0 approaches L_2.) As might be expected, one may combine the fields of two sources, say a second at $\mathbf{x}_1$, so that the combination of the $\partial q/\partial L_1$'s is zero at $x_0 = L_1$. This would be obvious if $\lim x_0 \to L_1 (\partial q/\partial L_1)$ existed. In fact, it does not, but the same reasoning that was used for the Dirichlet case shows that for any $\mathbf{x}'$ and $\mathbf{x}_1$ there exists a function $\alpha_N(\mathbf{x}', \mathbf{x}_1, L_1, L_2)$ such that

$$\lim_{x_0 \to L_1} [\partial_{L_1} q(x_0, \mathbf{x}') - \alpha_N \partial_{L_1} q(x_0, \mathbf{x}_1)] = 0. \tag{A16}$$

It follows from Eq. (14) that

$$0 = -\left[\frac{\partial^2}{\partial x^2} + k^2\right] \int_{L_2}^{L_1} dx_0 \frac{i}{4} H_0^{(1)}(k\,|x_0 - x|)$$
$$\times [\partial_{L_1} q(x_0, \mathbf{x}') - \alpha_N \partial_{L_1} q(x_0, \mathbf{x}_1)]. \tag{A17}$$

The unknown function in Eq. (A17), unlike that of Eq. (A14), is accompanied by boundary conditions of being zero at both ends of the strip. Hence, since the problem with the Neuman boundary conditions has a unique solution, it may readily be shown that

$$\partial_{L_1} q(x_0, \mathbf{x}') - \alpha_N \partial_{L_1} q(x_0, \mathbf{x}_1) = 0$$
$$\text{for} \quad L_2 < x_0 < L_1. \tag{A18}$$

It then follows from Eq. (A11) that

$$\partial_{L_1} \psi_N(\mathbf{x}, \mathbf{x}') - \alpha_N(\mathbf{x}', \mathbf{x}_1) \partial_{L_1} \psi_N(\mathbf{x}, \mathbf{x}_1) = 0. \tag{A19}$$